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# BIM2005: Homework I

> In this report, the 'we' term may be preferred by convention rather than by a result of collaboration.

## Preparation

- Headers are added to to the initial .gzmat code as below.

```
#

C2H4Cl2

0 1
  C
  C 1 1.54
  H 1 1.0 2 109.5
  H 1 1.0 2 109.5 3 120.0
  Cl 1 1.67 2 109.5 4 120.0
  H 2 1.0 1 109.5 5 -120.0
  H 2 1.0 1 109.5 5 120.0
  Cl 2 1.67 1 109.5 5 0.0
```

# Procedure

> Details of implementation could be found in the GitHub repository zcorn2017/BIM2001-HWK1 (github.com).
>
> **The comments to and styles of the code has been organised well to make it highly readable.**

1. We added the headers to the code manually for it to be recognised by OpenBabel
2. We modify the code in order to change $\tau(Cl^8 - C^2 - C^1 - Cl^5)$ by $20 \times N^\circ$. (As the reference plane, which is the $2 - 1 - 5$ plane, is the same for the last three definitions of atoms, we only need to change the dihedral angles of the last three lines by an increment of $20^\circ$.)
3. We convert the code from the .gzmat format to the .xyz. one via the Python bindings to the OpenBabel C++ library.
4. During the conversion, we use the python bindings to set up the force fields for MMFF94 and GAFF respectively, then calculating the energy, where the analysis process is recorded (See Appendix I).
5. The energy are stored in lists for further analysis.
6. We repeat the steps 2-5 for $N = 0 \ldots 18$, which means 19 times.
7. All the .xyz and .gzmat files could be found in Reuslts I.
8. Pre-processing of the data includes conversion between kcal/mol and kJ/mol and calculations of the relative energy.
9. A table where all the data for the angles is established by Pandas and it could be found in Results II.
10. A lineplot of relative energy in kcal/mol with respect to angle in degrees is displayed by [Seaborn] [https://seaborn.pydata.org/]. For details, please refer to Result III

# GitHub Repo File Hierarchy

```
.
├── C2H4Cl2_structure.png         // the 2D molecule structure overview
├── CODE                          // the directory containing all the .xyz and
.gzmat file
│   ├── C2H4Cl2_0_degrees.gzmat
│   ├── C2H4Cl2_0_degrees.xyz
```

```
6  │   ├── C2H4Cl2_100_degrees.gzmat
7  │   ├── C2H4Cl2_100_degrees.xyz
8  │   ├── C2H4Cl2_120_degrees.gzmat
9  │   ├── C2H4Cl2_120_degrees.xyz
10 │   ├── C2H4Cl2_140_degrees.gzmat
11 │   ├── C2H4Cl2_140_degrees.xyz
12 │   ├── C2H4Cl2_160_degrees.gzmat
13 │   ├── C2H4Cl2_160_degrees.xyz
14 │   ├── C2H4Cl2_180_degrees.gzmat
15 │   ├── C2H4Cl2_180_degrees.xyz
16 │   ├── C2H4Cl2_200_degrees.gzmat
17 │   ├── C2H4Cl2_200_degrees.xyz
18 │   ├── C2H4Cl2_20_degrees.gzmat
19 │   ├── C2H4Cl2_20_degrees.xyz
20 │   ├── C2H4Cl2_220_degrees.gzmat
21 │   ├── C2H4Cl2_220_degrees.xyz
22 │   ├── C2H4Cl2_240_degrees.gzmat
23 │   ├── C2H4Cl2_240_degrees.xyz
24 │   ├── C2H4Cl2_260_degrees.gzmat
25 │   ├── C2H4Cl2_260_degrees.xyz
26 │   ├── C2H4Cl2_280_degrees.gzmat
27 │   ├── C2H4Cl2_280_degrees.xyz
28 │   ├── C2H4Cl2_300_degrees.gzmat
29 │   ├── C2H4Cl2_300_degrees.xyz
30 │   ├── C2H4Cl2_320_degrees.gzmat
31 │   ├── C2H4Cl2_320_degrees.xyz
32 │   ├── C2H4Cl2_340_degrees.gzmat
33 │   ├── C2H4Cl2_340_degrees.xyz
34 │   ├── C2H4Cl2_360_degrees.gzmat
35 │   ├── C2H4Cl2_360_degrees.xyz
36 │   ├── C2H4Cl2_40_degrees.gzmat
37 │   ├── C2H4Cl2_40_degrees.xyz
38 │   ├── C2H4Cl2_60_degrees.gzmat
39 │   ├── C2H4Cl2_60_degrees.xyz
40 │   ├── C2H4Cl2_80_degrees.gzmat
41 │   └── C2H4Cl2_80_degrees.xyz
42 ├── DATA                          // .csv table file containing all the energy
   data
43 │   ├── data.csv
44 │   ├── data_in_KJ.csv
45 │   └── data_in_Kcal.csv
46 ├── README.md                     // This file you are in
47 ├── XYZ_GAMAT_SUMMARY.md          // (Not Important)
48 ├── code2mkdoc.py                 // The script used to facilitate the processing
   of the documentation
49 ├── file_tree.txt                // The file tree (Not Important)
50 └── requirements.txt             // All the requirements in my environment to run
   this script and some of them are redundant for you
51 ├── rel_energy.png                // Lineplot of the relative energy in kcal/mol
```

```
└── torsion_angle.py              // The main program to process the molecule

2 directories, 49 files
```

# Results

## I .gzmat and .xyz Files for a Specific Torsion Angle

### Torsion Angle at $0^\circ$

- ./CODE/C2H4Cl2_0_degrees.gzmat

```
#

C2H4Cl2-0-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 -120.0
H 2 1.0 1 109.5 5 120.0
Cl 2 1.67 1 109.5 5 0.0


```

- ./CODE/C2H4Cl2_0_degrees.xyz

```
8
./CODE/C2H4Cl2_0_degrees.gzmat
C          0.00000        0.00000        0.00000
C          1.54000        0.00000        0.00000
H         -0.33381        0.00000       -0.94264
H         -0.33381       -0.81635        0.47132
Cl        -0.55746        1.36331        0.78711
H          1.87381        0.00000       -0.94264
H          1.87381       -0.81635        0.47132
Cl         2.09746        1.36331        0.78711

```

## Torsion Angle at $20^\circ$

- ./CODE/C2H4Cl2_20_degrees.gzmat

```
#

C2H4Cl2-20-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 -100.0
H 2 1.0 1 109.5 5 140.0
Cl 2 1.67 1 109.5 5 20.0


```

- ./CODE/C2H4Cl2_20_degrees.xyz

```
8
./CODE/C2H4Cl2_20_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381         0.32240        -0.88579
H           1.87381        -0.92832         0.16369
Cl          2.09746         1.01188         1.20592

```

## Torsion Angle at $40^\circ$

- ./CODE/C2H4Cl2_40_degrees.gzmat

```

#

C2H4Cl2-40-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5

```

```
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 -80.0
H 2 1.0 1 109.5 5 160.0
Cl 2 1.67 1 109.5 5 40.0


```

- ./CODE/C2H4Cl2_40_degrees.xyz

```
8
./CODE/C2H4Cl2_40_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381         0.60592        -0.72211
H           1.87381        -0.92832        -0.16369
Cl          2.09746         0.53841         1.47927

```

## Torsion Angle at $60^\circ$

- ./CODE/C2H4Cl2_60_degrees.gzmat

```

#

C2H4Cl2-60-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 -60.0
H 2 1.0 1 109.5 5 180.0
Cl 2 1.67 1 109.5 5 60.0


```

- ./CODE/C2H4Cl2_60_degrees.xyz

```
8
./CODE/C2H4Cl2_60_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381         0.81635        -0.47132
H           1.87381        -0.81635        -0.47132
Cl          2.09746        -0.00000         1.57421

```

## Torsion Angle at $80^\circ$

- ./CODE/C2H4Cl2_80_degrees.gzmat

```

#

C2H4Cl2-80-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 -40.0
H 2 1.0 1 109.5 5 200.0
Cl 2 1.67 1 109.5 5 80.0


```

- ./CODE/C2H4Cl2_80_degrees.xyz

```
8
./CODE/C2H4Cl2_80_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381         0.92832        -0.16369
H           1.87381        -0.60592        -0.72211
Cl          2.09746        -0.53841         1.47927

```

## Torsion Angle at $100^\circ$

- ./CODE/C2H4Cl2_100_degrees.gzmat

```
#

C2H4Cl2-100-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 -20.0
H 2 1.0 1 109.5 5 220.0
Cl 2 1.67 1 109.5 5 100.0


```

- ./CODE/C2H4Cl2_100_degrees.xyz

```
8
./CODE/C2H4Cl2_100_degrees.gzmat
C          0.00000        0.00000        0.00000
C          1.54000        0.00000        0.00000
H         -0.33381        0.00000       -0.94264
H         -0.33381       -0.81635        0.47132
Cl        -0.55746        1.36331        0.78711
H          1.87381        0.92832        0.16369
H          1.87381       -0.32240       -0.88579
Cl         2.09746       -1.01188        1.20592

```

## Torsion Angle at $120^\circ$

- ./CODE/C2H4Cl2_120_degrees.gzmat

```

#

C2H4Cl2-120-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5

```

```
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 0.0
H 2 1.0 1 109.5 5 240.0
Cl 2 1.67 1 109.5 5 120.0


```

- ./CODE/C2H4Cl2_120_degrees.xyz

```
8
./CODE/C2H4Cl2_120_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381         0.81635         0.47132
H           1.87381         0.00000        -0.94264
Cl          2.09746        -1.36331         0.78711

```

## Torsion Angle at $140^\circ$

- ./CODE/C2H4Cl2_140_degrees.gzmat

```

#

C2H4Cl2-140-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 20.0
H 2 1.0 1 109.5 5 260.0
Cl 2 1.67 1 109.5 5 140.0


```

- ./CODE/C2H4Cl2_140_degrees.xyz

```
8
./CODE/C2H4Cl2_140_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381         0.60592         0.72211
H           1.87381         0.32240        -0.88579
Cl          2.09746        -1.55030         0.27336

```

## Torsion Angle at $160^\circ$

- ./CODE/C2H4Cl2_160_degrees.gzmat

```

#

C2H4Cl2-160-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 40.0
H 2 1.0 1 109.5 5 280.0
Cl 2 1.67 1 109.5 5 160.0


```

- ./CODE/C2H4Cl2_160_degrees.xyz

```
8
./CODE/C2H4Cl2_160_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381         0.32240         0.88579
H           1.87381         0.60592        -0.72211
Cl          2.09746        -1.55030        -0.27336

```

## Torsion Angle at $180^\circ$

- ./CODE/C2H4Cl2_180_degrees.gzmat

```
#

C2H4Cl2-180-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 60.0
H 2 1.0 1 109.5 5 300.0
Cl 2 1.67 1 109.5 5 180.0


```

- ./CODE/C2H4Cl2_180_degrees.xyz

```
8
./CODE/C2H4Cl2_180_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.00000         0.94264
H           1.87381         0.81635        -0.47132
Cl          2.09746        -1.36331        -0.78711

```

## Torsion Angle at $200^\circ$

- ./CODE/C2H4Cl2_200_degrees.gzmat

```

#

C2H4Cl2-200-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5

```

```
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 80.0
H 2 1.0 1 109.5 5 320.0
Cl 2 1.67 1 109.5 5 200.0


```

- ./CODE/C2H4Cl2_200_degrees.xyz

```
8
./CODE/C2H4Cl2_200_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.32240         0.88579
H           1.87381         0.92832        -0.16369
Cl          2.09746        -1.01188        -1.20592

```

## Torsion Angle at $220^\circ$

- ./CODE/C2H4Cl2_220_degrees.gzmat

```

#

C2H4Cl2-220-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 100.0
H 2 1.0 1 109.5 5 340.0
Cl 2 1.67 1 109.5 5 220.0


```

- ./CODE/C2H4Cl2_220_degrees.xyz

```
8
./CODE/C2H4Cl2_220_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.60592         0.72211
H           1.87381         0.92832         0.16369
Cl          2.09746        -0.53841        -1.47927

```

## Torsion Angle at $240^\circ$

- ./CODE/C2H4Cl2_240_degrees.gzmat

```


#

C2H4Cl2-240-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 120.0
H 2 1.0 1 109.5 5 0.0
Cl 2 1.67 1 109.5 5 240.0


```

- ./CODE/C2H4Cl2_240_degrees.xyz

```
8
./CODE/C2H4Cl2_240_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.81635         0.47132
H           1.87381         0.81635         0.47132
Cl          2.09746         0.00000        -1.57421

```

## Torsion Angle at $260^\circ$

- ./CODE/C2H4Cl2_260_degrees.gzmat

```
#

C2H4Cl2-260-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 140.0
H 2 1.0 1 109.5 5 20.0
Cl 2 1.67 1 109.5 5 260.0


```

- ./CODE/C2H4Cl2_260_degrees.xyz

```
8
./CODE/C2H4Cl2_260_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.92832         0.16369
H           1.87381         0.60592         0.72211
Cl          2.09746         0.53841        -1.47927

```

## Torsion Angle at $280^\circ$

- ./CODE/C2H4Cl2_280_degrees.gzmat

```
#

C2H4Cl2-280-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
```

```
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 160.0
H 2 1.0 1 109.5 5 40.0
Cl 2 1.67 1 109.5 5 280.0


```

- ./CODE/C2H4Cl2_280_degrees.xyz

```
8
./CODE/C2H4Cl2_280_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.92832        -0.16369
H           1.87381         0.32240         0.88579
Cl          2.09746         1.01188        -1.20592

```

## Torsion Angle at $300^\circ$

- ./CODE/C2H4Cl2_300_degrees.gzmat

```

#

C2H4Cl2-300-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 180.0
H 2 1.0 1 109.5 5 60.0
Cl 2 1.67 1 109.5 5 300.0


```

- ./CODE/C2H4Cl2_300_degrees.xyz

```
8
./CODE/C2H4Cl2_300_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.81635        -0.47132
H           1.87381        -0.00000         0.94264
Cl          2.09746         1.36331        -0.78711

```

## Torsion Angle at $320^\circ$

- ./CODE/C2H4Cl2_320_degrees.gzmat

```

#

C2H4Cl2-320-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 200.0
H 2 1.0 1 109.5 5 80.0
Cl 2 1.67 1 109.5 5 320.0


```

- ./CODE/C2H4Cl2_320_degrees.xyz

```
8
./CODE/C2H4Cl2_320_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.60592        -0.72211
H           1.87381        -0.32240         0.88579
Cl          2.09746         1.55030        -0.27336

```

## Torsion Angle at $340^\circ$

- ./CODE/C2H4Cl2_340_degrees.gzmat

```
#

C2H4Cl2-340-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 220.0
H 2 1.0 1 109.5 5 100.0
Cl 2 1.67 1 109.5 5 340.0


```

- ./CODE/C2H4Cl2_340_degrees.xyz

```
8
./CODE/C2H4Cl2_340_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H           1.87381        -0.32240        -0.88579
H           1.87381        -0.60592         0.72211
Cl          2.09746         1.55030         0.27336

```

## Torsion Angle at $360^\circ$

- ./CODE/C2H4Cl2_360_degrees.gzmat

```

#

C2H4Cl2-360-degrees

0 1
C
C 1 1.54
H 1 1.0 2 109.5

```

```
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 240.0
H 2 1.0 1 109.5 5 120.0
Cl 2 1.67 1 109.5 5 0.0


```

- ./CODE/C2H4Cl2_360_degrees.xyz

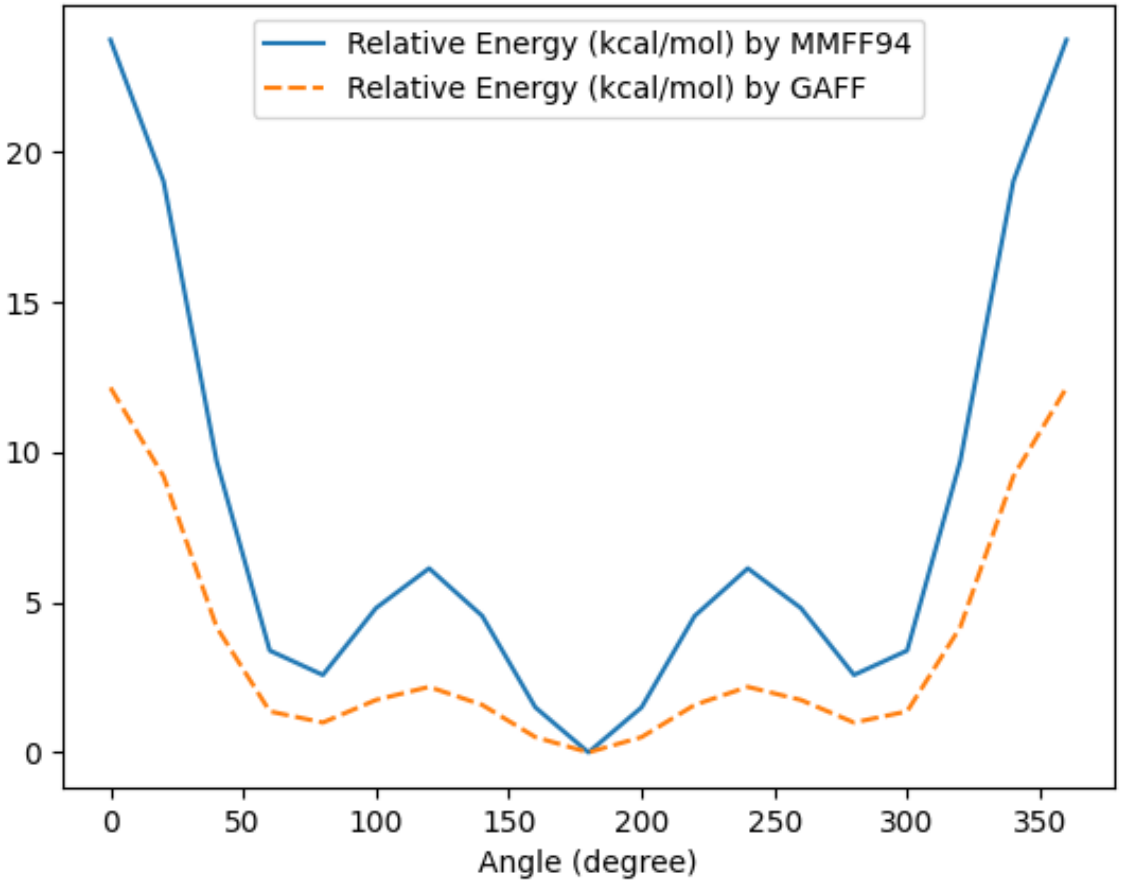
```
8
./CODE/C2H4Cl2_360_degrees.gzmat
C          0.00000        0.00000        0.00000
C          1.54000        0.00000        0.00000
H         -0.33381        0.00000       -0.94264
H         -0.33381       -0.81635        0.47132
Cl        -0.55746        1.36331        0.78711
H          1.87381        0.00000       -0.94264
H          1.87381       -0.81635        0.47132
Cl         2.09746        1.36331        0.78711

```

# II Energy Overview

| Angle (degree) | Absolute Energy (kcal/mol) by MMFF94 | Absolute Energy (kcal/mol) by GAFF | Relative Energy (kcal/mol) by MMFF94 | Relative Energy (kcal/mol) by GAFF | Absolute Energy (kJ/mol) by MMFF94 | Absolute Energy (kJ/mol) by GAFF | Relative Energy (kJ/mol) by MMFF94 | Relative Energy (kJ/mol) by GAFF |
|---|---|---|---|---|---|---|---|---|
| 0 | 50.104 | 32.032 | 23.741 | 12.153 | 209.633 | 134.023 | 99.331 | 50.847 |
| 20 | 45.389 | 29.078 | 19.027 | 9.198 | 189.91 | 121.662 | 79.607 | 38.485 |
| 40 | 36.065 | 24.052 | 9.702 | 4.172 | 150.897 | 100.634 | 40.595 | 17.458 |
| 60 | 29.755 | 21.245 | 3.392 | 1.366 | 124.494 | 88.891 | 14.192 | 5.715 |
| 80 | 28.942 | 20.874 | 2.579 | 0.994 | 121.095 | 87.337 | 10.792 | 4.16 |
| 100 | 31.171 | 21.627 | 4.808 | 1.747 | 130.418 | 90.486 | 20.115 | 7.31 |
| 120 | 32.494 | 22.063 | 6.131 | 2.183 | 135.953 | 92.31 | 25.651 | 9.133 |
| 140 | 30.91 | 21.462 | 4.547 | 1.582 | 129.326 | 89.796 | 19.023 | 6.62 |
| 160 | 27.863 | 20.389 | 1.5 | 0.509 | 116.58 | 85.306 | 6.278 | 2.129 |
| 180 | 26.363 | 19.88 | 0.0 | 0.0 | 110.302 | 83.176 | 0.0 | 0.0 |
| 200 | 27.863 | 20.389 | 1.5 | 0.509 | 116.58 | 85.306 | 6.278 | 2.129 |
| 220 | 30.91 | 21.462 | 4.547 | 1.582 | 129.326 | 89.796 | 19.023 | 6.62 |
| 240 | 32.494 | 22.063 | 6.131 | 2.183 | 135.953 | 92.31 | 25.651 | 9.133 |
| 260 | 31.171 | 21.627 | 4.808 | 1.747 | 130.418 | 90.486 | 20.115 | 7.31 |
| 280 | 28.942 | 20.874 | 2.579 | 0.994 | 121.095 | 87.337 | 10.792 | 4.16 |
| 300 | 29.755 | 21.245 | 3.392 | 1.366 | 124.494 | 88.891 | 14.192 | 5.715 |
| 320 | 36.065 | 24.052 | 9.702 | 4.172 | 150.897 | 100.634 | 40.595 | 17.458 |
| 340 | 45.389 | 29.078 | 19.027 | 9.198 | 189.91 | 121.662 | 79.607 | 38.485 |
| 360 | 50.104 | 32.032 | 23.741 | 12.153 | 209.633 | 134.023 | 99.331 | 50.847 |

## III Lineplot of Relative Energy in Kcal by MMFF94 and GAFF




# Appendix

## I Code

### torsion_angle.py

```
# This the main program to process the molecule.

from openbabel import openbabel
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt

# Set the constant used to convert kCal/mol to kJ/mol
KCAL2KJ_CONSTANT = 4.184

# The C2H4Cl2 molecule with the torsion angle at 0 degree
gzmat_code = """
#
```

```
C2H4Cl2

0 1
C
C 1 1.54
H 1 1.0 2 109.5
H 1 1.0 2 109.5 3 120.0
Cl 1 1.67 2 109.5 4 120.0
H 2 1.0 1 109.5 5 -120.0
H 2 1.0 1 109.5 5 120.0
Cl 2 1.67 1 109.5 5 0.0
"""

# Store the code of the 18 modified molecules as a list
code_list = []

for n in range(0, 19):
    # Count the reference number of the atoms to determine which atom to manipulate
    atom_counter = 0

    # .xyz code after conversion
    code_aft_cnv = ""
    for line in gzmat_code.split("\n"):
        words = line.split()

        # if the line is empty, do not make modifications
        if len(words) == 0:
            pass

        # if the title is met, rename the title to mark it with the torsion angle
        elif line.startswith("C2H4Cl2"):
            words.append(str(20 * n))
            words.append("degrees")
            code_aft_cnv = code_aft_cnv + "-".join(words) + "\n"
            continue

        elif words[0].isalpha() and len(words[0]) in [1, 2]:
            atom_counter = atom_counter + 1

            if atom_counter in [6, 7, 8]:

                words[-1] = str(float(words[-1]) + 20 * n)
                if float(words[-1]) >= 360:
                    words[-1] = str(float(words[-1]) - 360)

        code_aft_cnv = code_aft_cnv + " ".join(words) + "\n"
    code_list.append(code_aft_cnv)
```

```python

# Write the code to the .gzmat format
for code, angle in zip(code_list, range(0, 380, 20)):
    with open(f"./CODE/C2H4Cl2_{angle}_degrees.gzmat", "w") as gzmat_file:
        gzmat_file.write(code)

# Set the input format to gzmat and the output format to xyz
OB_converter = openbabel.OBConversion()
OB_converter.SetInAndOutFormats("gzmat", "xyz")

MMFF94_abs_energy_in_Kcal_list = []
GAFF_abs_energy_in_KJ_list = []

# Convert the .gzmat files to .xyz file via OpenBabel
for angle in range(0, 380, 20):
    mol_C2H4Cl2 = openbabel.OBMol()

    # Use MMFF94 and GAFF to calculate the absolute energy
    OB_converter.ReadFile(mol_C2H4Cl2, f"./CODE/C2H4Cl2_{angle}_degrees.gzmat")

    MMFF94_forcefield = openbabel.OBForceField.FindForceField("MMFF94")
    GAFF_forcefield = openbabel.OBForceField.FindForceField("GAFF")

    # Redirect the log output to std::cout
    MMFF94_forcefield.SetLogToStdOut()
    GAFF_forcefield.SetLogToStdOut()

    # Set the priority of log to high
    MMFF94_forcefield.SetLogLevel(openbabel.OBFF_LOGLVL_HIGH)
    GAFF_forcefield.SetLogLevel(openbabel.OBFF_LOGLVL_HIGH)

    # Specify the molecule we calculate the energy of
    MMFF94_forcefield.Setup(mol_C2H4Cl2)
    GAFF_forcefield.Setup(mol_C2H4Cl2)

    # Energy of C_2H_4Cl_2 with Torsion Angle at `angle` Degrees Starts
    # by MMFF94
    MMFF94_abs_energy_in_Kcal = MMFF94_forcefield.Energy()
    # by GAFF
    GAFF_abs_energy_in_KJ = GAFF_forcefield.Energy()

    MMFF94_abs_energy_in_Kcal_list.append(MMFF94_abs_energy_in_Kcal)
    GAFF_abs_energy_in_KJ_list.append(GAFF_abs_energy_in_KJ)

    OB_converter.WriteFile(mol_C2H4Cl2, f"./CODE/C2H4Cl2_{angle}_degrees.xyz")

# Construct a table containing the information required by the question
ref_MMFF94_energy_in_Kcal = min(MMFF94_abs_energy_in_Kcal_list)
ref_GAFF_energy_in_KJ = min(GAFF_abs_energy_in_KJ_list)
```

```
112
113 MMFF94_abs_energy_in_Kcal_vec = np.array(MMFF94_abs_energy_in_Kcal_list)
114 GAFF_abs_energy_in_KJ_vec = np.array(GAFF_abs_energy_in_KJ_list)
115
116 MMFF94_abs_energy_in_KJ_vec = KCAL2KJ_CONSTANT * MMFF94_abs_energy_in_Kcal_vec
117 GAFF_abs_energy_in_Kcal_vec = GAFF_abs_energy_in_KJ_vec / KCAL2KJ_CONSTANT
118
119 MMFF94_rel_energy_in_Kcal_vec = MMFF94_abs_energy_in_Kcal_vec -
    ref_MMFF94_energy_in_Kcal
120 GAFF_rel_energy_in_KJ_vec = GAFF_abs_energy_in_KJ_vec - ref_GAFF_energy_in_KJ
121
122 MMFF94_rel_energy_in_KJ_vec = MMFF94_abs_energy_in_KJ_vec - KCAL2KJ_CONSTANT *
    ref_MMFF94_energy_in_Kcal
123 GAFF_rel_energy_in_Kcal_vec = GAFF_abs_energy_in_Kcal_vec - ref_GAFF_energy_in_KJ
    / KCAL2KJ_CONSTANT
124
125 data_in_Kcal_dict = {
126     "Absolute Energy (kcal/mol) by MMFF94" :
    MMFF94_abs_energy_in_Kcal_vec.tolist(),
127     "Absolute Energy (kcal/mol) by GAFF" : GAFF_abs_energy_in_Kcal_vec.tolist(),
128     "Relative Energy (kcal/mol) by MMFF94" :
    MMFF94_rel_energy_in_Kcal_vec.tolist(),
129     "Relative Energy (kcal/mol) by GAFF" : GAFF_rel_energy_in_Kcal_vec.tolist()
130 }
131 data_in_KJ_dict = {
132     "Absolute Energy (kJ/mol) by MMFF94" : MMFF94_abs_energy_in_KJ_vec.tolist(),
133     "Absolute Energy (kJ/mol) by GAFF" : GAFF_abs_energy_in_KJ_vec.tolist(),
134     "Relative Energy (kJ/mol) by MMFF94" : MMFF94_rel_energy_in_KJ_vec.tolist(),
135     "Relative Energy (kJ/mol) by GAFF" : GAFF_rel_energy_in_KJ_vec.tolist()
136 }
137
138 data_in_Kcal_df = pd.DataFrame(data_in_Kcal_dict,index=[angle for angle in
    range(0, 380, 20)])
139 data_in_KJ_df = pd.DataFrame(data_in_KJ_dict,index=[angle for angle in range(0,
    380, 20)])
140
141 data_in_Kcal_df.to_csv("./DATA/data_in_Kcal.csv")
142 data_in_KJ_df.to_csv("./DATA/data_in_KJ.csv")
143
144 data_dict = {
145     "Absolute Energy (kcal/mol) by MMFF94":
    np.round(MMFF94_abs_energy_in_Kcal_vec.tolist(), 3),
146     "Absolute Energy (kcal/mol) by GAFF":
    np.round(GAFF_abs_energy_in_Kcal_vec.tolist(), 3),
147     "Relative Energy (kcal/mol) by MMFF94":
    np.round(MMFF94_rel_energy_in_Kcal_vec.tolist(), 3),
148     "Relative Energy (kcal/mol) by GAFF":
    np.round(GAFF_rel_energy_in_Kcal_vec.tolist(), 3),
```

```
    "Absolute Energy (kJ/mol) by MMFF94":
np.round(MMFF94_abs_energy_in_KJ_vec.tolist(), 3),
    "Absolute Energy (kJ/mol) by GAFF":
np.round(GAFF_abs_energy_in_KJ_vec.tolist(), 3),
    "Relative Energy (kJ/mol) by MMFF94":
np.round(MMFF94_rel_energy_in_KJ_vec.tolist(), 3),
    "Relative Energy (kJ/mol) by GAFF":
np.round(GAFF_rel_energy_in_KJ_vec.tolist(), 3)
}

data_df = pd.DataFrame(data_dict, index=[angle for angle in range(0, 380, 20)])
data_df.index.name = "Angle (degree)"
data_df.to_csv("./DATA/data.csv")

# Plot the lineplot of relative energy in kcal/mol with respect to angle in
degrees
lineplot_df = data_df.loc[:,["Relative Energy (kcal/mol) by MMFF94","Relative
Energy (kcal/mol) by GAFF"]]
sns.lineplot(data=lineplot_df)

plt.savefig("rel_energy.png")
```

## code2mkdoc.py

```
# This script aims to facilitate the gerneration of the documentation
# which is not part of the main program.
# For the homework solution,
# pls refer to torsion_angle.py

import sys

# Add heading to the Markdown file
def mkdoc_heading(heading, level=1):
    heading_level = "#" * level + " " + heading + "\n"
    print(f"""
{heading_level}""")

# Wrap the code to make it be recognised by the Markdown parser
def wrap_code(code, lang="python"):
    print(f"""```{lang}
{code}
    ```""")

# Redirect the output to the file writing object.
with open("XYZ_GAMAT_SUMMARY.md","w") as sys.stdout:
    for angle in range(0, 380, 20):
        mkdoc_heading(f"Torsion Angle at {angle}$\degree$", level= 4)

        print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.gzmat\n")
```
```

```
        with open(f"./CODE/C2H4Cl2_{angle}_degrees.gzmat", "r")  as gzmat:
            wrap_code(gzmat.read(), lang="gzmat")

        print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.xyz\n")
        with open(f"./CODE/C2H4Cl2_{angle}_degrees.xyz", "r") as xyz:
            wrap_code(xyz.read(), lang="xyz")
```

## II Analysis of the Energy

```

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

```

```
SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1      0      1.000      1.093        4.766     -0.093      3.578
```

```
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 1    1      0      1.540      1.508        4.258      0.032      0.294
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
```

```
 I    J    K    L     CLASS    ANGLE         V1   V2   V3     ENERGY
-------------------------------------------------------------------
 5    1    1    5       0      0.000    0.284   -1.386    0.314      0.598
 5    1    1    5       0   -120.000    0.284   -1.386    0.314     -0.655
 5    1    1   12       0    120.000    0.678   -0.602    0.398      0.116
 5    1    1    5       0    120.000    0.284   -1.386    0.314     -0.654
 5    1    1    5       0      0.000    0.284   -1.386    0.314      0.598
 5    1    1   12       0   -120.000    0.678   -0.602    0.398      0.116
12    1    1    5       0   -120.000    0.678   -0.602    0.398      0.116
12    1    1    5       0    120.000    0.678   -0.602    0.398      0.116
12    1    1   12       0     -0.000    0.000    0.000    0.893      0.893
     TOTAL TORSIONAL ENERGY =  1.24400 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.208     2.970     0.022     0.377
 5    5        2.746     2.970     0.022    -0.014
 5   12        3.280     3.713     0.053     0.009
 5    5        2.746     2.970     0.022    -0.014
 5    5        2.208     2.970     0.022     0.377
 5   12        3.280     3.713     0.053     0.009
12    5        3.280     3.713     0.053     0.009
12    5        3.280     3.713     0.053     0.009
12   12        2.655     4.089     0.276    20.655
     TOTAL VAN DER WAALS ENERGY = 21.41512 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      2.705    -0.290    -0.290     7.743
     TOTAL ELECTROSTATIC ENERGY =  7.74347 kcal/mol

TOTAL ENERGY = 50.10353 kcal/mol

E N E R G Y
```

```
B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
h1 c3 c3 h1     0.651        0      0.000   3      1.303
h1 c3 c3 h1     0.651        0   -120.000   3      1.303
h1 c3 c3 cl     0.000        0    120.000   3      0.000
h1 c3 c3 h1     0.651        0    120.000   3      1.303
h1 c3 c3 h1     0.651        0      0.000   3      1.303
h1 c3 c3 cl     0.000        0   -120.000   3      0.000
cl c3 c3 h1     0.000        0   -120.000   3      0.000
cl c3 c3 h1     0.000        0    120.000   3      0.000
cl c3 c3 cl     0.000        0     -0.000   3      0.000
     TOTAL TORSIONAL ENERGY =    5.210 kJ/mol
```

```
I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.208     0.251
h1 h1      2.746    -0.033
h1 cl      3.280    -0.134
h1 h1      2.746    -0.033
h1 h1      2.208     0.251
h1 cl      3.280    -0.134
cl h1      3.280    -0.134
cl h1      3.280    -0.134
cl cl      2.655    44.245
     TOTAL VAN DER WAALS ENERGY =   44.146 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.208     1.352     0.613
h1 h1      2.746     1.352     0.493
h1 cl      3.280    -3.809    -1.161
h1 h1      2.746     1.352     0.493
h1 h1      2.208     1.352     0.613
h1 cl      3.280    -3.809    -1.161
cl h1      3.280    -3.809    -1.161
cl h1      3.280    -3.809    -1.161
cl cl      2.655    10.728     4.041
     TOTAL ELECTROSTATIC ENERGY =    1.607 kJ/mol

TOTAL ENERGY =  134.023 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
```

```
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
```

```
7 0.044101
8 -0.124211

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
```

```
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE         V1    V2    V3     ENERGY
-----------------------------------------------------------------------
 5    1    1    5       0     20.000     0.284   -1.386    0.314      0.349
 5    1    1    5       0   -100.000     0.284   -1.386    0.314     -0.991
 5    1    1   12       0    140.000     0.678   -0.602    0.398      0.129
 5    1    1    5       0    140.000     0.284   -1.386    0.314     -0.304
 5    1    1    5       0     20.000     0.284   -1.386    0.314      0.349
 5    1    1   12       0   -100.000     0.678   -0.602    0.398     -0.005
12    1    1    5       0   -100.000     0.678   -0.602    0.398     -0.005
12    1    1    5       0    140.000     0.678   -0.602    0.398      0.129
12    1    1   12       0     20.000     0.000    0.000    0.893      0.670
     TOTAL TORSIONAL ENERGY =  0.31978 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
```

```
 5    5        2.232     2.970     0.022     0.328
 5    5        2.638     2.970     0.022     0.001
 5   12        3.399     3.713     0.053    -0.028
 5    5        2.831     2.970     0.022    -0.019
 5    5        2.232     2.970     0.022     0.328
 5   12        3.129     3.713     0.053     0.104
12    5        3.129     3.713     0.053     0.104
12    5        3.399     3.713     0.053    -0.028
12   12        2.711     4.089     0.276    16.993
     TOTAL VAN DER WAALS ENERGY = 17.78153 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      2.761    -0.290    -0.290     7.587
     TOTAL ELECTROSTATIC ENERGY =  7.58721 kcal/mol

TOTAL ENERGY = 45.38946 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
```

```
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
h1 c3 c3 h1     0.651        0     20.000   3      0.977
h1 c3 c3 h1     0.651        0   -100.000   3      0.977
h1 c3 c3 cl     0.000        0    140.000   3      0.000
h1 c3 c3 h1     0.651        0    140.000   3      0.977
h1 c3 c3 h1     0.651        0     20.000   3      0.977
h1 c3 c3 cl     0.000        0   -100.000   3      0.000
cl c3 c3 h1     0.000        0   -100.000   3      0.000
cl c3 c3 h1     0.000        0    140.000   3      0.000
cl c3 c3 cl     0.000        0     20.000   3      0.000
     TOTAL TORSIONAL ENERGY =    3.908 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.232     0.205
h1 h1      2.638    -0.029
h1 cl      3.399    -0.133
h1 h1      2.831    -0.032
h1 h1      2.232     0.205
h1 cl      3.129    -0.106
cl h1      3.129    -0.106
cl h1      3.399    -0.133
cl cl      2.711    33.340
     TOTAL VAN DER WAALS ENERGY =   33.209 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

```

```
ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-----------------------------------------
h1 h1      2.232     1.352     0.606
h1 h1      2.638     1.352     0.513
h1 cl      3.399    -3.809    -1.121
h1 h1      2.831     1.352     0.478
h1 h1      2.232     1.352     0.606
h1 cl      3.129    -3.809    -1.217
cl h1      3.129    -3.809    -1.217
cl h1      3.399    -3.809    -1.121
cl cl      2.711    10.728     3.958
     TOTAL ELECTROSTATIC ENERGY =    1.484 kJ/mol

TOTAL ENERGY =  121.662 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
```

```
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G
```

```
ATOM TYPES    FF     BOND        IDEAL        FORCE
 I    J      CLASS  LENGTH      LENGTH      CONSTANT      DELTA       ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000       1.093         4.766     -0.093       3.578
 5    1       0      1.000       1.093         4.766     -0.093       3.578
 5    1       0      1.000       1.093         4.766     -0.093       3.578
 1    1       0      1.540       1.508         4.258      0.032       0.294
 1    5       0      1.000       1.093         4.766     -0.093       3.578
 1   12       0      1.670       1.773         2.974     -0.103       2.795
 1   12       0      1.670       1.773         2.974     -0.103       2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES         FF     VALENCE      IDEAL       FORCE
 I    J    K      CLASS   ANGLE       ANGLE      CONSTANT      DELTA       ENERGY
-------------------------------------------------------------------------------
 1    1    5       0     109.500     110.549        0.636     -1.049       0.015
 5    1    5       0     109.442     108.836        0.516      0.606       0.004
 5    1   12       0     109.442     108.162        0.698      1.280       0.025
 1    1    5       0     109.500     110.549        0.636     -1.049       0.015
 1    1   12       0     109.500     108.679        1.056      0.821       0.016
 5    1   12       0     109.442     108.162        0.698      1.280       0.025
 5    1    5       0     109.442     108.836        0.516      0.606       0.004
 1    1    5       0     109.500     110.549        0.636     -1.049       0.015
 5    1   12       0     109.442     108.162        0.698      1.280       0.025
 1    1    5       0     109.500     110.549        0.636     -1.049       0.015
 5    1   12       0     109.442     108.162        0.698      1.280       0.025
 1    1   12       0     109.500     108.679        1.056      0.821       0.016
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES         FF     VALENCE      DELTA         FORCE CONSTANT
 I    J    K      CLASS   ANGLE       ANGLE         I J         J K       ENERGY
-------------------------------------------------------------------------------
 1    1    5       0     109.500     -1.049        0.227       0.070      -0.002
 5    1    5       0     109.442      0.606        0.115       0.115      -0.033
 5    1   12       0     109.442      1.280       -0.018       0.380      -0.121
 1    1    5       0     109.500     -1.049        0.227       0.070      -0.002
 1    1   12       0     109.500      0.821        0.176       0.386      -0.070
 5    1   12       0     109.442      1.280       -0.018       0.380      -0.121
 5    1    5       0     109.442      0.606        0.115       0.115      -0.033
 1    1    5       0     109.500     -1.049        0.227       0.070      -0.002
 5    1   12       0     109.442      1.280       -0.018       0.380      -0.121
 1    1    5       0     109.500     -1.049        0.227       0.070      -0.002
 5    1   12       0     109.442      1.280       -0.018       0.380      -0.121
 1    1   12       0     109.500      0.821        0.176       0.386      -0.070
```

```
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE         V1   V2   V3     ENERGY
-----------------------------------------------------------------------
 5    1    1    5       0     40.000    0.284   -1.386    0.314     -0.243
 5    1    1    5       0    -80.000    0.284   -1.386    0.314     -1.099
 5    1    1   12       0    160.000    0.678   -0.602    0.398      0.050
 5    1    1    5       0    160.000    0.284   -1.386    0.314     -0.075
 5    1    1    5       0     40.000    0.284   -1.386    0.314     -0.243
 5    1    1   12       0    -80.000    0.678   -0.602    0.398     -0.086
12    1    1    5       0    -80.000    0.678   -0.602    0.398     -0.086
12    1    1    5       0    160.000    0.678   -0.602    0.398      0.050
12    1    1   12       0     40.000    0.000    0.000    0.893      0.223
     TOTAL TORSIONAL ENERGY = -1.51155 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.300     2.970     0.022     0.215
 5    5        2.518     2.970     0.022     0.036
 5   12        3.474     3.713     0.053    -0.041
 5    5        2.885     2.970     0.022    -0.021
 5    5        2.300     2.970     0.022     0.215
 5   12        2.960     3.713     0.053     0.331
12    5        2.960     3.713     0.053     0.331
12    5        3.474     3.713     0.053    -0.041
12   12        2.865     4.089     0.276     9.664
     TOTAL VAN DER WAALS ENERGY = 10.69051 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      2.915    -0.290    -0.290     7.185
     TOTAL ELECTROSTATIC ENERGY =  7.18544 kcal/mol
```

```
TOTAL ENERGY = 36.06534 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
h1 c3 c3 h1     0.651        0     40.000   3      0.326
h1 c3 c3 h1     0.651        0    -80.000   3      0.326
h1 c3 c3 cl     0.000        0    160.000   3      0.000
h1 c3 c3 h1     0.651        0    160.000   3      0.326
h1 c3 c3 h1     0.651        0     40.000   3      0.326
h1 c3 c3 cl     0.000        0    -80.000   3      0.000
```

```
cl c3 c3 h1     0.000        0    -80.000   3      0.000
cl c3 c3 h1     0.000        0    160.000   3      0.000
cl c3 c3 cl     0.000        0     40.000   3      0.000
     TOTAL TORSIONAL ENERGY =    1.303 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
----------------------------------------
h1 h1      2.300     0.109
h1 h1      2.518    -0.013
h1 cl      3.474    -0.129
h1 h1      2.885    -0.031
h1 h1      2.300     0.109
h1 cl      2.960     0.012
cl h1      2.960     0.012
cl h1      3.474    -0.129
cl cl      2.865    15.169
     TOTAL VAN DER WAALS ENERGY =   15.111 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.300     1.352     0.588
h1 h1      2.518     1.352     0.537
h1 cl      3.474    -3.809    -1.097
h1 h1      2.885     1.352     0.469
h1 h1      2.300     1.352     0.588
h1 cl      2.960    -3.809    -1.287
cl h1      2.960    -3.809    -1.287
cl h1      3.474    -3.809    -1.097
cl cl      2.865    10.728     3.745
     TOTAL ELECTROSTATIC ENERGY =    1.160 kJ/mol

TOTAL ENERGY =  100.634 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
```

```
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.036009
```

```
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES    FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
 1   12       0      1.670      1.773        2.974     -0.103      2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES         FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
```

```
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1   12      0    109.500    108.679        1.056      0.821      0.016
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1    V2    V3     ENERGY
-----------------------------------------------------------------------
 5    1    1    5      0     60.000     0.284   -1.386    0.314     -0.827
 5    1    1    5      0    -60.000     0.284   -1.386    0.314     -0.826
 5    1    1   12      0   -180.000     0.678   -0.602    0.398      0.000
 5    1    1    5      0   -180.000     0.284   -1.386    0.314      0.000
 5    1    1    5      0     60.000     0.284   -1.386    0.314     -0.827
 5    1    1   12      0    -60.000     0.678   -0.602    0.398      0.057
12    1    1    5      0    -60.000     0.678   -0.602    0.398      0.057
12    1    1    5      0    180.000     0.678   -0.602    0.398      0.000
12    1    1   12      0     60.000     0.000    0.000    0.893      0.000
     TOTAL TORSIONAL ENERGY = -2.36550 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol
```

```
V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.400     2.970     0.022     0.107
 5    5        2.400     2.970     0.022     0.107
 5   12        3.499     3.713     0.053    -0.044
 5    5        2.903     2.970     0.022    -0.021
 5    5        2.400     2.970     0.022     0.107
 5   12        2.792     3.713     0.053     0.792
12    5        2.792     3.713     0.053     0.792
12    5        3.499     3.713     0.053    -0.044
12   12        3.087     4.089     0.276     3.947
     TOTAL VAN DER WAALS ENERGY =  5.74158 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      3.137    -0.290    -0.290     6.678
     TOTAL ELECTROSTATIC ENERGY =  6.67788 kcal/mol

TOTAL ENERGY = 29.75490 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
```

```
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------
h1 c3 c3 h1     0.651        0     60.000   3      0.000
h1 c3 c3 h1     0.651        0    -60.000   3      0.000
h1 c3 c3 cl     0.000        0   -180.000   3      0.000
h1 c3 c3 h1     0.651        0   -180.000   3      0.000
h1 c3 c3 h1     0.651        0     60.000   3      0.000
h1 c3 c3 cl     0.000        0    -60.000   3      0.000
cl c3 c3 h1     0.000        0    -60.000   3      0.000
cl c3 c3 h1     0.000        0    180.000   3      0.000
cl c3 c3 cl     0.000        0     60.000   3      0.000
     TOTAL TORSIONAL ENERGY =    0.000 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
----------------------------------------
h1 h1      2.400     0.030
h1 h1      2.400     0.030
h1 cl      3.499    -0.127
h1 h1      2.903    -0.031
h1 h1      2.400     0.030
h1 cl      2.792     0.356
cl h1      2.792     0.356
cl h1      3.499    -0.127
```

```
cl cl      3.087     4.588
     TOTAL VAN DER WAALS ENERGY =    5.105 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-----------------------------------------
h1 h1      2.400     1.352     0.563
h1 h1      2.400     1.352     0.563
h1 cl      3.499    -3.809    -1.089
h1 h1      2.903     1.352     0.466
h1 h1      2.400     1.352     0.563
h1 cl      2.792    -3.809    -1.364
cl h1      2.792    -3.809    -1.364
cl h1      3.499    -3.809    -1.089
cl cl      3.087    10.728     3.476
     TOTAL ELECTROSTATIC ENERGY =    0.726 kJ/mol

TOTAL ENERGY =   88.891 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
```

```
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

E N E R G Y


B O N D   S T R E T C H I N G

```

```
ATOM TYPES    FF     BOND        IDEAL        FORCE
 I    J      CLASS  LENGTH      LENGTH      CONSTANT       DELTA       ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000       1.093         4.766      -0.093       3.578
 5    1       0      1.000       1.093         4.766      -0.093       3.578
 5    1       0      1.000       1.093         4.766      -0.093       3.578
 1    1       0      1.540       1.508         4.258       0.032       0.294
 1    5       0      1.000       1.093         4.766      -0.093       3.578
 1   12       0      1.670       1.773         2.974      -0.103       2.795
 1   12       0      1.670       1.773         2.974      -0.103       2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES         FF     VALENCE      IDEAL       FORCE
 I    J    K      CLASS    ANGLE       ANGLE      CONSTANT       DELTA       ENERGY
-------------------------------------------------------------------------------
 1    1    5        0     109.500     110.549         0.636      -1.049       0.015
 5    1    5        0     109.442     108.836         0.516       0.606       0.004
 5    1   12        0     109.442     108.162         0.698       1.280       0.025
 1    1    5        0     109.500     110.549         0.636      -1.049       0.015
 1    1   12        0     109.500     108.679         1.056       0.821       0.016
 5    1   12        0     109.442     108.162         0.698       1.280       0.025
 5    1    5        0     109.442     108.836         0.516       0.606       0.004
 1    1    5        0     109.500     110.549         0.636      -1.049       0.015
 5    1   12        0     109.442     108.162         0.698       1.280       0.025
 1    1    5        0     109.500     110.549         0.636      -1.049       0.015
 5    1   12        0     109.442     108.162         0.698       1.280       0.025
 1    1   12        0     109.500     108.679         1.056       0.821       0.016
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES         FF     VALENCE      DELTA         FORCE CONSTANT
 I    J    K      CLASS    ANGLE       ANGLE         I J         J K       ENERGY
-------------------------------------------------------------------------------
 1    1    5        0     109.500      -1.049       0.227       0.070      -0.002
 5    1    5        0     109.442       0.606       0.115       0.115      -0.033
 5    1   12        0     109.442       1.280      -0.018       0.380      -0.121
 1    1    5        0     109.500      -1.049       0.227       0.070      -0.002
 1    1   12        0     109.500       0.821       0.176       0.386      -0.070
 5    1   12        0     109.442       1.280      -0.018       0.380      -0.121
 5    1    5        0     109.442       0.606       0.115       0.115      -0.033
 1    1    5        0     109.500      -1.049       0.227       0.070      -0.002
 5    1   12        0     109.442       1.280      -0.018       0.380      -0.121
 1    1    5        0     109.500      -1.049       0.227       0.070      -0.002
 5    1   12        0     109.442       1.280      -0.018       0.380      -0.121
 1    1   12        0     109.500       0.821       0.176       0.386      -0.070
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
```

```
T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1    V2    V3     ENERGY
-----------------------------------------------------------------------
 5    1    1    5       0      80.000     0.284   -1.386    0.314     -1.099
 5    1    1    5       0     -40.000     0.284   -1.386    0.314     -0.243
 5    1    1   12       0    -160.000     0.678   -0.602    0.398      0.050
 5    1    1    5       0    -160.000     0.284   -1.386    0.314     -0.075
 5    1    1    5       0      80.000     0.284   -1.386    0.314     -1.099
 5    1    1   12       0     -40.000     0.678   -0.602    0.398      0.449
12    1    1    5       0     -40.000     0.678   -0.602    0.398      0.449
12    1    1    5       0    -160.000     0.678   -0.602    0.398      0.050
12    1    1   12       0      80.000     0.000    0.000    0.893      0.223
     TOTAL TORSIONAL ENERGY = -1.29534 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.518     2.970     0.022     0.036
 5    5        2.300     2.970     0.022     0.215
 5   12        3.474     3.713     0.053    -0.041
 5    5        2.885     2.970     0.022    -0.021
 5    5        2.518     2.970     0.022     0.036
 5   12        2.647     3.713     0.053     1.520
12    5        2.647     3.713     0.053     1.520
12    5        3.474     3.713     0.053    -0.041
12   12        3.338     4.089     0.276     1.129
     TOTAL VAN DER WAALS ENERGY =  4.35500 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      3.388    -0.290    -0.290     6.182
     TOTAL ELECTROSTATIC ENERGY =  6.18170 kcal/mol

TOTAL ENERGY = 28.94230 kcal/mol
```

```
E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
h1 c3 c3 h1     0.651        0     80.000   3      0.326
h1 c3 c3 h1     0.651        0    -40.000   3      0.326
h1 c3 c3 cl     0.000        0   -160.000   3      0.000
h1 c3 c3 h1     0.651        0   -160.000   3      0.326
h1 c3 c3 h1     0.651        0     80.000   3      0.326
h1 c3 c3 cl     0.000        0    -40.000   3      0.000
cl c3 c3 h1     0.000        0    -40.000   3      0.000
```

```
cl c3 c3 h1     0.000        0   -160.000   3      0.000
cl c3 c3 cl     0.000        0     80.000   3      0.000
     TOTAL TORSIONAL ENERGY =    1.303 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.518    -0.013
h1 h1      2.300     0.109
h1 cl      3.474    -0.129
h1 h1      2.885    -0.031
h1 h1      2.518    -0.013
h1 cl      2.647     1.083
cl h1      2.647     1.083
cl h1      3.474    -0.129
cl cl      3.338     0.738
     TOTAL VAN DER WAALS ENERGY =    2.701 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.518     1.352     0.537
h1 h1      2.300     1.352     0.588
h1 cl      3.474    -3.809    -1.097
h1 h1      2.885     1.352     0.469
h1 h1      2.518     1.352     0.537
h1 cl      2.647    -3.809    -1.439
cl h1      2.647    -3.809    -1.439
cl h1      3.474    -3.809    -1.097
cl cl      3.338    10.728     3.214
     TOTAL ELECTROSTATIC ENERGY =    0.273 kJ/mol

TOTAL ENERGY =   87.337 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
```

```
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
```

```
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 1    1      0      1.540      1.508        4.258      0.032      0.294
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1    5      0    109.442    108.836        0.516      0.606      0.004
```

```
 5    1   12       0    109.442    108.162         0.698       1.280       0.025
 1    1    5       0    109.500    110.549         0.636      -1.049       0.015
 1    1   12       0    109.500    108.679         1.056       0.821       0.016
 5    1   12       0    109.442    108.162         0.698       1.280       0.025
 1    1    5       0    109.500    110.549         0.636      -1.049       0.015
 5    1    5       0    109.442    108.836         0.516       0.606       0.004
 5    1   12       0    109.442    108.162         0.698       1.280       0.025
 1    1    5       0    109.500    110.549         0.636      -1.049       0.015
 1    1   12       0    109.500    108.679         1.056       0.821       0.016
 5    1   12       0    109.442    108.162         0.698       1.280       0.025
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------
 1    1    5       0    109.500     -1.049       0.227      0.070     -0.002
 5    1    5       0    109.442      0.606       0.115      0.115     -0.033
 5    1   12       0    109.442      1.280      -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049       0.227      0.070     -0.002
 1    1   12       0    109.500      0.821       0.176      0.386     -0.070
 5    1   12       0    109.442      1.280      -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049       0.227      0.070     -0.002
 5    1    5       0    109.442      0.606       0.115      0.115     -0.033
 5    1   12       0    109.442      1.280      -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049       0.227      0.070     -0.002
 1    1   12       0    109.500      0.821       0.176      0.386     -0.070
 5    1   12       0    109.442      1.280      -0.018      0.380     -0.121
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1    V2    V3     ENERGY
-----------------------------------------------------------------------
 5    1    1    5       0    -20.000     0.284   -1.386    0.314      0.349
 5    1    1    5       0    100.000     0.284   -1.386    0.314     -0.991
 5    1    1   12       0   -140.000     0.678   -0.602    0.398      0.129
 5    1    1    5       0    100.000     0.284   -1.386    0.314     -0.991
 5    1    1    5       0   -140.000     0.284   -1.386    0.314     -0.304
 5    1    1   12       0    -20.000     0.678   -0.602    0.398      0.886
12    1    1    5       0   -140.000     0.678   -0.602    0.398      0.129
12    1    1    5       0    -20.000     0.678   -0.602    0.398      0.886
12    1    1   12       0    100.000     0.000    0.000    0.893      0.670
     TOTAL TORSIONAL ENERGY =  0.76131 kcal/mol

O U T - O F - P L A N E   B E N D I N G
```

```
ATOM TYPES              FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-----------------------------------------------
 5    5        2.638     2.970     0.022     0.001
 5    5        2.232     2.970     0.022     0.328
 5   12        3.399     3.713     0.053    -0.028
 5    5        2.831     2.970     0.022    -0.019
 5    5        2.638     2.970     0.022     0.001
 5   12        2.547     3.713     0.053     2.298
12    5        2.547     3.713     0.053     2.298
12    5        3.399     3.713     0.053    -0.028
12   12        3.587     4.089     0.276     0.100
     TOTAL VAN DER WAALS ENERGY =  4.94916 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-------------------------------------------------
12   12      3.637    -0.290    -0.290     5.759
     TOTAL ELECTROSTATIC ENERGY =  5.75922 kcal/mol

TOTAL ENERGY = 31.17064 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G
```

```
ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
h1 c3 c3 h1     0.651        0    -20.000   3      0.977
h1 c3 c3 h1     0.651        0    100.000   3      0.977
h1 c3 c3 cl     0.000        0   -140.000   3      0.000
h1 c3 c3 h1     0.651        0    100.000   3      0.977
h1 c3 c3 h1     0.651        0   -140.000   3      0.977
h1 c3 c3 cl     0.000        0    -20.000   3      0.000
cl c3 c3 h1     0.000        0   -140.000   3      0.000
cl c3 c3 h1     0.000        0    -20.000   3      0.000
cl c3 c3 cl     0.000        0    100.000   3      0.000
     TOTAL TORSIONAL ENERGY =    3.908 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
----------------------------------------
h1 h1      2.638    -0.029
h1 h1      2.232     0.205
h1 cl      3.399    -0.133
```

```
h1 h1      2.831    -0.032
h1 h1      2.638    -0.029
h1 cl      2.547     2.064
cl h1      2.547     2.064
cl h1      3.399    -0.133
cl cl      3.587    -0.326
     TOTAL VAN DER WAALS ENERGY =    3.650 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.638     1.352     0.513
h1 h1      2.232     1.352     0.606
h1 cl      3.399    -3.809    -1.121
h1 h1      2.831     1.352     0.478
h1 h1      2.638     1.352     0.513
h1 cl      2.547    -3.809    -1.495
cl h1      2.547    -3.809    -1.495
cl h1      3.399    -3.809    -1.121
cl cl      3.587    10.728     2.991
     TOTAL ELECTROSTATIC ENERGY =   -0.132 kJ/mol

TOTAL ENERGY =   90.486 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000
```

```
P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211
```

E N E R G Y

B O N D  S T R E T C H I N G

| ATOM TYPES I | J | FF CLASS | BOND LENGTH | IDEAL LENGTH | FORCE CONSTANT | DELTA | ENERGY |
|---|---|---|---|---|---|---|---|
| 5 | 1 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 5 | 1 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 1 | 1 | 0 | 1.540 | 1.508 | 4.258 | 0.032 | 0.294 |
| 1 | 5 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 1 | 12 | 0 | 1.670 | 1.773 | 2.974 | -0.103 | 2.795 |
| 1 | 5 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 1 | 12 | 0 | 1.670 | 1.773 | 2.974 | -0.103 | 2.795 |

TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E  B E N D I N G

| ATOM TYPES I | J | K | FF CLASS | VALENCE ANGLE | IDEAL ANGLE | FORCE CONSTANT | DELTA | ENERGY |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 5 | 1 | 5 | 0 | 109.442 | 108.836 | 0.516 | 0.606 | 0.004 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 1 | 1 | 12 | 0 | 109.500 | 108.679 | 1.056 | 0.821 | 0.016 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 5 | 1 | 5 | 0 | 109.442 | 108.836 | 0.516 | 0.606 | 0.004 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 1 | 1 | 12 | 0 | 109.500 | 108.679 | 1.056 | 0.821 | 0.016 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |

TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

S T R E T C H  B E N D I N G

| ATOM TYPES I | J | K | FF CLASS | VALENCE ANGLE | DELTA ANGLE | FORCE CONSTANT I J | FORCE CONSTANT J K | ENERGY |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 5 | 1 | 5 | 0 | 109.442 | 0.606 | 0.115 | 0.115 | -0.033 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 1 | 1 | 12 | 0 | 109.500 | 0.821 | 0.176 | 0.386 | -0.070 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 5 | 1 | 5 | 0 | 109.442 | 0.606 | 0.115 | 0.115 | -0.033 |

```
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1    V2    V3      ENERGY
-----------------------------------------------------------------------
 5    1    1    5       0      0.000     0.284   -1.386     0.314      0.598
 5    1    1    5       0    120.000     0.284   -1.386     0.314     -0.654
 5    1    1   12       0   -120.000     0.678   -0.602     0.398      0.116
 5    1    1    5       0    120.000     0.284   -1.386     0.314     -0.655
 5    1    1    5       0   -120.000     0.284   -1.386     0.314     -0.655
 5    1    1   12       0      0.000     0.678   -0.602     0.398      1.076
12    1    1    5       0   -120.000     0.678   -0.602     0.398      0.116
12    1    1    5       0     -0.000     0.678   -0.602     0.398      1.076
12    1    1   12       0    120.000     0.000    0.000     0.893      0.893
     TOTAL TORSIONAL ENERGY =  1.91150 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.746     2.970     0.022    -0.014
 5    5        2.208     2.970     0.022     0.377
 5   12        3.280     3.713     0.053     0.009
 5    5        2.746     2.970     0.022    -0.014
 5    5        2.746     2.970     0.022    -0.014
 5   12        2.512     3.713     0.053     2.649
12    5        2.512     3.713     0.053     2.649
12    5        3.280     3.713     0.053     0.009
12   12        3.806     4.089     0.276    -0.201
     TOTAL VAN DER WAALS ENERGY =  5.44875 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
```

```
-------------------------------------------------
12   12      3.856    -0.290    -0.290     5.432
     TOTAL ELECTROSTATIC ENERGY =  5.43239 kcal/mol

TOTAL ENERGY = 32.49359 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K       ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------
h1 c3 c3 h1     0.651        0      0.000   3      1.303
h1 c3 c3 h1     0.651        0    120.000   3      1.303
```

```
h1 c3 c3 cl     0.000        0   -120.000   3      0.000
h1 c3 c3 h1     0.651        0    120.000   3      1.303
h1 c3 c3 h1     0.651        0   -120.000   3      1.303
h1 c3 c3 cl     0.000        0      0.000   3      0.000
cl c3 c3 h1     0.000        0   -120.000   3      0.000
cl c3 c3 h1     0.000        0     -0.000   3      0.000
cl c3 c3 cl     0.000        0    120.000   3      0.000
     TOTAL TORSIONAL ENERGY =    5.210 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.746    -0.033
h1 h1      2.208     0.251
h1 cl      3.280    -0.134
h1 h1      2.746    -0.033
h1 h1      2.746    -0.033
h1 cl      2.512     2.571
cl h1      2.512     2.571
cl h1      3.280    -0.134
cl cl      3.806    -0.542
     TOTAL VAN DER WAALS ENERGY =    4.485 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.746     1.352     0.493
h1 h1      2.208     1.352     0.613
h1 cl      3.280    -3.809    -1.161
h1 h1      2.746     1.352     0.493
h1 h1      2.746     1.352     0.493
h1 cl      2.512    -3.809    -1.516
cl h1      2.512    -3.809    -1.516
cl h1      3.280    -3.809    -1.161
cl cl      3.806    10.728     2.819
     TOTAL ELECTROSTATIC ENERGY =   -0.446 kJ/mol

TOTAL ENERGY =   92.310 kJ/mol
```

```
A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
```

```
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 1    1      0      1.540      1.508        4.258      0.032      0.294
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1    5      0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

```

```
ATOM TYPES          FF    VALENCE     IDEAL      FORCE
 I    J    K      CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5        0    109.500    110.549       0.636     -1.049       0.015
 5    1    5        0    109.442    108.836       0.516      0.606       0.004
 5    1   12        0    109.442    108.162       0.698      1.280       0.025
 1    1    5        0    109.500    110.549       0.636     -1.049       0.015
 1    1   12        0    109.500    108.679       1.056      0.821       0.016
 5    1   12        0    109.442    108.162       0.698      1.280       0.025
 1    1    5        0    109.500    110.549       0.636     -1.049       0.015
 5    1   12        0    109.442    108.162       0.698      1.280       0.025
 5    1    5        0    109.442    108.836       0.516      0.606       0.004
 1    1   12        0    109.500    108.679       1.056      0.821       0.016
 1    1    5        0    109.500    110.549       0.636     -1.049       0.015
 5    1   12        0    109.442    108.162       0.698      1.280       0.025
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES          FF    VALENCE     DELTA         FORCE CONSTANT
 I    J    K      CLASS   ANGLE      ANGLE         I J         J K       ENERGY
-------------------------------------------------------------------------------
 1    1    5        0    109.500     -1.049       0.227       0.070      -0.002
 5    1    5        0    109.442      0.606       0.115       0.115      -0.033
 5    1   12        0    109.442      1.280      -0.018       0.380      -0.121
 1    1    5        0    109.500     -1.049       0.227       0.070      -0.002
 1    1   12        0    109.500      0.821       0.176       0.386      -0.070
 5    1   12        0    109.442      1.280      -0.018       0.380      -0.121
 1    1    5        0    109.500     -1.049       0.227       0.070      -0.002
 5    1   12        0    109.442      1.280      -0.018       0.380      -0.121
 5    1    5        0    109.442      0.606       0.115       0.115      -0.033
 1    1   12        0    109.500      0.821       0.176       0.386      -0.070
 1    1    5        0    109.500     -1.049       0.227       0.070      -0.002
 5    1   12        0    109.442      1.280      -0.018       0.380      -0.121
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES              FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS     ANGLE          V1    V2    V3      ENERGY
-------------------------------------------------------------------------------
 5    1    1    5       0      20.000      0.284   -1.386    0.314       0.349
 5    1    1   12       0    -100.000      0.678   -0.602    0.398      -0.005
 5    1    1    5       0     140.000      0.284   -1.386    0.314      -0.304
 5    1    1    5       0     140.000      0.284   -1.386    0.314      -0.304
 5    1    1   12       0      20.000      0.678   -0.602    0.398       0.886
 5    1    1    5       0    -100.000      0.284   -1.386    0.314      -0.991
12    1    1    5       0    -100.000      0.678   -0.602    0.398      -0.005
12    1    1   12       0     140.000      0.000    0.000    0.893       0.670
```

```
12    1    1    5      0     20.000    0.678   -0.602    0.398      0.886
     TOTAL TORSIONAL ENERGY =  1.18015 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.831     2.970     0.022    -0.019
 5    5        2.232     2.970     0.022     0.328
 5   12        3.129     3.713     0.053     0.104
 5    5        2.638     2.970     0.022     0.001
 5    5        2.831     2.970     0.022    -0.019
 5   12        2.547     3.713     0.053     2.298
12    5        2.547     3.713     0.053     2.298
12    5        3.129     3.713     0.053     0.104
12   12        3.975     4.089     0.276    -0.269
     TOTAL VAN DER WAALS ENERGY =  4.82482 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      4.025    -0.290    -0.290     5.204
     TOTAL ELECTROSTATIC ENERGY =  5.20367 kcal/mol

TOTAL ENERGY = 30.90959 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
```

```
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
------------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
------------------------------------------------------------------
h1 c3 c3 h1     0.651        0     20.000   3      0.977
h1 c3 c3 cl     0.000        0   -100.000   3      0.000
h1 c3 c3 h1     0.651        0    140.000   3      0.977
h1 c3 c3 h1     0.651        0    140.000   3      0.977
h1 c3 c3 cl     0.000        0     20.000   3      0.000
h1 c3 c3 h1     0.651        0   -100.000   3      0.977
cl c3 c3 h1     0.000        0   -100.000   3      0.000
cl c3 c3 cl     0.000        0    140.000   3      0.000
cl c3 c3 h1     0.000        0     20.000   3      0.000
     TOTAL TORSIONAL ENERGY =    3.908 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
```

```
 I    J        Rij       kij       ENERGY
---------------------------------------
h1 h1      2.831    -0.032
h1 h1      2.232     0.205
h1 cl      3.129    -0.106
h1 h1      2.638    -0.029
h1 h1      2.831    -0.032
h1 cl      2.547     2.064
cl h1      2.547     2.064
cl h1      3.129    -0.106
cl cl      3.975    -0.548
     TOTAL VAN DER WAALS ENERGY =    3.480 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-----------------------------------------
h1 h1      2.831     1.352     0.478
h1 h1      2.232     1.352     0.606
h1 cl      3.129    -3.809    -1.217
h1 h1      2.638     1.352     0.513
h1 h1      2.831     1.352     0.478
h1 cl      2.547    -3.809    -1.495
cl h1      2.547    -3.809    -1.495
cl h1      3.129    -3.809    -1.217
cl cl      3.975    10.728     2.699
     TOTAL ELECTROSTATIC ENERGY =   -0.652 kJ/mol

TOTAL ENERGY =   89.796 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
```

```
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
```

```
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES    FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 5    1       0      1.000      1.093        4.766     -0.093      3.578
12    1       0      1.670      1.773        2.974     -0.103      2.795
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
 1    5       0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES         FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G
```

```
ATOM TYPES          FF     VALENCE      DELTA          FORCE CONSTANT
 I     J     K      CLASS    ANGLE       ANGLE          I J          J K       ENERGY
-------------------------------------------------------------------------------
 1     1     5        0     109.500     -1.049        0.227        0.070      -0.002
 5     1     5        0     109.442      0.606        0.115        0.115      -0.033
 5     1    12        0     109.442      1.280       -0.018        0.380      -0.121
 1     1     5        0     109.500     -1.049        0.227        0.070      -0.002
 1     1    12        0     109.500      0.821        0.176        0.386      -0.070
 5     1    12        0     109.442      1.280       -0.018        0.380      -0.121
 5     1    12        0     109.442      1.280       -0.018        0.380      -0.121
 1     1     5        0     109.500     -1.049        0.227        0.070      -0.002
 5     1     5        0     109.442      0.606        0.115        0.115      -0.033
 1     1    12        0     109.500      0.821        0.176        0.386      -0.070
 5     1    12        0     109.442      1.280       -0.018        0.380      -0.121
 1     1     5        0     109.500     -1.049        0.227        0.070      -0.002
      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES              FF      TORSION        FORCE CONSTANT
 I     J     K     L     CLASS     ANGLE          V1    V2    V3      ENERGY
-----------------------------------------------------------------------
 5     1     1     5       0      40.000      0.284   -1.386    0.314     -0.243
 5     1     1    12       0     -80.000      0.678   -0.602    0.398     -0.086
 5     1     1     5       0     160.000      0.284   -1.386    0.314     -0.075
 5     1     1     5       0     160.000      0.284   -1.386    0.314     -0.075
 5     1     1    12       0      40.000      0.678   -0.602    0.398      0.449
 5     1     1     5       0     -80.000      0.284   -1.386    0.314     -1.099
12     1     1     5       0     -80.000      0.678   -0.602    0.398     -0.086
12     1     1    12       0     160.000      0.000    0.000    0.893      0.223
12     1     1     5       0      40.000      0.678   -0.602    0.398      0.449
      TOTAL TORSIONAL ENERGY = -0.54336 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES              FF       OOP      FORCE
 I     J     K     L     CLASS     ANGLE    CONSTANT      ENERGY
-----------------------------------------------------------------
      TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I     J         Rij        R*IJ     EPSILON     ENERGY
-------------------------------------------------------
 5     5         2.885      2.970      0.022     -0.021
 5     5         2.300      2.970      0.022      0.215
 5    12         2.960      3.713      0.053      0.331
 5     5         2.518      2.970      0.022      0.036
```

```
 5    5        2.885     2.970     0.022    -0.021
 5   12        2.647     3.713     0.053     1.520
12    5        2.647     3.713     0.053     1.520
12    5        2.960     3.713     0.053     0.331
12   12        4.082     4.089     0.276    -0.276
     TOTAL VAN DER WAALS ENERGY =  3.63663 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      4.132    -0.290    -0.290     5.069
     TOTAL ELECTROSTATIC ENERGY =  5.06915 kcal/mol

TOTAL ENERGY = 27.86335 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
cl c3     1.670      1.786     1168.117     -0.116     15.718
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
```

```
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
h1 c3 c3 h1     0.651        0     40.000   3      0.326
h1 c3 c3 cl     0.000        0    -80.000   3      0.000
h1 c3 c3 h1     0.651        0    160.000   3      0.326
h1 c3 c3 h1     0.651        0    160.000   3      0.326
h1 c3 c3 cl     0.000        0     40.000   3      0.000
h1 c3 c3 h1     0.651        0    -80.000   3      0.326
cl c3 c3 h1     0.000        0    -80.000   3      0.000
cl c3 c3 cl     0.000        0    160.000   3      0.000
cl c3 c3 h1     0.000        0     40.000   3      0.000
     TOTAL TORSIONAL ENERGY =    1.303 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.885    -0.031
h1 h1      2.300     0.109
h1 cl      2.960     0.012
h1 h1      2.518    -0.013
h1 h1      2.885    -0.031
h1 cl      2.647     1.083
cl h1      2.647     1.083
cl h1      2.960     0.012
cl cl      4.082    -0.522
     TOTAL VAN DER WAALS ENERGY =    1.704 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.885     1.352     0.469
```

```
h1 h1      2.300     1.352     0.588
h1 cl      2.960    -3.809    -1.287
h1 h1      2.518     1.352     0.537
h1 h1      2.885     1.352     0.469
h1 cl      2.647    -3.809    -1.439
cl h1      2.647    -3.809    -1.439
cl h1      2.960    -3.809    -1.287
cl cl      4.082    10.728     2.628
     TOTAL ELECTROSTATIC ENERGY =   -0.761 kJ/mol

TOTAL ENERGY =   85.306 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S
```

```
2490
2491 SETTING UP BOND CALCULATIONS...
2492 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
2493 SETTING UP TORSION CALCULATIONS...
2494 SETTING UP OOP CALCULATIONS...
2495 SETTING UP VAN DER WAALS CALCULATIONS...
2496 SETTING UP ELECTROSTATIC CALCULATIONS...
2497
2498 A T O M   T Y P E S
2499
2500 IDX TYPE  RING
2501 1 c3  NO
2502 2 c3  NO
2503 3 h1  NO
2504 4 h1  NO
2505 5 cl  NO
2506 6 h1  NO
2507 7 h1  NO
2508 8 cl  NO
2509
2510 C H A R G E S
2511
2512 IDX CHARGE
2513 1 0.036009
2514 2 0.036009
2515 3 0.044101
2516 4 0.044101
2517 5 -0.124211
2518 6 0.044101
2519 7 0.044101
2520 8 -0.124211
2521
2522 S E T T I N G   U P   C A L C U L A T I O N S
2523
2524 SETTING UP BOND CALCULATIONS...
2525 SETTING UP ANGLE CALCULATIONS...
2526 SETTING UP TORSION CALCULATIONS...
2527 SETTING UP IMPROPER TORSION CALCULATIONS...
2528 SETTING UP VAN DER WAALS CALCULATIONS...
2529 SETTING UP ELECTROSTATIC CALCULATIONS...
2530
2531 E N E R G Y
2532
2533
2534 B O N D   S T R E T C H I N G
2535
2536 ATOM TYPES   FF    BOND       IDEAL       FORCE
2537  I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
2538 ---------------------------------------------------------------------------
```

```
 5    1      0      1.000      1.093        4.766     -0.093      3.578
12    1      0      1.670      1.773        2.974     -0.103      2.795
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 1    1      0      1.540      1.508        4.258      0.032      0.294
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1    5      0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L
```

```
ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1    V2    V3      ENERGY
-----------------------------------------------------------------------
 5    1    1   12       0    -60.000     0.678   -0.602    0.398       0.057
 5    1    1    5       0     60.000     0.284   -1.386    0.314      -0.827
 5    1    1    5       0   -180.000     0.284   -1.386    0.314       0.000
 5    1    1   12       0     60.000     0.678   -0.602    0.398       0.057
 5    1    1    5       0   -180.000     0.284   -1.386    0.314       0.000
 5    1    1    5       0    -60.000     0.284   -1.386    0.314      -0.826
12    1    1   12       0    180.000     0.000    0.000    0.893       0.000
12    1    1    5       0    -60.000     0.678   -0.602    0.398       0.057
12    1    1    5       0     60.000     0.678   -0.602    0.398       0.057
     TOTAL TORSIONAL ENERGY = -1.42500 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.903     2.970     0.022    -0.021
 5    5        2.400     2.970     0.022     0.107
 5   12        2.792     3.713     0.053     0.792
 5    5        2.400     2.970     0.022     0.107
 5    5        2.903     2.970     0.022    -0.021
 5   12        2.792     3.713     0.053     0.792
12    5        2.792     3.713     0.053     0.792
12    5        2.792     3.713     0.053     0.792
12   12        4.118     4.089     0.276    -0.275
     TOTAL VAN DER WAALS ENERGY =  3.06216 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      4.168    -0.290    -0.290     5.025
     TOTAL ELECTROSTATIC ENERGY =  5.02482 kcal/mol

TOTAL ENERGY = 26.36292 kcal/mol

E N E R G Y
```

```
B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
cl c3     1.670      1.786     1168.117     -0.116     15.718
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
h1 c3 c3 cl     0.000        0    -60.000   3      0.000
h1 c3 c3 h1     0.651        0     60.000   3      0.000
h1 c3 c3 h1     0.651        0   -180.000   3      0.000
h1 c3 c3 cl     0.000        0     60.000   3      0.000
h1 c3 c3 h1     0.651        0   -180.000   3      0.000
h1 c3 c3 h1     0.651        0    -60.000   3      0.000
cl c3 c3 cl     0.000        0    180.000   3      0.000
cl c3 c3 h1     0.000        0    -60.000   3      0.000
cl c3 c3 h1     0.000        0     60.000   3      0.000
     TOTAL TORSIONAL ENERGY =    0.000 kJ/mol
```

```
I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.903    -0.031
h1 h1      2.400     0.030
h1 cl      2.792     0.356
h1 h1      2.400     0.030
h1 h1      2.903    -0.031
h1 cl      2.792     0.356
cl h1      2.792     0.356
cl h1      2.792     0.356
cl cl      4.118    -0.510
     TOTAL VAN DER WAALS ENERGY =    0.910 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.903     1.352     0.466
h1 h1      2.400     1.352     0.563
h1 cl      2.792    -3.809    -1.364
h1 h1      2.400     1.352     0.563
h1 h1      2.903     1.352     0.466
h1 cl      2.792    -3.809    -1.364
cl h1      2.792    -3.809    -1.364
cl h1      2.792    -3.809    -1.364
cl cl      4.118    10.728     2.605
     TOTAL ELECTROSTATIC ENERGY =   -0.794 kJ/mol

TOTAL ENERGY =   83.176 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
```

```
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO
```

```
C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
12    1      0      1.670      1.773        2.974     -0.103      2.795
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 1    1      0      1.540      1.508        4.258      0.032      0.294
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1    5      0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1    5      0    109.442    108.836        0.516      0.606      0.004
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 1    1   12      0    109.500    108.679        1.056      0.821      0.016
```

```
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1   12      0    109.500    108.679        1.056      0.821      0.016
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1    5      0    109.442    108.836        0.516      0.606      0.004
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE         V1    V2    V3     ENERGY
-----------------------------------------------------------------------
 5    1    1   12      0    -40.000    0.678   -0.602    0.398      0.449
 5    1    1    5      0     80.000    0.284   -1.386    0.314     -1.099
 5    1    1    5      0   -160.000    0.284   -1.386    0.314     -0.075
 5    1    1   12      0     80.000    0.678   -0.602    0.398     -0.086
 5    1    1    5      0   -160.000    0.284   -1.386    0.314     -0.075
 5    1    1    5      0    -40.000    0.284   -1.386    0.314     -0.243
12    1    1   12      0   -160.000    0.000    0.000    0.893      0.223
12    1    1    5      0    -40.000    0.678   -0.602    0.398      0.449
12    1    1    5      0     80.000    0.678   -0.602    0.398     -0.086
     TOTAL TORSIONAL ENERGY = -0.54336 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
```

```
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.885     2.970     0.022    -0.021
 5    5        2.518     2.970     0.022     0.036
 5   12        2.647     3.713     0.053     1.520
 5    5        2.300     2.970     0.022     0.215
 5    5        2.885     2.970     0.022    -0.021
 5   12        2.960     3.713     0.053     0.331
12    5        2.960     3.713     0.053     0.331
12    5        2.647     3.713     0.053     1.520
12   12        4.082     4.089     0.276    -0.276
     TOTAL VAN DER WAALS ENERGY =  3.63663 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      4.132    -0.290    -0.290     5.069
     TOTAL ELECTROSTATIC ENERGY =  5.06915 kcal/mol

TOTAL ENERGY = 27.86335 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
cl c3     1.670      1.786     1168.117     -0.116     15.718
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
```

```
-------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
h1 c3 c3 cl     0.000        0    -40.000   3      0.000
h1 c3 c3 h1     0.651        0     80.000   3      0.326
h1 c3 c3 h1     0.651        0   -160.000   3      0.326
h1 c3 c3 cl     0.000        0     80.000   3      0.000
h1 c3 c3 h1     0.651        0   -160.000   3      0.326
h1 c3 c3 h1     0.651        0    -40.000   3      0.326
cl c3 c3 cl     0.000        0   -160.000   3      0.000
cl c3 c3 h1     0.000        0    -40.000   3      0.000
cl c3 c3 h1     0.000        0     80.000   3      0.000
     TOTAL TORSIONAL ENERGY =    1.303 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
----------------------------------------
h1 h1      2.885    -0.031
h1 h1      2.518    -0.013
h1 cl      2.647     1.083
h1 h1      2.300     0.109
h1 h1      2.885    -0.031
h1 cl      2.960     0.012
```

```
cl h1      2.960     0.012
cl h1      2.647     1.083
cl cl      4.082    -0.522
     TOTAL VAN DER WAALS ENERGY =    1.704 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-----------------------------------------
h1 h1      2.885     1.352     0.469
h1 h1      2.518     1.352     0.537
h1 cl      2.647    -3.809    -1.439
h1 h1      2.300     1.352     0.588
h1 h1      2.885     1.352     0.469
h1 cl      2.960    -3.809    -1.287
cl h1      2.960    -3.809    -1.287
cl h1      2.647    -3.809    -1.439
cl cl      4.082    10.728     2.628
     TOTAL ELECTROSTATIC ENERGY =   -0.761 kJ/mol

TOTAL ENERGY =   85.306 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

```

```
IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
```

```
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES    FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
12    1       0      1.670      1.773        2.974     -0.103      2.795
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES         FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES         FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
```

```
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1   V2   V3     ENERGY
-------------------------------------------------------------------
12    1    1    5       0    -20.000    0.678   -0.602    0.398      0.886
12    1    1    5       0    100.000    0.678   -0.602    0.398     -0.005
12    1    1   12       0   -140.000    0.000    0.000    0.893      0.670
 5    1    1    5       0    100.000    0.284   -1.386    0.314     -0.991
 5    1    1    5       0   -140.000    0.284   -1.386    0.314     -0.304
 5    1    1   12       0    -20.000    0.678   -0.602    0.398      0.886
 5    1    1    5       0   -140.000    0.284   -1.386    0.314     -0.304
 5    1    1    5       0    -20.000    0.284   -1.386    0.314      0.349
 5    1    1   12       0    100.000    0.678   -0.602    0.398     -0.005
     TOTAL TORSIONAL ENERGY =  1.18015 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.831     2.970     0.022    -0.019
 5    5        2.638     2.970     0.022     0.001
 5   12        2.547     3.713     0.053     2.298
 5    5        2.232     2.970     0.022     0.328
 5    5        2.831     2.970     0.022    -0.019
 5   12        3.129     3.713     0.053     0.104
12    5        3.129     3.713     0.053     0.104
12    5        2.547     3.713     0.053     2.298
12   12        3.975     4.089     0.276    -0.269
     TOTAL VAN DER WAALS ENERGY =  4.82482 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S
```

```
ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      4.025    -0.290    -0.290     5.204
     TOTAL ELECTROSTATIC ENERGY =  5.20367 kcal/mol

TOTAL ENERGY = 30.90959 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
cl c3     1.670      1.786     1168.117     -0.116     15.718
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
```

```
3225 ------------------------------------------------------------------
3226 cl c3 c3 h1     0.000        0    -20.000   3      0.000
3227 cl c3 c3 h1     0.000        0    100.000   3      0.000
3228 cl c3 c3 cl     0.000        0   -140.000   3      0.000
3229 h1 c3 c3 h1     0.651        0    100.000   3      0.977
3230 h1 c3 c3 h1     0.651        0   -140.000   3      0.977
3231 h1 c3 c3 cl     0.000        0    -20.000   3      0.000
3232 h1 c3 c3 h1     0.651        0   -140.000   3      0.977
3233 h1 c3 c3 h1     0.651        0    -20.000   3      0.977
3234 h1 c3 c3 cl     0.000        0    100.000   3      0.000
3235      TOTAL TORSIONAL ENERGY =    3.908 kJ/mol
3236
3237 I M P R O P E R   T O R S I O N A L
3238
3239 ----ATOM TYPES-----    FORCE     IMPROPER_TORSION
3240  I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
3241 ------------------------------------------------------------------
3242      TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol
3243
3244 V A N   D E R   W A A L S
3245
3246 ATOM TYPES
3247  I    J        Rij       kij       ENERGY
3248 ----------------------------------------
3249 h1 h1      2.831    -0.032
3250 h1 h1      2.638    -0.029
3251 h1 cl      2.547     2.064
3252 h1 h1      2.232     0.205
3253 h1 h1      2.831    -0.032
3254 h1 cl      3.129    -0.106
3255 cl h1      3.129    -0.106
3256 cl h1      2.547     2.064
3257 cl cl      3.975    -0.548
3258      TOTAL VAN DER WAALS ENERGY =    3.480 kJ/mol
3259
3260 E L E C T R O S T A T I C   I N T E R A C T I O N S
3261
3262 ATOM TYPES
3263  I    J           Rij   332.17*QiQj  ENERGY
3264 ----------------------------------------
3265 h1 h1      2.831     1.352     0.478
3266 h1 h1      2.638     1.352     0.513
3267 h1 cl      2.547    -3.809    -1.495
3268 h1 h1      2.232     1.352     0.606
3269 h1 h1      2.831     1.352     0.478
3270 h1 cl      3.129    -3.809    -1.217
3271 cl h1      3.129    -3.809    -1.217
3272 cl h1      2.547    -3.809    -1.495
3273 cl cl      3.975    10.728     2.699
```

```
     TOTAL ELECTROSTATIC ENERGY =   -0.652 kJ/mol

TOTAL ENERGY =   89.796 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
```

```
7 h1  NO
8 cl  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
12    1       0      1.670      1.773        2.974     -0.103      2.795
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
```

```
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1    5      0    109.442    108.836        0.516      0.606      0.004
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 1    1   12      0    109.500    108.679        1.056      0.821      0.016
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1   12      0    109.500    108.679        1.056      0.821      0.016
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1    5      0    109.442    108.836        0.516      0.606      0.004
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE         V1    V2    V3     ENERGY
-----------------------------------------------------------------------
12    1    1    5      0      0.000     0.678   -0.602    0.398      1.076
12    1    1    5      0    120.000     0.678   -0.602    0.398      0.116
12    1    1   12      0   -120.000     0.000    0.000    0.893      0.893
 5    1    1    5      0    120.000     0.284   -1.386    0.314     -0.654
 5    1    1    5      0   -120.000     0.284   -1.386    0.314     -0.655
 5    1    1   12      0     -0.000     0.678   -0.602    0.398      1.076
 5    1    1    5      0   -120.000     0.284   -1.386    0.314     -0.655
 5    1    1    5      0      0.000     0.284   -1.386    0.314      0.598
 5    1    1   12      0    120.000     0.678   -0.602    0.398      0.116
     TOTAL TORSIONAL ENERGY =  1.91150 kcal/mol
```

```
O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-------------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.746     2.970     0.022    -0.014
 5    5        2.746     2.970     0.022    -0.014
 5   12        2.512     3.713     0.053     2.649
 5    5        2.208     2.970     0.022     0.377
 5    5        2.746     2.970     0.022    -0.014
 5   12        3.280     3.713     0.053     0.009
12    5        3.280     3.713     0.053     0.009
12    5        2.512     3.713     0.053     2.649
12   12        3.806     4.089     0.276    -0.201
     TOTAL VAN DER WAALS ENERGY =  5.44875 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      3.856    -0.290    -0.290     5.432
     TOTAL ELECTROSTATIC ENERGY =  5.43239 kcal/mol

TOTAL ENERGY = 32.49359 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
cl c3     1.670      1.786     1168.117     -0.116     15.718
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol
```

```
A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
cl c3 c3 h1     0.000        0      0.000   3      0.000
cl c3 c3 h1     0.000        0    120.000   3      0.000
cl c3 c3 cl     0.000        0   -120.000   3      0.000
h1 c3 c3 h1     0.651        0    120.000   3      1.303
h1 c3 c3 h1     0.651        0   -120.000   3      1.303
h1 c3 c3 cl     0.000        0     -0.000   3      0.000
h1 c3 c3 h1     0.651        0   -120.000   3      1.303
h1 c3 c3 h1     0.651        0      0.000   3      1.303
h1 c3 c3 cl     0.000        0    120.000   3      0.000
     TOTAL TORSIONAL ENERGY =    5.210 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.746    -0.033
```

```
h1 h1      2.746    -0.033
h1 cl      2.512     2.571
h1 h1      2.208     0.251
h1 h1      2.746    -0.033
h1 cl      3.280    -0.134
cl h1      3.280    -0.134
cl h1      2.512     2.571
cl cl      3.806    -0.542
     TOTAL VAN DER WAALS ENERGY =    4.485 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-----------------------------------------
h1 h1      2.746     1.352     0.493
h1 h1      2.746     1.352     0.493
h1 cl      2.512    -3.809    -1.516
h1 h1      2.208     1.352     0.613
h1 h1      2.746     1.352     0.493
h1 cl      3.280    -3.809    -1.161
cl h1      3.280    -3.809    -1.161
cl h1      2.512    -3.809    -1.516
cl cl      3.806    10.728     2.819
     TOTAL ELECTROSTATIC ENERGY =   -0.446 kJ/mol

TOTAL ENERGY =   92.310 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
```

```
7 0.000000
8 -0.290000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
```

8 -0.124211

E N E R G Y

B O N D  S T R E T C H I N G

| ATOM TYPES I | J | FF CLASS | BOND LENGTH | IDEAL LENGTH | FORCE CONSTANT | DELTA | ENERGY |
|---|---|---|---|---|---|---|---|
| 12 | 1 | 0 | 1.670 | 1.773 | 2.974 | -0.103 | 2.795 |
| 5 | 1 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 1 | 1 | 0 | 1.540 | 1.508 | 4.258 | 0.032 | 0.294 |
| 1 | 5 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 1 | 5 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 1 | 5 | 0 | 1.000 | 1.093 | 4.766 | -0.093 | 3.578 |
| 1 | 12 | 0 | 1.670 | 1.773 | 2.974 | -0.103 | 2.795 |

TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E  B E N D I N G

| ATOM TYPES I | J | K | FF CLASS | VALENCE ANGLE | IDEAL ANGLE | FORCE CONSTANT | DELTA | ENERGY |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 5 | 1 | 5 | 0 | 109.442 | 108.836 | 0.516 | 0.606 | 0.004 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 1 | 1 | 12 | 0 | 109.500 | 108.679 | 1.056 | 0.821 | 0.016 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 12 | 0 | 109.500 | 108.679 | 1.056 | 0.821 | 0.016 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 5 | 1 | 5 | 0 | 109.442 | 108.836 | 0.516 | 0.606 | 0.004 |

TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

S T R E T C H  B E N D I N G

| ATOM TYPES I | J | K | FF CLASS | VALENCE ANGLE | DELTA ANGLE | FORCE CONSTANT I J | FORCE CONSTANT J K | ENERGY |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 5 | 1 | 5 | 0 | 109.442 | 0.606 | 0.115 | 0.115 | -0.033 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 1 | 1 | 12 | 0 | 109.500 | 0.821 | 0.176 | 0.386 | -0.070 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |

```
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1    V2    V3     ENERGY
-----------------------------------------------------------------------
12    1    1    5       0     20.000     0.678   -0.602    0.398      0.886
12    1    1    5       0    140.000     0.678   -0.602    0.398      0.129
12    1    1   12       0   -100.000     0.000    0.000    0.893      0.670
 5    1    1    5       0    140.000     0.284   -1.386    0.314     -0.304
 5    1    1    5       0   -100.000     0.284   -1.386    0.314     -0.991
 5    1    1   12       0     20.000     0.678   -0.602    0.398      0.886
 5    1    1    5       0   -100.000     0.284   -1.386    0.314     -0.991
 5    1    1    5       0     20.000     0.284   -1.386    0.314      0.349
 5    1    1   12       0    140.000     0.678   -0.602    0.398      0.129
     TOTAL TORSIONAL ENERGY =  0.76131 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.638     2.970     0.022     0.001
 5    5        2.831     2.970     0.022    -0.019
 5   12        2.547     3.713     0.053     2.298
 5    5        2.232     2.970     0.022     0.328
 5    5        2.638     2.970     0.022     0.001
 5   12        3.399     3.713     0.053    -0.028
12    5        3.399     3.713     0.053    -0.028
12    5        2.547     3.713     0.053     2.298
12   12        3.587     4.089     0.276     0.100
     TOTAL VAN DER WAALS ENERGY =  4.94916 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S
```

```
ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      3.637    -0.290    -0.290     5.759
     TOTAL ELECTROSTATIC ENERGY =  5.75922 kcal/mol

TOTAL ENERGY = 31.17064 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------
cl c3     1.670      1.786     1168.117     -0.116     15.718
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------
```

```
cl c3 c3 h1     0.000        0     20.000   3      0.000
cl c3 c3 h1     0.000        0    140.000   3      0.000
cl c3 c3 cl     0.000        0   -100.000   3      0.000
h1 c3 c3 h1     0.651        0    140.000   3      0.977
h1 c3 c3 h1     0.651        0   -100.000   3      0.977
h1 c3 c3 cl     0.000        0     20.000   3      0.000
h1 c3 c3 h1     0.651        0   -100.000   3      0.977
h1 c3 c3 h1     0.651        0     20.000   3      0.977
h1 c3 c3 cl     0.000        0    140.000   3      0.000
     TOTAL TORSIONAL ENERGY =    3.908 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.638    -0.029
h1 h1      2.831    -0.032
h1 cl      2.547     2.064
h1 h1      2.232     0.205
h1 h1      2.638    -0.029
h1 cl      3.399    -0.133
cl h1      3.399    -0.133
cl h1      2.547     2.064
cl cl      3.587    -0.326
     TOTAL VAN DER WAALS ENERGY =    3.650 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.638     1.352     0.513
h1 h1      2.831     1.352     0.478
h1 cl      2.547    -3.809    -1.495
h1 h1      2.232     1.352     0.606
h1 h1      2.638     1.352     0.513
h1 cl      3.399    -3.809    -1.121
cl h1      3.399    -3.809    -1.121
cl h1      2.547    -3.809    -1.495
cl cl      3.587    10.728     2.991
     TOTAL ELECTROSTATIC ENERGY =   -0.132 kJ/mol
```

```
3813
3814 TOTAL ENERGY =   90.486 kJ/mol
3815
3816 A T O M   T Y P E S
3817
3818 IDX TYPE  RING
3819 1 1 NO
3820 2 1 NO
3821 3 5 NO
3822 4 5 NO
3823 5 12  NO
3824 6 5 NO
3825 7 5 NO
3826 8 12  NO
3827
3828 F O R M A L   C H A R G E S
3829
3830 IDX CHARGE
3831 1 0.000000
3832 2 0.000000
3833 3 0.000000
3834 4 0.000000
3835 5 0.000000
3836 6 0.000000
3837 7 0.000000
3838 8 0.000000
3839
3840 P A R T I A L   C H A R G E S
3841
3842 IDX CHARGE
3843 1 0.290000
3844 2 0.290000
3845 3 0.000000
3846 4 0.000000
3847 5 -0.290000
3848 6 0.000000
3849 7 0.000000
3850 8 -0.290000
3851
3852 S E T T I N G   U P   C A L C U L A T I O N S
3853
3854 SETTING UP BOND CALCULATIONS...
3855 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
3856 SETTING UP TORSION CALCULATIONS...
3857 SETTING UP OOP CALCULATIONS...
3858 SETTING UP VAN DER WAALS CALCULATIONS...
3859 SETTING UP ELECTROSTATIC CALCULATIONS...
3860
3861 A T O M   T Y P E S
```

```
IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
12    1      0      1.670      1.773        2.974     -0.103      2.795
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 1    1      0      1.540      1.508        4.258      0.032      0.294
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1    5      0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

```

A N G L E  B E N D I N G

| ATOM TYPES I | J | K | FF CLASS | VALENCE ANGLE | IDEAL ANGLE | FORCE CONSTANT | DELTA | ENERGY |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 5 | 1 | 5 | 0 | 109.442 | 108.836 | 0.516 | 0.606 | 0.004 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 1 | 1 | 12 | 0 | 109.500 | 108.679 | 1.056 | 0.821 | 0.016 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 12 | 0 | 109.500 | 108.679 | 1.056 | 0.821 | 0.016 |
| 5 | 1 | 12 | 0 | 109.442 | 108.162 | 0.698 | 1.280 | 0.025 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |
| 5 | 1 | 5 | 0 | 109.442 | 108.836 | 0.516 | 0.606 | 0.004 |
| 1 | 1 | 5 | 0 | 109.500 | 110.549 | 0.636 | -1.049 | 0.015 |

TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

S T R E T C H  B E N D I N G

| ATOM TYPES I | J | K | FF CLASS | VALENCE ANGLE | DELTA ANGLE | FORCE CONSTANT I J | J K | ENERGY |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 5 | 1 | 5 | 0 | 109.442 | 0.606 | 0.115 | 0.115 | -0.033 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 1 | 1 | 12 | 0 | 109.500 | 0.821 | 0.176 | 0.386 | -0.070 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 12 | 0 | 109.500 | 0.821 | 0.176 | 0.386 | -0.070 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 5 | 1 | 5 | 0 | 109.442 | 0.606 | 0.115 | 0.115 | -0.033 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |

TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

| ATOM TYPES I | J | K | L | FF CLASS | TORSION ANGLE | FORCE CONSTANT V1 | V2 | V3 | ENERGY |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 1 | 1 | 12 | 0 | 40.000 | 0.678 | -0.602 | 0.398 | 0.449 |
| 5 | 1 | 1 | 5 | 0 | -80.000 | 0.284 | -1.386 | 0.314 | -1.099 |
| 5 | 1 | 1 | 5 | 0 | 160.000 | 0.284 | -1.386 | 0.314 | -0.075 |
| 5 | 1 | 1 | 12 | 0 | 160.000 | 0.678 | -0.602 | 0.398 | 0.050 |
| 5 | 1 | 1 | 5 | 0 | 40.000 | 0.284 | -1.386 | 0.314 | -0.243 |
| 5 | 1 | 1 | 5 | 0 | -80.000 | 0.284 | -1.386 | 0.314 | -1.099 |

```
12    1    1   12      0    -80.000    0.000    0.000    0.893      0.223
12    1    1    5      0    160.000    0.678   -0.602    0.398      0.050
12    1    1    5      0     40.000    0.678   -0.602    0.398      0.449
     TOTAL TORSIONAL ENERGY = -1.29534 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.518     2.970     0.022     0.036
 5    5        2.885     2.970     0.022    -0.021
 5   12        2.647     3.713     0.053     1.520
 5    5        2.300     2.970     0.022     0.215
 5    5        2.518     2.970     0.022     0.036
 5   12        3.474     3.713     0.053    -0.041
12    5        3.474     3.713     0.053    -0.041
12    5        2.647     3.713     0.053     1.520
12   12        3.338     4.089     0.276     1.129
     TOTAL VAN DER WAALS ENERGY =  4.35500 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      3.388    -0.290    -0.290     6.182
     TOTAL ELECTROSTATIC ENERGY =  6.18170 kcal/mol

TOTAL ENERGY = 28.94230 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
cl c3     1.670      1.786     1168.117     -0.116     15.718
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
```

```
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K       ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
h1 c3 c3 cl     0.000        0     40.000   3      0.000
h1 c3 c3 h1     0.651        0    -80.000   3      0.326
h1 c3 c3 h1     0.651        0    160.000   3      0.326
h1 c3 c3 cl     0.000        0    160.000   3      0.000
h1 c3 c3 h1     0.651        0     40.000   3      0.326
h1 c3 c3 h1     0.651        0    -80.000   3      0.326
cl c3 c3 cl     0.000        0    -80.000   3      0.000
cl c3 c3 h1     0.000        0    160.000   3      0.000
cl c3 c3 h1     0.000        0     40.000   3      0.000
     TOTAL TORSIONAL ENERGY =    1.303 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S
```

```
4058
4059 ATOM TYPES
4060  I    J        Rij       kij       ENERGY
4061 ----------------------------------------
4062 h1 h1      2.518    -0.013
4063 h1 h1      2.885    -0.031
4064 h1 cl      2.647     1.083
4065 h1 h1      2.300     0.109
4066 h1 h1      2.518    -0.013
4067 h1 cl      3.474    -0.129
4068 cl h1      3.474    -0.129
4069 cl h1      2.647     1.083
4070 cl cl      3.338     0.738
4071      TOTAL VAN DER WAALS ENERGY =    2.701 kJ/mol
4072
4073 E L E C T R O S T A T I C   I N T E R A C T I O N S
4074
4075 ATOM TYPES
4076  I    J           Rij   332.17*QiQj  ENERGY
4077 ----------------------------------------
4078 h1 h1      2.518     1.352     0.537
4079 h1 h1      2.885     1.352     0.469
4080 h1 cl      2.647    -3.809    -1.439
4081 h1 h1      2.300     1.352     0.588
4082 h1 h1      2.518     1.352     0.537
4083 h1 cl      3.474    -3.809    -1.097
4084 cl h1      3.474    -3.809    -1.097
4085 cl h1      2.647    -3.809    -1.439
4086 cl cl      3.338    10.728     3.214
4087      TOTAL ELECTROSTATIC ENERGY =    0.273 kJ/mol
4088
4089 TOTAL ENERGY =   87.337 kJ/mol
4090
4091 A T O M   T Y P E S
4092
4093 IDX TYPE  RING
4094 1 1 NO
4095 2 1 NO
4096 3 5 NO
4097 4 5 NO
4098 5 12  NO
4099 6 5 NO
4100 7 5 NO
4101 8 12  NO
4102
4103 F O R M A L   C H A R G E S
4104
4105 IDX CHARGE
4106 1 0.000000
```

```
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
```

```
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES    FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000      1.093        4.766     -0.093      3.578
12    1       0      1.670      1.773        2.974     -0.103      2.795
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
 1    5       0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES         FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol
```

S T R E T C H   B E N D I N G

| ATOM TYPES I | J | K | FF CLASS | VALENCE ANGLE | DELTA ANGLE | FORCE CONSTANT I J | J K | ENERGY |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 5 | 1 | 5 | 0 | 109.442 | 0.606 | 0.115 | 0.115 | -0.033 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 1 | 1 | 12 | 0 | 109.500 | 0.821 | 0.176 | 0.386 | -0.070 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 12 | 0 | 109.500 | 0.821 | 0.176 | 0.386 | -0.070 |
| 5 | 1 | 12 | 0 | 109.442 | 1.280 | -0.018 | 0.380 | -0.121 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |
| 5 | 1 | 5 | 0 | 109.442 | 0.606 | 0.115 | 0.115 | -0.033 |
| 1 | 1 | 5 | 0 | 109.500 | -1.049 | 0.227 | 0.070 | -0.002 |

TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

| ATOM TYPES I | J | K | L | FF CLASS | TORSION ANGLE | FORCE CONSTANT V1 | V2 | V3 | ENERGY |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 1 | 1 | 12 | 0 | 60.000 | 0.678 | -0.602 | 0.398 | 0.057 |
| 5 | 1 | 1 | 5 | 0 | -60.000 | 0.284 | -1.386 | 0.314 | -0.826 |
| 5 | 1 | 1 | 5 | 0 | -180.000 | 0.284 | -1.386 | 0.314 | 0.000 |
| 5 | 1 | 1 | 12 | 0 | -180.000 | 0.678 | -0.602 | 0.398 | 0.000 |
| 5 | 1 | 1 | 5 | 0 | 60.000 | 0.284 | -1.386 | 0.314 | -0.827 |
| 5 | 1 | 1 | 5 | 0 | -60.000 | 0.284 | -1.386 | 0.314 | -0.826 |
| 12 | 1 | 1 | 12 | 0 | -60.000 | 0.000 | 0.000 | 0.893 | 0.000 |
| 12 | 1 | 1 | 5 | 0 | 180.000 | 0.678 | -0.602 | 0.398 | 0.000 |
| 12 | 1 | 1 | 5 | 0 | 60.000 | 0.678 | -0.602 | 0.398 | 0.057 |

TOTAL TORSIONAL ENERGY = -2.36550 kcal/mol

O U T - O F - P L A N E   B E N D I N G

| ATOM TYPES I | J | K | L | FF CLASS | OOP ANGLE | FORCE CONSTANT | ENERGY |
|---|---|---|---|---|---|---|---|

TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol

V A N   D E R   W A A L S

| ATOM TYPES I | J | Rij | R*IJ | EPSILON | ENERGY |
|---|---|---|---|---|---|
| 5 | 5 | 2.400 | 2.970 | 0.022 | 0.107 |
| 5 | 5 | 2.903 | 2.970 | 0.022 | -0.021 |

```
 5   12        2.792     3.713     0.053     0.792
 5    5        2.400     2.970     0.022     0.107
 5    5        2.400     2.970     0.022     0.107
 5   12        3.499     3.713     0.053    -0.044
12    5        3.499     3.713     0.053    -0.044
12    5        2.792     3.713     0.053     0.792
12   12        3.087     4.089     0.276     3.947
     TOTAL VAN DER WAALS ENERGY =  5.74158 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      3.137    -0.290    -0.290     6.678
     TOTAL ELECTROSTATIC ENERGY =  6.67788 kcal/mol

TOTAL ENERGY = 29.75490 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
cl c3     1.670      1.786     1168.117     -0.116     15.718
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES       VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
```

```
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
h1 c3 c3 cl     0.000        0     60.000   3      0.000
h1 c3 c3 h1     0.651        0    -60.000   3      0.000
h1 c3 c3 h1     0.651        0   -180.000   3      0.000
h1 c3 c3 cl     0.000        0   -180.000   3      0.000
h1 c3 c3 h1     0.651        0     60.000   3      0.000
h1 c3 c3 h1     0.651        0    -60.000   3      0.000
cl c3 c3 cl     0.000        0    -60.000   3      0.000
cl c3 c3 h1     0.000        0    180.000   3      0.000
cl c3 c3 h1     0.000        0     60.000   3      0.000
     TOTAL TORSIONAL ENERGY =    0.000 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.400     0.030
h1 h1      2.903    -0.031
h1 cl      2.792     0.356
h1 h1      2.400     0.030
h1 h1      2.400     0.030
h1 cl      3.499    -0.127
cl h1      3.499    -0.127
cl h1      2.792     0.356
cl cl      3.087     4.588
     TOTAL VAN DER WAALS ENERGY =    5.105 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
```

```
4352 ----------------------------------------
4353 h1 h1      2.400     1.352     0.563
4354 h1 h1      2.903     1.352     0.466
4355 h1 cl      2.792    -3.809    -1.364
4356 h1 h1      2.400     1.352     0.563
4357 h1 h1      2.400     1.352     0.563
4358 h1 cl      3.499    -3.809    -1.089
4359 cl h1      3.499    -3.809    -1.089
4360 cl h1      2.792    -3.809    -1.364
4361 cl cl      3.087    10.728     3.476
4362      TOTAL ELECTROSTATIC ENERGY =    0.726 kJ/mol
4363
4364 TOTAL ENERGY =   88.891 kJ/mol
4365
4366 A T O M   T Y P E S
4367
4368 IDX TYPE  RING
4369 1 1 NO
4370 2 1 NO
4371 3 5 NO
4372 4 5 NO
4373 5 12  NO
4374 6 5 NO
4375 7 5 NO
4376 8 12  NO
4377
4378 F O R M A L   C H A R G E S
4379
4380 IDX CHARGE
4381 1 0.000000
4382 2 0.000000
4383 3 0.000000
4384 4 0.000000
4385 5 0.000000
4386 6 0.000000
4387 7 0.000000
4388 8 0.000000
4389
4390 P A R T I A L   C H A R G E S
4391
4392 IDX CHARGE
4393 1 0.290000
4394 2 0.290000
4395 3 0.000000
4396 4 0.000000
4397 5 -0.290000
4398 6 0.000000
4399 7 0.000000
4400 8 -0.290000
```

```
4401
4402 S E T T I N G   U P   C A L C U L A T I O N S
4403
4404 SETTING UP BOND CALCULATIONS...
4405 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4406 SETTING UP TORSION CALCULATIONS...
4407 SETTING UP OOP CALCULATIONS...
4408 SETTING UP VAN DER WAALS CALCULATIONS...
4409 SETTING UP ELECTROSTATIC CALCULATIONS...
4410
4411 A T O M   T Y P E S
4412
4413 IDX TYPE  RING
4414 1 c3  NO
4415 2 c3  NO
4416 3 h1  NO
4417 4 h1  NO
4418 5 cl  NO
4419 6 h1  NO
4420 7 h1  NO
4421 8 cl  NO
4422
4423 C H A R G E S
4424
4425 IDX CHARGE
4426 1 0.036009
4427 2 0.036009
4428 3 0.044101
4429 4 0.044101
4430 5 -0.124211
4431 6 0.044101
4432 7 0.044101
4433 8 -0.124211
4434
4435 S E T T I N G   U P   C A L C U L A T I O N S
4436
4437 SETTING UP BOND CALCULATIONS...
4438 SETTING UP ANGLE CALCULATIONS...
4439 SETTING UP TORSION CALCULATIONS...
4440 SETTING UP IMPROPER TORSION CALCULATIONS...
4441 SETTING UP VAN DER WAALS CALCULATIONS...
4442 SETTING UP ELECTROSTATIC CALCULATIONS...
4443
4444 E N E R G Y
4445
4446
4447 B O N D   S T R E T C H I N G
4448
4449 ATOM TYPES   FF    BOND       IDEAL       FORCE
```

```
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 5    1       0      1.000      1.093        4.766     -0.093      3.578
12    1       0      1.670      1.773        2.974     -0.103      2.795
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
 1    5       0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5       0    109.442      0.606      0.115      0.115     -0.033
 1    1   12       0    109.500      0.821      0.176      0.386     -0.070
 5    1   12       0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5       0    109.500     -1.049      0.227      0.070     -0.002
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
```

```
T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE         V1    V2    V3     ENERGY
-------------------------------------------------------------------------
 5    1    1    5       0    -40.000     0.284   -1.386    0.314     -0.243
 5    1    1   12       0     80.000     0.678   -0.602    0.398     -0.086
 5    1    1    5       0   -160.000     0.284   -1.386    0.314     -0.075
 5    1    1    5       0     80.000     0.284   -1.386    0.314     -1.099
 5    1    1   12       0   -160.000     0.678   -0.602    0.398      0.050
 5    1    1    5       0    -40.000     0.284   -1.386    0.314     -0.243
12    1    1    5       0   -160.000     0.678   -0.602    0.398      0.050
12    1    1   12       0    -40.000     0.000    0.000    0.893      0.223
12    1    1    5       0     80.000     0.678   -0.602    0.398     -0.086
     TOTAL TORSIONAL ENERGY = -1.51155 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.300     2.970     0.022     0.215
 5    5        2.885     2.970     0.022    -0.021
 5   12        2.960     3.713     0.053     0.331
 5    5        2.518     2.970     0.022     0.036
 5    5        2.300     2.970     0.022     0.215
 5   12        3.474     3.713     0.053    -0.041
12    5        3.474     3.713     0.053    -0.041
12    5        2.960     3.713     0.053     0.331
12   12        2.865     4.089     0.276     9.664
     TOTAL VAN DER WAALS ENERGY = 10.69051 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      2.915    -0.290    -0.290     7.185
     TOTAL ELECTROSTATIC ENERGY =  7.18544 kcal/mol

TOTAL ENERGY = 36.06534 kcal/mol
```

```
E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
cl c3     1.670      1.786     1168.117     -0.116     15.718
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G

ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-----------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-----------------------------------------------------------------
h1 c3 c3 h1     0.651        0    -40.000   3      0.326
h1 c3 c3 cl     0.000        0     80.000   3      0.000
h1 c3 c3 h1     0.651        0   -160.000   3      0.326
h1 c3 c3 h1     0.651        0     80.000   3      0.326
h1 c3 c3 cl     0.000        0   -160.000   3      0.000
h1 c3 c3 h1     0.651        0    -40.000   3      0.326
cl c3 c3 h1     0.000        0   -160.000   3      0.000
cl c3 c3 cl     0.000        0    -40.000   3      0.000
```

```
cl c3 c3 h1     0.000        0     80.000   3      0.000
     TOTAL TORSIONAL ENERGY =    1.303 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.300     0.109
h1 h1      2.885    -0.031
h1 cl      2.960     0.012
h1 h1      2.518    -0.013
h1 h1      2.300     0.109
h1 cl      3.474    -0.129
cl h1      3.474    -0.129
cl h1      2.960     0.012
cl cl      2.865    15.169
     TOTAL VAN DER WAALS ENERGY =   15.111 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-------------------------------------------
h1 h1      2.300     1.352     0.588
h1 h1      2.885     1.352     0.469
h1 cl      2.960    -3.809    -1.287
h1 h1      2.518     1.352     0.537
h1 h1      2.300     1.352     0.588
h1 cl      3.474    -3.809    -1.097
cl h1      3.474    -3.809    -1.097
cl h1      2.960    -3.809    -1.287
cl cl      2.865    10.728     3.745
     TOTAL ELECTROSTATIC ENERGY =    1.160 kJ/mol

TOTAL ENERGY =  100.634 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
```

```
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000

P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
```

```
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES   FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 5    1      0      1.000      1.093        4.766     -0.093      3.578
 1    1      0      1.540      1.508        4.258      0.032      0.294
 1    5      0      1.000      1.093        4.766     -0.093      3.578
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1   12      0      1.670      1.773        2.974     -0.103      2.795
 1    5      0      1.000      1.093        4.766     -0.093      3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES        FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1    5      0    109.442    108.836        0.516      0.606      0.004
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
```

```
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 1    1   12      0    109.500    108.679        1.056      0.821      0.016
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
 5    1    5      0    109.442    108.836        0.516      0.606      0.004
 1    1   12      0    109.500    108.679        1.056      0.821      0.016
 1    1    5      0    109.500    110.549        0.636     -1.049      0.015
 5    1   12      0    109.442    108.162        0.698      1.280      0.025
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES        FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K      ENERGY
-------------------------------------------------------------------------
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE         V1    V2    V3     ENERGY
-----------------------------------------------------------------------
 5    1    1    5      0    -20.000    0.284   -1.386    0.314      0.349
 5    1    1   12      0    100.000    0.678   -0.602    0.398     -0.005
 5    1    1    5      0   -140.000    0.284   -1.386    0.314     -0.304
 5    1    1    5      0    100.000    0.284   -1.386    0.314     -0.991
 5    1    1   12      0   -140.000    0.678   -0.602    0.398      0.129
 5    1    1    5      0    -20.000    0.284   -1.386    0.314      0.349
12    1    1    5      0   -140.000    0.678   -0.602    0.398      0.129
12    1    1   12      0    -20.000    0.000    0.000    0.893      0.670
12    1    1    5      0    100.000    0.678   -0.602    0.398     -0.005
     TOTAL TORSIONAL ENERGY =  0.31978 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
```

```
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.232     2.970     0.022     0.328
 5    5        2.831     2.970     0.022    -0.019
 5   12        3.129     3.713     0.053     0.104
 5    5        2.638     2.970     0.022     0.001
 5    5        2.232     2.970     0.022     0.328
 5   12        3.399     3.713     0.053    -0.028
12    5        3.399     3.713     0.053    -0.028
12    5        3.129     3.713     0.053     0.104
12   12        2.711     4.089     0.276    16.993
     TOTAL VAN DER WAALS ENERGY = 17.78153 kcal/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J        Rij        Qi         Qj        ENERGY
-----------------------------------------------------
12   12      2.761    -0.290    -0.290     7.587
     TOTAL ELECTROSTATIC ENERGY =  7.58721 kcal/mol

TOTAL ENERGY = 45.38946 kcal/mol

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES  BOND       IDEAL       FORCE
 I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
h1 c3     1.000      1.093     1406.346     -0.093     12.163
h1 c3     1.000      1.093     1406.346     -0.093     12.163
c3 c3     1.540      1.535     1269.019      0.005      0.032
c3 h1     1.000      1.093     1406.346     -0.093     12.163
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 cl     1.670      1.786     1168.117     -0.116     15.718
c3 h1     1.000      1.093     1406.346     -0.093     12.163
     TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol

A N G L E   B E N D I N G
```

```
ATOM TYPES        VALENCE     IDEAL      FORCE
 I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
h1 c3 cl   109.442    105.930      183.005      0.061      0.688
     TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol

T O R S I O N A L

----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
h1 c3 c3 h1     0.651        0    -20.000   3      0.977
h1 c3 c3 cl     0.000        0    100.000   3      0.000
h1 c3 c3 h1     0.651        0   -140.000   3      0.977
h1 c3 c3 h1     0.651        0    100.000   3      0.977
h1 c3 c3 cl     0.000        0   -140.000   3      0.000
h1 c3 c3 h1     0.651        0    -20.000   3      0.977
cl c3 c3 h1     0.000        0   -140.000   3      0.000
cl c3 c3 cl     0.000        0    -20.000   3      0.000
cl c3 c3 h1     0.000        0    100.000   3      0.000
     TOTAL TORSIONAL ENERGY =    3.908 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.232     0.205
h1 h1      2.831    -0.032
h1 cl      3.129    -0.106
h1 h1      2.638    -0.029
```

```
h1 h1      2.232     0.205
h1 cl      3.399    -0.133
cl h1      3.399    -0.133
cl h1      3.129    -0.106
cl cl      2.711    33.340
     TOTAL VAN DER WAALS ENERGY =   33.209 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-----------------------------------------
h1 h1      2.232     1.352     0.606
h1 h1      2.831     1.352     0.478
h1 cl      3.129    -3.809    -1.217
h1 h1      2.638     1.352     0.513
h1 h1      2.232     1.352     0.606
h1 cl      3.399    -3.809    -1.121
cl h1      3.399    -3.809    -1.121
cl h1      3.129    -3.809    -1.217
cl cl      2.711    10.728     3.958
     TOTAL ELECTROSTATIC ENERGY =    1.484 kJ/mol

TOTAL ENERGY =  121.662 kJ/mol

A T O M   T Y P E S

IDX TYPE  RING
1 1 NO
2 1 NO
3 5 NO
4 5 NO
5 12  NO
6 5 NO
7 5 NO
8 12  NO

F O R M A L   C H A R G E S

IDX CHARGE
1 0.000000
2 0.000000
3 0.000000
4 0.000000
5 0.000000
6 0.000000
7 0.000000
8 0.000000
```

```
P A R T I A L   C H A R G E S

IDX CHARGE
1 0.290000
2 0.290000
3 0.000000
4 0.000000
5 -0.290000
6 0.000000
7 0.000000
8 -0.290000

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
SETTING UP OOP CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

A T O M   T Y P E S

IDX TYPE  RING
1 c3  NO
2 c3  NO
3 h1  NO
4 h1  NO
5 cl  NO
6 h1  NO
7 h1  NO
8 cl  NO

C H A R G E S

IDX CHARGE
1 0.036009
2 0.036009
3 0.044101
4 0.044101
5 -0.124211
6 0.044101
7 0.044101
8 -0.124211

S E T T I N G   U P   C A L C U L A T I O N S

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE CALCULATIONS...
```

```
SETTING UP TORSION CALCULATIONS...
SETTING UP IMPROPER TORSION CALCULATIONS...
SETTING UP VAN DER WAALS CALCULATIONS...
SETTING UP ELECTROSTATIC CALCULATIONS...

E N E R G Y


B O N D   S T R E T C H I N G

ATOM TYPES    FF    BOND       IDEAL       FORCE
 I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 5    1       0      1.000      1.093        4.766     -0.093      3.578
 1    1       0      1.540      1.508        4.258      0.032      0.294
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
 1    5       0      1.000      1.093        4.766     -0.093      3.578
 1   12       0      1.670      1.773        2.974     -0.103      2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

A N G L E   B E N D I N G

ATOM TYPES         FF    VALENCE     IDEAL      FORCE
 I    J    K     CLASS   ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 5    1    5       0    109.442    108.836        0.516      0.606      0.004
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
 1    1    5       0    109.500    110.549        0.636     -1.049      0.015
 1    1   12       0    109.500    108.679        1.056      0.821      0.016
 5    1   12       0    109.442    108.162        0.698      1.280      0.025
     TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol

S T R E T C H   B E N D I N G

ATOM TYPES         FF    VALENCE     DELTA        FORCE CONSTANT
 I    J    K     CLASS   ANGLE      ANGLE        I J        J K       ENERGY
-------------------------------------------------------------------------------
 1    1    5       0    109.500     -1.049      0.227      0.070      -0.002
 5    1    5       0    109.442      0.606      0.115      0.115      -0.033
 5    1   12       0    109.442      1.280     -0.018      0.380      -0.121
```

```
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 5    1    5      0    109.442      0.606      0.115      0.115     -0.033
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
 1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
 1    1   12      0    109.500      0.821      0.176      0.386     -0.070
 5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES             FF     TORSION       FORCE CONSTANT
 I    J    K    L     CLASS    ANGLE          V1    V2    V3     ENERGY
-------------------------------------------------------------------------
 5    1    1    5       0      0.000     0.284   -1.386    0.314      0.598
 5    1    1    5       0   -120.000     0.284   -1.386    0.314     -0.655
 5    1    1   12       0    120.000     0.678   -0.602    0.398      0.116
 5    1    1    5       0    120.000     0.284   -1.386    0.314     -0.655
 5    1    1    5       0      0.000     0.284   -1.386    0.314      0.598
 5    1    1   12       0   -120.000     0.678   -0.602    0.398      0.116
12    1    1    5       0   -120.000     0.678   -0.602    0.398      0.116
12    1    1    5       0    120.000     0.678   -0.602    0.398      0.116
12    1    1   12       0     -0.000     0.000    0.000    0.893      0.893
     TOTAL TORSIONAL ENERGY =  1.24400 kcal/mol

O U T - O F - P L A N E   B E N D I N G

ATOM TYPES             FF       OOP     FORCE
 I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
-----------------------------------------------------------
     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       R*IJ    EPSILON    ENERGY
-------------------------------------------------
 5    5        2.208     2.970     0.022     0.377
 5    5        2.746     2.970     0.022    -0.014
 5   12        3.280     3.713     0.053     0.009
 5    5        2.746     2.970     0.022    -0.014
 5    5        2.208     2.970     0.022     0.377
 5   12        3.280     3.713     0.053     0.009
12    5        3.280     3.713     0.053     0.009
12    5        3.280     3.713     0.053     0.009
12   12        2.655     4.089     0.276    20.655
     TOTAL VAN DER WAALS ENERGY = 21.41512 kcal/mol
```

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5087
5088 E L E C T R O S T A T I C   I N T E R A C T I O N S
5089
5090 ATOM TYPES
5091  I    J        Rij        Qi         Qj        ENERGY
5092 ---------------------------------------------------
5093 12   12      2.705    -0.290    -0.290     7.743
5094      TOTAL ELECTROSTATIC ENERGY =  7.74347 kcal/mol
5095
5096 TOTAL ENERGY = 50.10353 kcal/mol
5097
5098 E N E R G Y
5099
5100
5101 B O N D   S T R E T C H I N G
5102
5103 ATOM TYPES  BOND       IDEAL       FORCE
5104  I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
5105 ------------------------------------------------------------------------
5106 h1 c3     1.000      1.093     1406.346     -0.093     12.163
5107 h1 c3     1.000      1.093     1406.346     -0.093     12.163
5108 c3 c3     1.540      1.535     1269.019      0.005      0.032
5109 c3 h1     1.000      1.093     1406.346     -0.093     12.163
5110 c3 cl     1.670      1.786     1168.117     -0.116     15.718
5111 c3 h1     1.000      1.093     1406.346     -0.093     12.163
5112 c3 cl     1.670      1.786     1168.117     -0.116     15.718
5113      TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol
5114
5115 A N G L E   B E N D I N G
5116
5117 ATOM TYPES        VALENCE     IDEAL      FORCE
5118  I    J    K      ANGLE      ANGLE     CONSTANT      DELTA      ENERGY
5119 ------------------------------------------------------------------------------
5120 c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
5121 h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
5122 h1 c3 cl   109.442    105.930      183.005      0.061      0.688
5123 c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
5124 c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
5125 h1 c3 cl   109.442    105.930      183.005      0.061      0.688
5126 c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
5127 h1 c3 h1   109.442    109.550      164.039     -0.002      0.001
5128 h1 c3 cl   109.442    105.930      183.005      0.061      0.688
5129 c3 c3 h1   109.500    110.070      194.100     -0.010      0.019
5130 c3 c3 cl   109.500    110.330      260.419     -0.014      0.055
5131 h1 c3 cl   109.442    105.930      183.005      0.061      0.688
5132      TOTAL ANGLE BENDING ENERGY =    2.938 kJ/mol
5133
5134 T O R S I O N A L
5135
```

```
----ATOM TYPES-----    FORCE              TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
h1 c3 c3 h1     0.651        0      0.000   3      1.303
h1 c3 c3 h1     0.651        0   -120.000   3      1.303
h1 c3 c3 cl     0.000        0    120.000   3      0.000
h1 c3 c3 h1     0.651        0    120.000   3      1.303
h1 c3 c3 h1     0.651        0      0.000   3      1.303
h1 c3 c3 cl     0.000        0   -120.000   3      0.000
cl c3 c3 h1     0.000        0   -120.000   3      0.000
cl c3 c3 h1     0.000        0    120.000   3      0.000
cl c3 c3 cl     0.000        0     -0.000   3      0.000
     TOTAL TORSIONAL ENERGY =    5.210 kJ/mol

I M P R O P E R   T O R S I O N A L

----ATOM TYPES-----    FORCE     IMPROPER_TORSION
 I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
-------------------------------------------------------------------
     TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol

V A N   D E R   W A A L S

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
h1 h1      2.208     0.251
h1 h1      2.746    -0.033
h1 cl      3.280    -0.134
h1 h1      2.746    -0.033
h1 h1      2.208     0.251
h1 cl      3.280    -0.134
cl h1      3.280    -0.134
cl h1      3.280    -0.134
cl cl      2.655    44.245
     TOTAL VAN DER WAALS ENERGY =   44.146 kJ/mol

E L E C T R O S T A T I C   I N T E R A C T I O N S

ATOM TYPES
 I    J           Rij   332.17*QiQj  ENERGY
-----------------------------------------
h1 h1      2.208     1.352     0.613
h1 h1      2.746     1.352     0.493
h1 cl      3.280    -3.809    -1.161
h1 h1      2.746     1.352     0.493
h1 h1      2.208     1.352     0.613
h1 cl      3.280    -3.809    -1.161
cl h1      3.280    -3.809    -1.161
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cl h1      3.280    -3.809    -1.161
cl cl      2.655    10.728     4.041
     TOTAL ELECTROSTATIC ENERGY =    1.607 kJ/mol

TOTAL ENERGY =  134.023 kJ/mol
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