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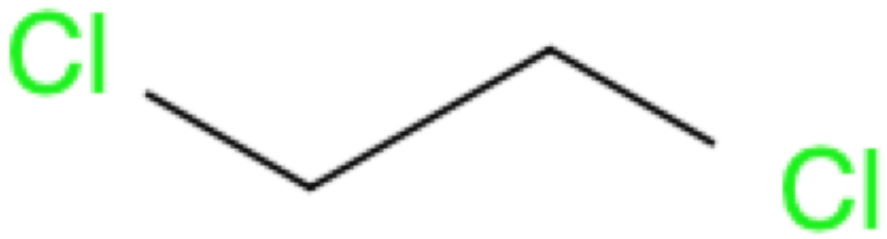
BIM2005: Homework I

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

Preparation

- Structure of $C_2H_4Cl_2$ (For reference)



- 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/BIM2005-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°.)
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. 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
│   ├── C2H4Cl2_100_degrees.gzmat
│   ├── C2H4Cl2_100_degrees.xyz
│   ├── C2H4Cl2_120_degrees.gzmat
│   ├── C2H4Cl2_120_degrees.xyz
│   ├── C2H4Cl2_140_degrees.gzmat
│   ├── C2H4Cl2_140_degrees.xyz
│   ├── C2H4Cl2_160_degrees.gzmat
│   ├── C2H4Cl2_160_degrees.xyz
│   ├── C2H4Cl2_180_degrees.gzmat
│   ├── C2H4Cl2_180_degrees.xyz
│   ├── C2H4Cl2_200_degrees.gzmat
│   ├── C2H4Cl2_200_degrees.xyz
│   ├── C2H4Cl2_20_degrees.gzmat
│   ├── C2H4Cl2_20_degrees.xyz
│   ├── C2H4Cl2_220_degrees.gzmat
│   ├── C2H4Cl2_220_degrees.xyz
│   ├── C2H4Cl2_240_degrees.gzmat
```

```
│   ├── C2H4Cl2_240_degrees.xyz
│   ├── C2H4Cl2_260_degrees.gzmat
│   ├── C2H4Cl2_260_degrees.xyz
│   ├── C2H4Cl2_280_degrees.gzmat
│   ├── C2H4Cl2_280_degrees.xyz
│   ├── C2H4Cl2_300_degrees.gzmat
│   ├── C2H4Cl2_300_degrees.xyz
│   ├── C2H4Cl2_320_degrees.gzmat
│   ├── C2H4Cl2_320_degrees.xyz
│   ├── C2H4Cl2_340_degrees.gzmat
│   ├── C2H4Cl2_340_degrees.xyz
│   ├── C2H4Cl2_360_degrees.gzmat
│   ├── C2H4Cl2_360_degrees.xyz
│   ├── C2H4Cl2_40_degrees.gzmat
│   ├── C2H4Cl2_40_degrees.xyz
│   ├── C2H4Cl2_60_degrees.gzmat
│   ├── C2H4Cl2_60_degrees.xyz
│   ├── C2H4Cl2_80_degrees.gzmat
│   └── C2H4Cl2_80_degrees.xyz
├── DATA                            // .csv table file containing all the energy
data
│   ├── data.csv
│   ├── data_in_KJ.csv
│   └── data_in_Kcal.csv
├── README.md                       // This file you are in
├── XYZ_GAMAT_SUMMARY.md            // (Not Important)
├── code2mkdoc.py                    // The script used to facilitate the processing
of the documentation
├── file_tree.txt                  // The file tree (Not Important)
└── requirements.txt               // All the requirements in my environment to run
this script and some of them are redundant for you
├── 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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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°

- ./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

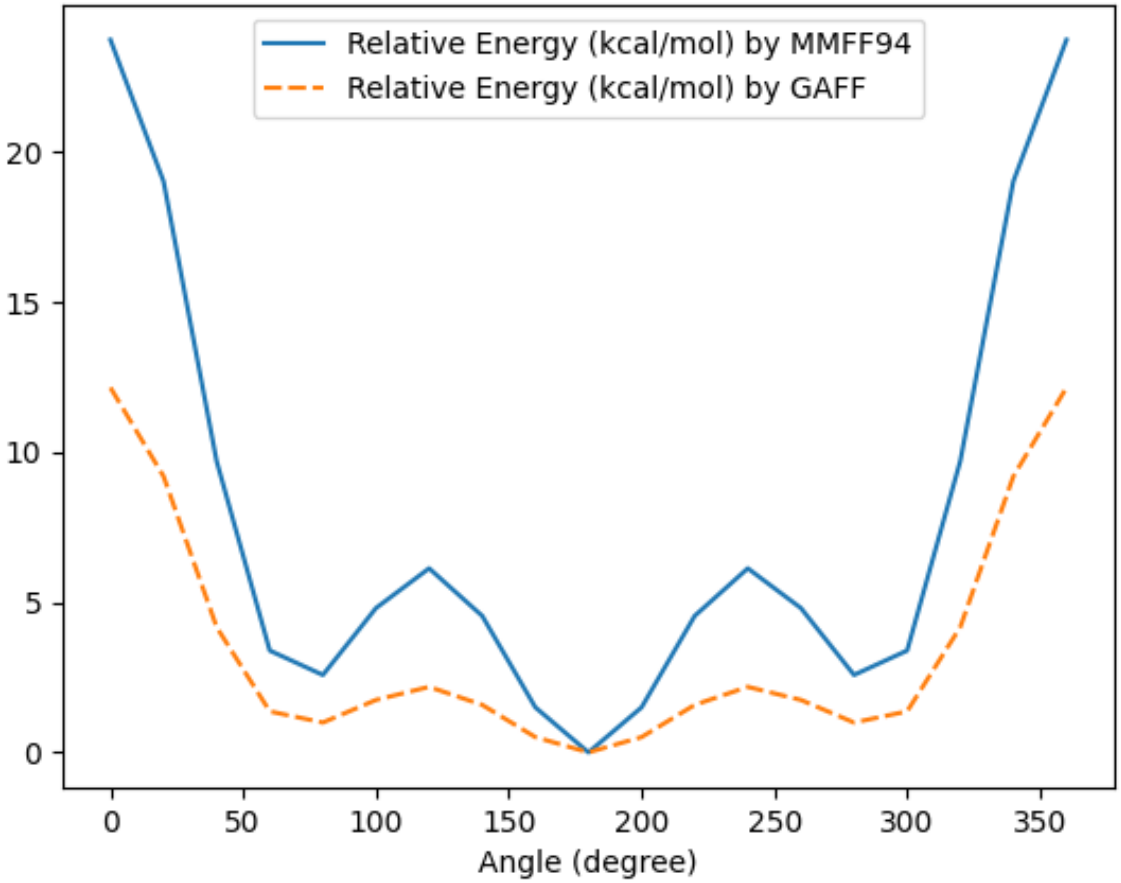
```
8
./CODE/C2H4Cl2_360_degrees.gzmat
C           0.00000         0.00000         0.00000
C           1.54000         0.00000         0.00000
H          -0.33381         0.00000        -0.94264
H          -0.33381        -0.81635         0.47132
Cl         -0.55746         1.36331         0.78711
H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

# 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)

MMFF94_abs_energy_in_Kcal_vec = np.array(MMFF94_abs_energy_in_Kcal_list)
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),
149     "Absolute Energy (kJ/mol) by MMFF94":
    np.round(MMFF94_abs_energy_in_KJ_vec.tolist(), 3),
150     "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
```

```
583
584 SETTING UP BOND CALCULATIONS...
585 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
586 SETTING UP TORSION CALCULATIONS...
587 SETTING UP OOP CALCULATIONS...
588 SETTING UP VAN DER WAALS CALCULATIONS...
589 SETTING UP ELECTROSTATIC CALCULATIONS...
590
591 A T O M   T Y P E S
592
593 IDX TYPE  RING
594 1 c3  NO
595 2 c3  NO
596 3 h1  NO
597 4 h1  NO
598 5 cl  NO
599 6 h1  NO
600 7 h1  NO
601 8 cl  NO
602
603 C H A R G E S
604
605 IDX CHARGE
606 1 0.036009
607 2 0.036009
608 3 0.044101
609 4 0.044101
610 5 -0.124211
611 6 0.044101
612 7 0.044101
613 8 -0.124211
614
615 S E T T I N G   U P   C A L C U L A T I O N S
616
617 SETTING UP BOND CALCULATIONS...
618 SETTING UP ANGLE CALCULATIONS...
619 SETTING UP TORSION CALCULATIONS...
620 SETTING UP IMPROPER TORSION CALCULATIONS...
621 SETTING UP VAN DER WAALS CALCULATIONS...
622 SETTING UP ELECTROSTATIC CALCULATIONS...
623
624 E N E R G Y
625
626
627 B O N D   S T R E T C H I N G
628
629 ATOM TYPES   FF    BOND       IDEAL       FORCE
630  I    J     CLASS  LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
631 ---------------------------------------------------------------------------
```

```
 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 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
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 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	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
```

```
1073
1074 ATOM TYPES
1075  I    J           Rij   332.17*QiQj  ENERGY
1076 ------------------------------------------
1077 h1 h1      2.400     1.352     0.563
1078 h1 h1      2.400     1.352     0.563
1079 h1 cl      3.499    -3.809    -1.089
1080 h1 h1      2.903     1.352     0.466
1081 h1 h1      2.400     1.352     0.563
1082 h1 cl      2.792    -3.809    -1.364
1083 cl h1      2.792    -3.809    -1.364
1084 cl h1      3.499    -3.809    -1.089
1085 cl cl      3.087    10.728     3.476
1086      TOTAL ELECTROSTATIC ENERGY =    0.726 kJ/mol
1087
1088 TOTAL ENERGY =   88.891 kJ/mol
1089
1090 A T O M   T Y P E S
1091
1092 IDX TYPE  RING
1093 1 1 NO
1094 2 1 NO
1095 3 5 NO
1096 4 5 NO
1097 5 12  NO
1098 6 5 NO
1099 7 5 NO
1100 8 12  NO
1101
1102 F O R M A L   C H A R G E S
1103
1104 IDX CHARGE
1105 1 0.290000
1106 2 0.290000
1107 3 0.000000
1108 4 0.000000
1109 5 -0.290000
1110 6 0.000000
1111 7 0.000000
1112 8 -0.290000
1113
1114 P A R T I A L   C H A R G E S
1115
1116 IDX CHARGE
1117 1 0.290000
1118 2 0.290000
1119 3 0.000000
1120 4 0.000000
1121 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 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        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
```

```
1710
1711 ATOM TYPES    FF     BOND        IDEAL        FORCE
1712  I    J      CLASS  LENGTH      LENGTH      CONSTANT       DELTA       ENERGY
1713 ---------------------------------------------------------------------------
1714  5    1       0      1.000       1.093         4.766      -0.093       3.578
1715  5    1       0      1.000       1.093         4.766      -0.093       3.578
1716  1    1       0      1.540       1.508         4.258       0.032       0.294
1717  1    5       0      1.000       1.093         4.766      -0.093       3.578
1718  1   12       0      1.670       1.773         2.974      -0.103       2.795
1719  1    5       0      1.000       1.093         4.766      -0.093       3.578
1720  1   12       0      1.670       1.773         2.974      -0.103       2.795
1721      TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
1722
1723 A N G L E   B E N D I N G
1724
1725 ATOM TYPES         FF     VALENCE      IDEAL       FORCE
1726  I    J    K      CLASS   ANGLE       ANGLE      CONSTANT       DELTA       ENERGY
1727 ---------------------------------------------------------------------------------
1728  1    1    5       0     109.500     110.549         0.636      -1.049       0.015
1729  5    1    5       0     109.442     108.836         0.516       0.606       0.004
1730  5    1   12       0     109.442     108.162         0.698       1.280       0.025
1731  1    1    5       0     109.500     110.549         0.636      -1.049       0.015
1732  1    1   12       0     109.500     108.679         1.056       0.821       0.016
1733  5    1   12       0     109.442     108.162         0.698       1.280       0.025
1734  1    1    5       0     109.500     110.549         0.636      -1.049       0.015
1735  5    1    5       0     109.442     108.836         0.516       0.606       0.004
1736  5    1   12       0     109.442     108.162         0.698       1.280       0.025
1737  1    1    5       0     109.500     110.549         0.636      -1.049       0.015
1738  1    1   12       0     109.500     108.679         1.056       0.821       0.016
1739  5    1   12       0     109.442     108.162         0.698       1.280       0.025
1740      TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol
1741
1742 S T R E T C H   B E N D I N G
1743
1744 ATOM TYPES         FF     VALENCE      DELTA          FORCE CONSTANT
1745  I    J    K      CLASS   ANGLE       ANGLE          I J          J K        ENERGY
1746 ---------------------------------------------------------------------------------
1747  1    1    5       0     109.500      -1.049        0.227        0.070       -0.002
1748  5    1    5       0     109.442       0.606        0.115        0.115       -0.033
1749  5    1   12       0     109.442       1.280       -0.018        0.380       -0.121
1750  1    1    5       0     109.500      -1.049        0.227        0.070       -0.002
1751  1    1   12       0     109.500       0.821        0.176        0.386       -0.070
1752  5    1   12       0     109.442       1.280       -0.018        0.380       -0.121
1753  1    1    5       0     109.500      -1.049        0.227        0.070       -0.002
1754  5    1    5       0     109.442       0.606        0.115        0.115       -0.033
1755  5    1   12       0     109.442       1.280       -0.018        0.380       -0.121
1756  1    1    5       0     109.500      -1.049        0.227        0.070       -0.002
1757  1    1   12       0     109.500       0.821        0.176        0.386       -0.070
1758  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

SETTING UP BOND CALCULATIONS...
SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
SETTING UP TORSION CALCULATIONS...
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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        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 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    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
-----------------------------------------------------------------
cl c3 c3 h1     0.000        0    -20.000   3      0.000
cl c3 c3 h1     0.000        0    100.000   3      0.000
cl 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
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
     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      2.638    -0.029
h1 cl      2.547     2.064
h1 h1      2.232     0.205
h1 h1      2.831    -0.032
h1 cl      3.129    -0.106
cl h1      3.129    -0.106
cl h1      2.547     2.064
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      2.638     1.352     0.513
h1 cl      2.547    -3.809    -1.495
h1 h1      2.232     1.352     0.606
h1 h1      2.831     1.352     0.478
h1 cl      3.129    -3.809    -1.217
cl h1      3.129    -3.809    -1.217
cl h1      2.547    -3.809    -1.495
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
```

```
3425 ------------------------------------------------------------
3426      TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol
3427
3428 V A N   D E R   W A A L S
3429
3430 ATOM TYPES
3431  I    J        Rij       R*IJ    EPSILON    ENERGY
3432 ------------------------------------------------
3433  5    5        2.746     2.970     0.022    -0.014
3434  5    5        2.746     2.970     0.022    -0.014
3435  5   12        2.512     3.713     0.053     2.649
3436  5    5        2.208     2.970     0.022     0.377
3437  5    5        2.746     2.970     0.022    -0.014
3438  5   12        3.280     3.713     0.053     0.009
3439 12    5        3.280     3.713     0.053     0.009
3440 12    5        2.512     3.713     0.053     2.649
3441 12   12        3.806     4.089     0.276    -0.201
3442      TOTAL VAN DER WAALS ENERGY =  5.44875 kcal/mol
3443
3444 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
3445
3446 ATOM TYPES
3447  I    J        Rij        Qi         Qj        ENERGY
3448 ------------------------------------------------------
3449 12   12      3.856    -0.290    -0.290     5.432
3450      TOTAL ELECTROSTATIC ENERGY =  5.43239 kcal/mol
3451
3452 TOTAL ENERGY = 32.49359 kcal/mol
3453
3454 E N E R G Y
3455
3456
3457 B O N D   S T R E T C H I N G
3458
3459 ATOM TYPES  BOND       IDEAL       FORCE
3460  I    J     LENGTH     LENGTH     CONSTANT      DELTA      ENERGY
3461 ------------------------------------------------------------------------
3462 cl c3     1.670      1.786     1168.117     -0.116     15.718
3463 h1 c3     1.000      1.093     1406.346     -0.093     12.163
3464 c3 c3     1.540      1.535     1269.019      0.005      0.032
3465 c3 h1     1.000      1.093     1406.346     -0.093     12.163
3466 c3 h1     1.000      1.093     1406.346     -0.093     12.163
3467 c3 h1     1.000      1.093     1406.346     -0.093     12.163
3468 c3 cl     1.670      1.786     1168.117     -0.116     15.718
3469      TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol
3470
3471 A N G L E   B E N D I N G
3472
3473 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

TOTAL ENERGY =   90.486 kJ/mol

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
3862
3863 IDX TYPE  RING
3864 1 c3  NO
3865 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    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

ATOM TYPES
 I    J        Rij       kij       ENERGY
-----------------------------------------
```

```
h1 h1      2.518    -0.013
h1 h1      2.885    -0.031
h1 cl      2.647     1.083
h1 h1      2.300     0.109
h1 h1      2.518    -0.013
h1 cl      3.474    -0.129
cl h1      3.474    -0.129
cl h1      2.647     1.083
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      2.885     1.352     0.469
h1 cl      2.647    -3.809    -1.439
h1 h1      2.300     1.352     0.588
h1 h1      2.518     1.352     0.537
h1 cl      3.474    -3.809    -1.097
cl h1      3.474    -3.809    -1.097
cl h1      2.647    -3.809    -1.439
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
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
```

```
4209 ------------------------------------------------------------------------
4210  1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
4211  5    1    5      0    109.442      0.606      0.115      0.115     -0.033
4212  5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
4213  1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
4214  1    1   12      0    109.500      0.821      0.176      0.386     -0.070
4215  5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
4216  5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
4217  1    1   12      0    109.500      0.821      0.176      0.386     -0.070
4218  5    1   12      0    109.442      1.280     -0.018      0.380     -0.121
4219  1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
4220  5    1    5      0    109.442      0.606      0.115      0.115     -0.033
4221  1    1    5      0    109.500     -1.049      0.227      0.070     -0.002
4222      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
4223
4224 T O R S I O N A L
4225
4226 ATOM TYPES             FF     TORSION       FORCE CONSTANT
4227  I    J    K    L     CLASS    ANGLE          V1    V2    V3     ENERGY
4228 ------------------------------------------------------------------------
4229  5    1    1   12       0     60.000     0.678   -0.602    0.398      0.057
4230  5    1    1    5       0    -60.000     0.284   -1.386    0.314     -0.826
4231  5    1    1    5       0   -180.000     0.284   -1.386    0.314      0.000
4232  5    1    1   12       0   -180.000     0.678   -0.602    0.398      0.000
4233  5    1    1    5       0     60.000     0.284   -1.386    0.314     -0.827
4234  5    1    1    5       0    -60.000     0.284   -1.386    0.314     -0.826
4235 12    1    1   12       0    -60.000     0.000    0.000    0.893      0.000
4236 12    1    1    5       0    180.000     0.678   -0.602    0.398      0.000
4237 12    1    1    5       0     60.000     0.678   -0.602    0.398      0.057
4238      TOTAL TORSIONAL ENERGY = -2.36550 kcal/mol
4239
4240 O U T - O F - P L A N E   B E N D I N G
4241
4242 ATOM TYPES             FF       OOP     FORCE
4243  I    J    K    L     CLASS    ANGLE   CONSTANT     ENERGY
4244 ------------------------------------------------------------
4245      TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol
4246
4247 V A N   D E R   W A A L S
4248
4249 ATOM TYPES
4250  I    J        Rij       R*IJ    EPSILON    ENERGY
4251 -------------------------------------------------
4252  5    5        2.400     2.970     0.022     0.107
4253  5    5        2.903     2.970     0.022    -0.021
4254  5   12        2.792     3.713     0.053     0.792
4255  5    5        2.400     2.970     0.022     0.107
4256  5    5        2.400     2.970     0.022     0.107
4257  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
-----------------------------------------
h1 h1      2.400     1.352     0.563
h1 h1      2.903     1.352     0.466
h1 cl      2.792    -3.809    -1.364
```

```
h1 h1      2.400     1.352     0.563
h1 h1      2.400     1.352     0.563
h1 cl      3.499    -3.809    -1.089
cl h1      3.499    -3.809    -1.089
cl h1      2.792    -3.809    -1.364
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 0.000000
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...
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```
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     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
```

```
4601
4602 ----ATOM TYPES-----    FORCE     IMPROPER_TORSION
4603  I    J    K    L     CONSTANT     s       ANGLE    n    ENERGY
4604 ---------------------------------------------------------------
4605      TOTAL IMPROPER-TORSIONAL ENERGY =    0.000 kJ/mol
4606
4607 V A N   D E R   W A A L S
4608
4609 ATOM TYPES
4610  I    J        Rij       kij       ENERGY
4611 ----------------------------------------
4612 h1 h1      2.300     0.109
4613 h1 h1      2.885    -0.031
4614 h1 cl      2.960     0.012
4615 h1 h1      2.518    -0.013
4616 h1 h1      2.300     0.109
4617 h1 cl      3.474    -0.129
4618 cl h1      3.474    -0.129
4619 cl h1      2.960     0.012
4620 cl cl      2.865    15.169
4621      TOTAL VAN DER WAALS ENERGY =   15.111 kJ/mol
4622
4623 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
4624
4625 ATOM TYPES
4626  I    J           Rij   332.17*QiQj  ENERGY
4627 ----------------------------------------
4628 h1 h1      2.300     1.352     0.588
4629 h1 h1      2.885     1.352     0.469
4630 h1 cl      2.960    -3.809    -1.287
4631 h1 h1      2.518     1.352     0.537
4632 h1 h1      2.300     1.352     0.588
4633 h1 cl      3.474    -3.809    -1.097
4634 cl h1      3.474    -3.809    -1.097
4635 cl h1      2.960    -3.809    -1.287
4636 cl cl      2.865    10.728     3.745
4637      TOTAL ELECTROSTATIC ENERGY =    1.160 kJ/mol
4638
4639 TOTAL ENERGY =  100.634 kJ/mol
4640
4641 A T O M   T Y P E S
4642
4643 IDX TYPE  RING
4644 1 1 NO
4645 2 1 NO
4646 3 5 NO
4647 4 5 NO
4648 5 12  NO
4649 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 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     -0.655
 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

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
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5189 TOTAL ENERGY =  134.023 kJ/mol
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