

Table of Contents

- [BIM2005: Homework I](#)
 - [Preparation](#)
 - [Procedure](#)
 - [GitHub Repo File Hierarchy](#)
 - [Results](#)
 - [I.gzmat and .xyz Files for a Specific Torsion Angle](#)
 - [Torsion Angle at 0°](#)
 - [Torsion Angle at 20°](#)
 - [Torsion Angle at 40°](#)
 - [Torsion Angle at 60°](#)
 - [Torsion Angle at 80°](#)
 - [Torsion Angle at 100°](#)
 - [Torsion Angle at 120°](#)
 - [Torsion Angle at 140°](#)
 - [Torsion Angle at 160°](#)
 - [Torsion Angle at 180°](#)
 - [Torsion Angle at 200°](#)
 - [Torsion Angle at 220°](#)
 - [Torsion Angle at 240°](#)
 - [Torsion Angle at 260°](#)
 - [Torsion Angle at 280°](#)
 - [Torsion Angle at 300°](#)
 - [Torsion Angle at 320°](#)
 - [Torsion Angle at 340°](#)
 - [Torsion Angle at 360°](#)
 - [II Energy Overview](#)
 - [III Lineplot of Relative Energy in Kcal by MMFF94 and GAFF](#)
 - [Appendix](#)
 - [I Code](#)
 - [torsion_angle.py](#)
 - [code2mkdoc.py](#)
 - [II Analysis of the Energy](#)

BIM2005: Homework I

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

Preparation

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

```

1  #
2
3  C2H4Cl2
4
5  0 1
6  C
7  C 1 1.54
8  H 1 1.0 2 109.5
9  H 1 1.0 2 109.5 3 120.0
10 C1 1 1.67 2 109.5 4 120.0
11 H 2 1.0 1 109.5 5 -120.0
12 H 2 1.0 1 109.5 5 120.0
13 C1 2 1.67 1 109.5 5 0.0

```

Procedure

Details of implementation could be found in the GitHub repository [zcorn2017/BIM2001-HWK1](https://github.com/zcorn2017/BIM2001-HWK1) (github.com).

The comments to and styles of the code has been organised well to make it highly readable.

1. We [added the headers to the code manually](#) for it to be recognised by [OpenBabel](#)
2. We modify the code in order to change $\tau(Cl^8 - C^2 - C^1 - Cl^5)$ by $20 \times N^\circ$. (As the reference plane, which is the 2 – 1 – 5 plane, is the same for the last three definitions of atoms, we only need to change the dihedral angles of the last three lines by an increment of 20° .)
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 $N = 0 \dots 18$, which means 19 times.
7. All the .xyz and .gzmat files could be found in [Reuslts I](#).
8. Pre-processing of the data includes conversion between kcal/mol and kj/mol and calculations of the relative energy.
9. A table where all the data for the angles is established by [Pandas](#) and it could be found in [Results II](#).
10. A lineplot of relative energy in kcal/mol with respect to angle in degrees is displayed by [Seaborn] [<https://seaborn.pydata.org/>]. For details, please refer to [Result III](#)

GitHub Repo File Hierarchy

```

1  .
2  ├── C2H4Cl2_structure.png           // the 2D molecule structure overview
3  ├── CODE                           // the directory containing all the .xyz and
   .gzmat file
4  |   ├── C2H4Cl2_0_degrees.gzmat
5  |   └── C2H4Cl2_0_degrees.xyz

```

```

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

```

```

52 | └─ torsion_angle.py           // The main program to process the molecule
53 |
54 | 2 directories, 49 files

```

Results

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

Torsion Angle at 0°

- ./CODE/C2H4Cl2_0_degrees.gzmat

```

1 |
2 | #
3 |
4 | C2H4Cl2-0-degrees
5 |
6 | 0 1
7 | C
8 | C 1 1.54
9 | H 1 1.0 2 109.5
10 | H 1 1.0 2 109.5 3 120.0
11 | Cl 1 1.67 2 109.5 4 120.0
12 | H 2 1.0 1 109.5 5 -120.0
13 | H 2 1.0 1 109.5 5 120.0
14 | Cl 2 1.67 1 109.5 5 0.0
15 |
16 |

```

- ./CODE/C2H4Cl2_0_degrees.xyz

```

1 | 8
2 | ./CODE/C2H4Cl2_0_degrees.gzmat
3 | C      0.00000      0.00000      0.00000
4 | C      1.54000      0.00000      0.00000
5 | H     -0.33381      0.00000     -0.94264
6 | H     -0.33381     -0.81635      0.47132
7 | Cl    -0.55746      1.36331      0.78711
8 | H      1.87381      0.00000     -0.94264
9 | H      1.87381     -0.81635      0.47132
10 | Cl     2.09746      1.36331      0.78711
11 |

```

Torsion Angle at 20°

- ./CODE/C2H4Cl2_20_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-20-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 -100.0
13 H 2 1.0 1 109.5 5 140.0
14 Cl 2 1.67 1 109.5 5 20.0
15
16
```

- ./CODE/C2H4Cl2_20_degrees.xyz

```
1 8
2 ./CODE/C2H4Cl2_20_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 0.32240 -0.88579
9 H 1.87381 -0.92832 0.16369
10 Cl 2.09746 1.01188 1.20592
11
```

Torsion Angle at 40°

- ./CODE/C2H4Cl2_40_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-40-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```

10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 -80.0
13 H 2 1.0 1 109.5 5 160.0
14 Cl 2 1.67 1 109.5 5 40.0
15
16

```

- ./CODE/C2H4Cl2_40_degrees.xyz

```

1 8
2 ./CODE/C2H4Cl2_40_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 0.60592 -0.72211
9 H 1.87381 -0.92832 -0.16369
10 Cl 2.09746 0.53841 1.47927
11

```

Torsion Angle at 60°

- ./CODE/C2H4Cl2_60_degrees.gzmat

```

1
2 #
3
4 C2H4Cl2-60-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 -60.0
13 H 2 1.0 1 109.5 5 180.0
14 Cl 2 1.67 1 109.5 5 60.0
15
16

```

- ./CODE/C2H4Cl2_60_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_60_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381      0.81635     -0.47132
9  H      1.87381     -0.81635     -0.47132
10 Cl      2.09746     -0.00000      1.57421
11

```

Torsion Angle at 80°

- ./CODE/C2H4Cl2_80_degrees.gzmat

```

1
2  #
3
4  C2H4Cl2-80-degrees
5
6  0 1
7  C
8  C 1 1.54
9  H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 -40.0
13 H 2 1.0 1 109.5 5 200.0
14 Cl 2 1.67 1 109.5 5 80.0
15
16

```

- ./CODE/C2H4Cl2_80_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_80_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381      0.92832     -0.16369
9  H      1.87381     -0.60592     -0.72211
10 Cl      2.09746     -0.53841      1.47927
11

```

Torsion Angle at 100°

- ./CODE/C2H4Cl2_100_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-100-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 -20.0
13 H 2 1.0 1 109.5 5 220.0
14 Cl 2 1.67 1 109.5 5 100.0
15
16
```

- ./CODE/C2H4Cl2_100_degrees.xyz

```
1 8
2 ./CODE/C2H4Cl2_100_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 0.92832 0.16369
9 H 1.87381 -0.32240 -0.88579
10 Cl 2.09746 -1.01188 1.20592
11
```

Torsion Angle at 120°

- ./CODE/C2H4Cl2_120_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-120-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```



```

10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 0.0
13 H 2 1.0 1 109.5 5 240.0
14 Cl 2 1.67 1 109.5 5 120.0
15
16

```

- ./CODE/C2H4Cl2_120_degrees.xyz

```

1 8
2 ./CODE/C2H4Cl2_120_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 0.81635 0.47132
9 H 1.87381 0.00000 -0.94264
10 Cl 2.09746 -1.36331 0.78711
11

```

Torsion Angle at 140°

- ./CODE/C2H4Cl2_140_degrees.gzmat

```

1
2 #
3
4 C2H4Cl2-140-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 20.0
13 H 2 1.0 1 109.5 5 260.0
14 Cl 2 1.67 1 109.5 5 140.0
15
16

```

- ./CODE/C2H4Cl2_140_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_140_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381      0.60592      0.72211
9  H      1.87381      0.32240     -0.88579
10 Cl      2.09746     -1.55030      0.27336
11

```

Torsion Angle at 160°

- ./CODE/C2H4Cl2_160_degrees.gzmat

```

1
2  #
3
4  C2H4Cl2-160-degrees
5
6  0 1
7  C
8  C 1 1.54
9  H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 40.0
13 H 2 1.0 1 109.5 5 280.0
14 Cl 2 1.67 1 109.5 5 160.0
15
16

```

- ./CODE/C2H4Cl2_160_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_160_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381      0.32240      0.88579
9  H      1.87381      0.60592     -0.72211
10 Cl      2.09746     -1.55030     -0.27336
11

```

Torsion Angle at 180°

- ./CODE/C2H4Cl2_180_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-180-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 60.0
13 H 2 1.0 1 109.5 5 300.0
14 Cl 2 1.67 1 109.5 5 180.0
15
16
```

- ./CODE/C2H4Cl2_180_degrees.xyz

```
1 8
2 ./CODE/C2H4Cl2_180_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 -0.00000 0.94264
9 H 1.87381 0.81635 -0.47132
10 Cl 2.09746 -1.36331 -0.78711
11
```

Torsion Angle at 200°

- ./CODE/C2H4Cl2_200_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-200-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```

10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 80.0
13 H 2 1.0 1 109.5 5 320.0
14 Cl 2 1.67 1 109.5 5 200.0
15
16

```

- ./CODE/C2H4Cl2_200_degrees.xyz

```

1 8
2 ./CODE/C2H4Cl2_200_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 -0.32240 0.88579
9 H 1.87381 0.92832 -0.16369
10 Cl 2.09746 -1.01188 -1.20592
11

```

Torsion Angle at 220°

- ./CODE/C2H4Cl2_220_degrees.gzmat

```

1
2 #
3
4 C2H4Cl2-220-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 100.0
13 H 2 1.0 1 109.5 5 340.0
14 Cl 2 1.67 1 109.5 5 220.0
15
16

```

- ./CODE/C2H4Cl2_220_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_220_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381     -0.60592      0.72211
9  H      1.87381      0.92832      0.16369
10 Cl      2.09746     -0.53841     -1.47927
11

```

Torsion Angle at 240°

- ./CODE/C2H4Cl2_240_degrees.gzmat

```

1
2  #
3
4  C2H4Cl2-240-degrees
5
6  0 1
7  C
8  C 1 1.54
9  H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 120.0
13 H 2 1.0 1 109.5 5 0.0
14 Cl 2 1.67 1 109.5 5 240.0
15
16

```

- ./CODE/C2H4Cl2_240_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_240_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381     -0.81635      0.47132
9  H      1.87381      0.81635      0.47132
10 Cl      2.09746      0.00000     -1.57421
11

```

Torsion Angle at 260°

- ./CODE/C2H4Cl2_260_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-260-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 140.0
13 H 2 1.0 1 109.5 5 20.0
14 Cl 2 1.67 1 109.5 5 260.0
15
16
```

- ./CODE/C2H4Cl2_260_degrees.xyz

```
1 8
2 ./CODE/C2H4Cl2_260_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 -0.92832 0.16369
9 H 1.87381 0.60592 0.72211
10 Cl 2.09746 0.53841 -1.47927
11
```

Torsion Angle at 280°

- ./CODE/C2H4Cl2_280_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-280-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```

10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 160.0
13 H 2 1.0 1 109.5 5 40.0
14 Cl 2 1.67 1 109.5 5 280.0
15
16

```

- ./CODE/C2H4Cl2_280_degrees.xyz

```

1 8
2 ./CODE/C2H4Cl2_280_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 -0.92832 -0.16369
9 H 1.87381 0.32240 0.88579
10 Cl 2.09746 1.01188 -1.20592
11

```

Torsion Angle at 300°

- ./CODE/C2H4Cl2_300_degrees.gzmat

```

1
2 #
3
4 C2H4Cl2-300-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 180.0
13 H 2 1.0 1 109.5 5 60.0
14 Cl 2 1.67 1 109.5 5 300.0
15
16

```

- ./CODE/C2H4Cl2_300_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_300_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381     -0.81635     -0.47132
9  H      1.87381     -0.00000      0.94264
10 Cl      2.09746      1.36331     -0.78711
11

```

Torsion Angle at 320°

- ./CODE/C2H4Cl2_320_degrees.gzmat

```

1
2  #
3
4  C2H4Cl2-320-degrees
5
6  0 1
7  C
8  C 1 1.54
9  H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 200.0
13 H 2 1.0 1 109.5 5 80.0
14 Cl 2 1.67 1 109.5 5 320.0
15
16

```

- ./CODE/C2H4Cl2_320_degrees.xyz

```

1  8
2  ./CODE/C2H4Cl2_320_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381     -0.60592     -0.72211
9  H      1.87381     -0.32240      0.88579
10 Cl      2.09746      1.55030     -0.27336
11

```


Torsion Angle at 340°

- ./CODE/C2H4Cl2_340_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-340-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 220.0
13 H 2 1.0 1 109.5 5 100.0
14 Cl 2 1.67 1 109.5 5 340.0
15
16
```

- ./CODE/C2H4Cl2_340_degrees.xyz

```
1 8
2 ./CODE/C2H4Cl2_340_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 -0.32240 -0.88579
9 H 1.87381 -0.60592 0.72211
10 Cl 2.09746 1.55030 0.27336
11
```

Torsion Angle at 360°

- ./CODE/C2H4Cl2_360_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-360-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```
10 H 1 1.0 2 109.5 3 120.0
11 Cl 1 1.67 2 109.5 4 120.0
12 H 2 1.0 1 109.5 5 240.0
13 H 2 1.0 1 109.5 5 120.0
14 Cl 2 1.67 1 109.5 5 0.0
15
16
```

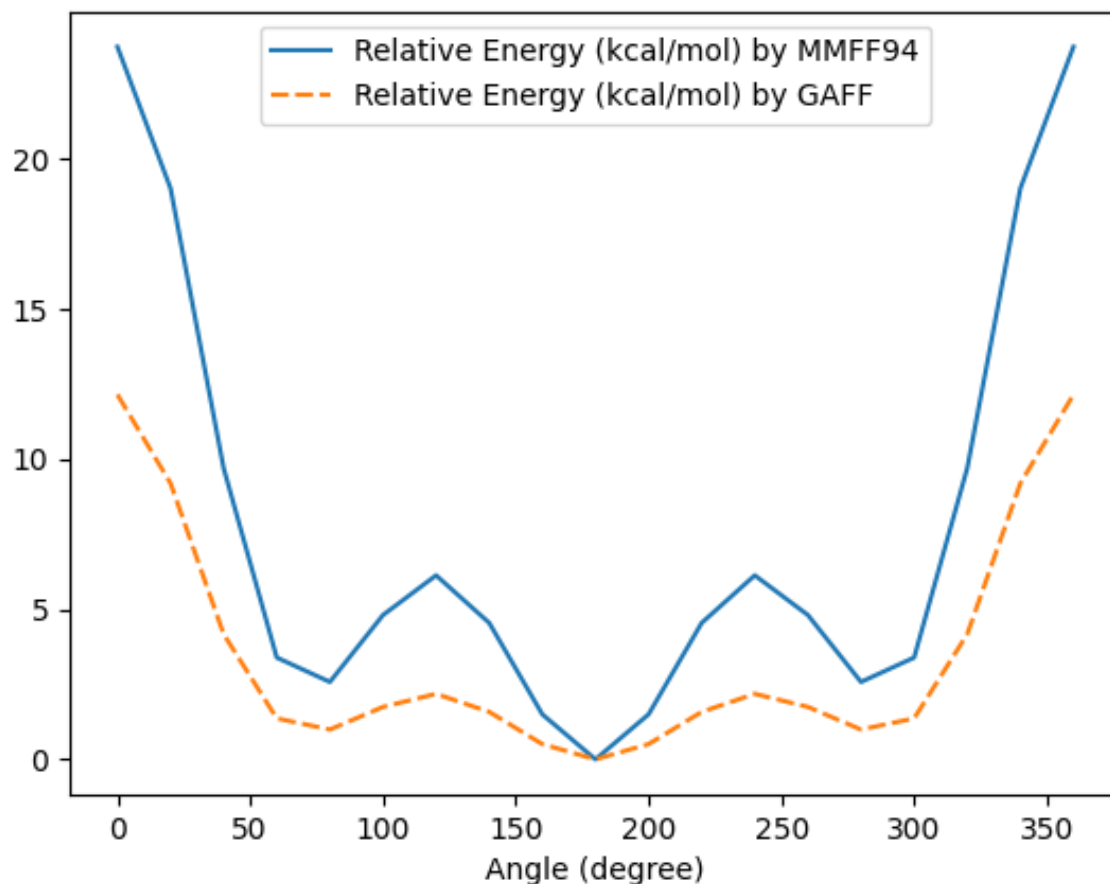
- ./CODE/C2H4Cl2_360_degrees.xyz

```
1 8
2 ./CODE/C2H4Cl2_360_degrees.gzmat
3 C 0.00000 0.00000 0.00000
4 C 1.54000 0.00000 0.00000
5 H -0.33381 0.00000 -0.94264
6 H -0.33381 -0.81635 0.47132
7 Cl -0.55746 1.36331 0.78711
8 H 1.87381 0.00000 -0.94264
9 H 1.87381 -0.81635 0.47132
10 Cl 2.09746 1.36331 0.78711
11
```

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

```
1  # This the main program to process the molecule.
2
3  from openbabel import openbabel
4  import numpy as np
5  import pandas as pd
6  import seaborn as sns
7  import matplotlib.pyplot as plt
8
9  # Set the constant used to convert kcal/mol to kJ/mol
10 KCAL2KJ_CONSTANT = 4.184
11
12 # The C2H4Cl2 molecule with the torsion angle at 0 degree
13 gzmata_code = """
14 #
```

```

15
16 C2H4Cl2
17
18 0 1
19 C
20 C 1 1.54
21 H 1 1.0 2 109.5
22 H 1 1.0 2 109.5 3 120.0
23 Cl 1 1.67 2 109.5 4 120.0
24 H 2 1.0 1 109.5 5 -120.0
25 H 2 1.0 1 109.5 5 120.0
26 Cl 2 1.67 1 109.5 5 0.0
27 ""
28
29 # Store the code of the 18 modified molecules as a list
30 code_list = []
31
32 for n in range(0, 19):
33     # Count the reference number of the atoms to determine which atom to
34     # manipulate
35     atom_counter = 0
36
37     # .xyz code after conversion
38     code_aft_cnv = ""
39     for line in gzmat_code.split("\n"):
40         words = line.split()
41
42         # if the line is empty, do not make modifications
43         if len(words) == 0:
44             pass
45
46         # if the title is met, rename the title to mark it with the torsion angle
47         elif line.startswith("C2H4Cl2"):
48             words.append(str(20 * n))
49             words.append("degrees")
50             code_aft_cnv = code_aft_cnv + "-".join(words) + "\n"
51             continue
52
53         elif words[0].isalpha() and len(words[0]) in [1, 2]:
54             atom_counter = atom_counter + 1
55
56             if atom_counter in [6, 7, 8]:
57
58                 words[-1] = str(float(words[-1]) + 20 * n)
59                 if float(words[-1]) >= 360:
60                     words[-1] = str(float(words[-1]) - 360)
61
62             code_aft_cnv = code_aft_cnv + " ".join(words) + "\n"
63     code_list.append(code_aft_cnv)

```

```

63
64 # Write the code to the .gzmat format
65 for code, angle in zip(code_list, range(0, 380, 20)):
66     with open(f"./CODE/C2H4Cl2_{angle}_degrees.gzmat", "w") as gzmat_file:
67         gzmat_file.write(code)
68
69 # Set the input format to gzmat and the output format to xyz
70 OB_converter = openbabel.OBConversion()
71 OB_converter.SetInAndOutFormats("gzmat", "xyz")
72
73 MMFF94_abs_energy_in_Kcal_list = []
74 GAFF_abs_energy_in_KJ_list = []
75
76 # Convert the .gzmat files to .xyz file via OpenBabel
77 for angle in range(0, 380, 20):
78     mol_C2H4Cl2 = openbabel.OBMol()
79
80     # Use MMFF94 and GAFF to calculate the absolute energy
81     OB_converter.ReadFile(mol_C2H4Cl2, f"./CODE/C2H4Cl2_{angle}_degrees.gzmat")
82
83     MMFF94_forcefield = openbabel.OBForceField.FindForceField("MMFF94")
84     GAFF_forcefield = openbabel.OBForceField.FindForceField("GAFF")
85
86     # Redirect the log output to std::cout
87     MMFF94_forcefield.SetLogToStdOut()
88     GAFF_forcefield.SetLogToStdOut()
89
90     # Set the priority of log to high
91     MMFF94_forcefield.SetLogLevel(openbabel.OBFF_LOGLVL_HIGH)
92     GAFF_forcefield.SetLogLevel(openbabel.OBFF_LOGLVL_HIGH)
93
94     # Specify the molecule we calculate the energy of
95     MMFF94_forcefield.Setup(mol_C2H4Cl2)
96     GAFF_forcefield.Setup(mol_C2H4Cl2)
97
98     # Energy of C_2H_4Cl_2 with Torsion Angle at `angle` Degrees Starts
99     # by MMFF94
100    MMFF94_abs_energy_in_Kcal = MMFF94_forcefield.Energy()
101    # by GAFF
102    GAFF_abs_energy_in_KJ = GAFF_forcefield.Energy()
103
104    MMFF94_abs_energy_in_Kcal_list.append(MMFF94_abs_energy_in_Kcal)
105    GAFF_abs_energy_in_KJ_list.append(GAFF_abs_energy_in_KJ)
106
107    OB_converter.WriteFile(mol_C2H4Cl2, f"./CODE/C2H4Cl2_{angle}_degrees.xyz")
108
109 # Construct a table containing the information required by the question
110 ref_MMFF94_energy_in_Kcal = min(MMFF94_abs_energy_in_Kcal_list)
111 ref_GAFF_energy_in_KJ = min(GAFF_abs_energy_in_KJ_list)

```

```

112
113 MMFF94_abs_energy_in_Kcal_vec = np.array(MMFF94_abs_energy_in_Kcal_list)
114 GAFF_abs_energy_in_KJ_vec = np.array(GAFF_abs_energy_in_KJ_list)
115
116 MMFF94_abs_energy_in_KJ_vec = KCAL2KJ_CONSTANT * MMFF94_abs_energy_in_Kcal_vec
117 GAFF_abs_energy_in_Kcal_vec = GAFF_abs_energy_in_KJ_vec / KCAL2KJ_CONSTANT
118
119 MMFF94_rel_energy_in_Kcal_vec = MMFF94_abs_energy_in_Kcal_vec -
    ref_MMFF94_energy_in_Kcal
120 GAFF_rel_energy_in_KJ_vec = GAFF_abs_energy_in_KJ_vec - ref_GAFF_energy_in_KJ
121
122 MMFF94_rel_energy_in_KJ_vec = MMFF94_abs_energy_in_KJ_vec - KCAL2KJ_CONSTANT *
    ref_MMFF94_energy_in_Kcal
123 GAFF_rel_energy_in_Kcal_vec = GAFF_abs_energy_in_Kcal_vec - ref_GAFF_energy_in_KJ
    / KCAL2KJ_CONSTANT
124
125 data_in_Kcal_dict = {
126     "Absolute Energy (kcal/mol) by MMFF94" :
127     MMFF94_abs_energy_in_Kcal_vec.tolist(),
128     "Absolute Energy (kcal/mol) by GAFF" : GAFF_abs_energy_in_Kcal_vec.tolist(),
129     "Relative Energy (kcal/mol) by MMFF94" :
130     MMFF94_rel_energy_in_Kcal_vec.tolist(),
131     "Relative Energy (kcal/mol) by GAFF" : GAFF_rel_energy_in_Kcal_vec.tolist()
132 }
133
134 data_in_KJ_dict = {
135     "Absolute Energy (kJ/mol) by MMFF94" : MMFF94_abs_energy_in_KJ_vec.tolist(),
136     "Absolute Energy (kJ/mol) by GAFF" : GAFF_abs_energy_in_KJ_vec.tolist(),
137     "Relative Energy (kJ/mol) by MMFF94" : MMFF94_rel_energy_in_KJ_vec.tolist(),
138     "Relative Energy (kJ/mol) by GAFF" : GAFF_rel_energy_in_KJ_vec.tolist()
139 }
140
141 data_in_Kcal_df = pd.DataFrame(data_in_Kcal_dict, index=[angle for angle in
142     range(0, 380, 20)])
143 data_in_KJ_df = pd.DataFrame(data_in_KJ_dict, index=[angle for angle in range(0,
144     380, 20)])
145
146 data_in_Kcal_df.to_csv("./DATA/data_in_Kcal.csv")
147 data_in_KJ_df.to_csv("./DATA/data_in_KJ.csv")
148
149 data_dict = {
150     "Absolute Energy (kcal/mol) by MMFF94":
151     np.round(MMFF94_abs_energy_in_Kcal_vec.tolist(), 3),
152     "Absolute Energy (kcal/mol) by GAFF":
153     np.round(GAFF_abs_energy_in_Kcal_vec.tolist(), 3),
154     "Relative Energy (kcal/mol) by MMFF94":
155     np.round(MMFF94_rel_energy_in_Kcal_vec.tolist(), 3),
156     "Relative Energy (kcal/mol) by GAFF":
157     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),
151     "Relative Energy (kJ/mol) by MMFF94":
np.round(MMFF94_rel_energy_in_KJ_vec.tolist(), 3),
152     "Relative Energy (kJ/mol) by GAFF":
np.round(GAFF_rel_energy_in_KJ_vec.tolist(), 3)
153 }
154
155 data_df = pd.DataFrame(data_dict, index=[angle for angle in range(0, 380, 20)])
156 data_df.index.name = "Angle (degree)"
157 data_df.to_csv("./DATA/data.csv")
158
159 # Plot the lineplot of relative energy in kcal/mol with respect to angle in
degrees
160 lineplot_df = data_df.loc[:,["Relative Energy (kcal/mol) by MMFF94", "Relative
Energy (kcal/mol) by GAFF"]]
161 sns.lineplot(data=lineplot_df)
162
163 plt.savefig("rel_energy.png")

```

code2mkdoc.py

```

1  # This script aims to facilitate the generation of the documentation
2  # which is not part of the main program.
3  # For the homework solution,
4  # pls refer to torsion_angle.py
5
6  import sys
7
8  # Add heading to the Markdown file
9  def mkdoc_heading(heading, level=1):
10     heading_level = "#" * level + " " + heading + "\n"
11     print(f"""
12 {heading_level}""")
13
14 # Wrap the code to make it be recognised by the Markdown parser
15 def wrap_code(code, lang="python"):
16     print(f"```\n{code}\n```\n")
17
18 # Redirect the output to the file writing object.
19
20 with open("XYZ_GAMAT_SUMMARY.md", "w") as sys.stdout:
21     for angle in range(0, 380, 20):
22         mkdoc_heading(f"Torsion Angle at {angle}$\degree$", level= 4)
23
24         print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.gzmat\n")
25

```

```

26         with open(f"./CODE/C2H4Cl2_{angle}_degrees.gzmat", "r") as gzmat:
27             wrap_code(gzmat.read(), lang="gzmat")
28
29         print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.xyz\n")
30         with open(f"./CODE/C2H4Cl2_{angle}_degrees.xyz", "r") as xyz:
31             wrap_code(xyz.read(), lang="xyz")

```

II Analysis of the Energy

```

1
2  A T O M   T Y P E S
3
4  IDX TYPE  RING
5  1 1 NO
6  2 1 NO
7  3 5 NO
8  4 5 NO
9  5 12  NO
10 6 5 NO
11 7 5 NO
12 8 12  NO
13
14 F O R M A L   C H A R G E S
15
16 IDX CHARGE
17 1 0.000000
18 2 0.000000
19 3 0.000000
20 4 0.000000
21 5 0.000000
22 6 0.000000
23 7 0.000000
24 8 0.000000
25
26 P A R T I A L   C H A R G E S
27
28 IDX CHARGE
29 1 0.290000
30 2 0.290000
31 3 0.000000
32 4 0.000000
33 5 -0.290000
34 6 0.000000
35 7 0.000000
36 8 -0.290000
37
38 S E T T I N G   U P   C A L C U L A T I O N S
39

```



```

40  SETTING UP BOND CALCULATIONS...
41  SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
42  SETTING UP TORSION CALCULATIONS...
43  SETTING UP OOP CALCULATIONS...
44  SETTING UP VAN DER WAALS CALCULATIONS...
45  SETTING UP ELECTROSTATIC CALCULATIONS...
46
47  A T O M   T Y P E S
48
49  IDX TYPE  RING
50  1 c3  NO
51  2 c3  NO
52  3 h1  NO
53  4 h1  NO
54  5 c1  NO
55  6 h1  NO
56  7 h1  NO
57  8 c1  NO
58
59  C H A R G E S
60
61  IDX CHARGE
62  1 0.036009
63  2 0.036009
64  3 0.044101
65  4 0.044101
66  5 -0.124211
67  6 0.044101
68  7 0.044101
69  8 -0.124211
70
71  S E T T I N G   U P   C A L C U L A T I O N S
72
73  SETTING UP BOND CALCULATIONS...
74  SETTING UP ANGLE CALCULATIONS...
75  SETTING UP TORSION CALCULATIONS...
76  SETTING UP IMPROPER TORSION CALCULATIONS...
77  SETTING UP VAN DER WAALS CALCULATIONS...
78  SETTING UP ELECTROSTATIC CALCULATIONS...
79
80  E N E R G Y
81
82
83  B O N D   S T R E T C H I N G
84
85  ATOM TYPES      FF      BOND      IDEAL      FORCE
86  I      J      CLASS  LENGTH  LENGTH  CONSTANT      DELTA      ENERGY
87  -----
88  5      1      0      1.000    1.093    4.766    -0.093    3.578

```

89	5	1	0	1.000	1.093	4.766	-0.093	3.578
90	1	1	0	1.540	1.508	4.258	0.032	0.294
91	1	5	0	1.000	1.093	4.766	-0.093	3.578
92	1	12	0	1.670	1.773	2.974	-0.103	2.795
93	1	5	0	1.000	1.093	4.766	-0.093	3.578
94	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

102	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
103	5	1	5	0	109.442	108.836	0.516	0.606	0.004
104	5	1	12	0	109.442	108.162	0.698	1.280	0.025
105	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
106	1	1	12	0	109.500	108.679	1.056	0.821	0.016
107	5	1	12	0	109.442	108.162	0.698	1.280	0.025
108	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
109	5	1	5	0	109.442	108.836	0.516	0.606	0.004
110	5	1	12	0	109.442	108.162	0.698	1.280	0.025
111	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
112	1	1	12	0	109.500	108.679	1.056	0.821	0.016
113	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

121	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
122	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
123	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
124	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
125	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
126	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
127	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
128	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
129	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
130	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
131	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
132	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

```

187 B O N D   S T R E T C H I N G
188
189 ATOM TYPES      BOND      IDEAL      FORCE
190 I      J      LENGTH      LENGTH      CONSTANT      DELTA      ENERGY
191 -----
192 h1 c3      1.000      1.093      1406.346      -0.093      12.163
193 h1 c3      1.000      1.093      1406.346      -0.093      12.163
194 c3 c3      1.540      1.535      1269.019      0.005      0.032
195 c3 h1      1.000      1.093      1406.346      -0.093      12.163
196 c3 c1      1.670      1.786      1168.117      -0.116      15.718
197 c3 h1      1.000      1.093      1406.346      -0.093      12.163
198 c3 c1      1.670      1.786      1168.117      -0.116      15.718
199      TOTAL BOND STRETCHING ENERGY =      80.122 kJ/mol
200
201 A N G L E   B E N D I N G
202
203 ATOM TYPES      VALENCE      IDEAL      FORCE
204 I      J      K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
205 -----
206 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
207 h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
208 h1 c3 c1      109.442      105.930      183.005      0.061      0.688
209 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
210 c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
211 h1 c3 c1      109.442      105.930      183.005      0.061      0.688
212 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
213 h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
214 h1 c3 c1      109.442      105.930      183.005      0.061      0.688
215 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
216 c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
217 h1 c3 c1      109.442      105.930      183.005      0.061      0.688
218      TOTAL ANGLE BENDING ENERGY =      2.938 kJ/mol
219
220 T O R S I O N A L
221
222 ----ATOM TYPES-----      FORCE      TORSION
223 I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
224 -----
225 h1 c3 c3 h1      0.651      0      0.000      3      1.303
226 h1 c3 c3 h1      0.651      0      -120.000      3      1.303
227 h1 c3 c3 c1      0.000      0      120.000      3      0.000
228 h1 c3 c3 h1      0.651      0      120.000      3      1.303
229 h1 c3 c3 h1      0.651      0      0.000      3      1.303
230 h1 c3 c3 c1      0.000      0      -120.000      3      0.000
231 c1 c3 c3 h1      0.000      0      -120.000      3      0.000
232 c1 c3 c3 h1      0.000      0      120.000      3      0.000
233 c1 c3 c3 c1      0.000      0      -0.000      3      0.000
234      TOTAL TORSIONAL ENERGY =      5.210 kJ/mol
235

```

```

236 I M P R O P E R   T O R S I O N A L
237
238 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
239 I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
240 -----
241          TOTAL IMPROPER-TORSIONAL ENERGY =          0.000 kJ/mol
242
243 V A N   D E R   W A A L S
244
245 ATOM TYPES
246 I      J      Rij      kij      ENERGY
247 -----
248 h1 h1      2.208      0.251
249 h1 h1      2.746     -0.033
250 h1 c1      3.280     -0.134
251 h1 h1      2.746     -0.033
252 h1 h1      2.208      0.251
253 h1 c1      3.280     -0.134
254 c1 h1      3.280     -0.134
255 c1 h1      3.280     -0.134
256 c1 c1      2.655     44.245
257          TOTAL VAN DER WAALS ENERGY =          44.146 kJ/mol
258
259 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
260
261 ATOM TYPES
262 I      J      Rij      332.17*QiQj      ENERGY
263 -----
264 h1 h1      2.208      1.352      0.613
265 h1 h1      2.746      1.352      0.493
266 h1 c1      3.280     -3.809     -1.161
267 h1 h1      2.746      1.352      0.493
268 h1 h1      2.208      1.352      0.613
269 h1 c1      3.280     -3.809     -1.161
270 c1 h1      3.280     -3.809     -1.161
271 c1 h1      3.280     -3.809     -1.161
272 c1 c1      2.655     10.728      4.041
273          TOTAL ELECTROSTATIC ENERGY =          1.607 kJ/mol
274
275 TOTAL ENERGY =  134.023 kJ/mol
276
277 A T O M   T Y P E S
278
279 IDX TYPE  RING
280 1 1 NO
281 2 1 NO
282 3 5 NO
283 4 5 NO
284 5 12 NO

```

```
285 6 5 NO
286 7 5 NO
287 8 12 NO
288
289 F O R M A L C H A R G E S
290
291 IDX CHARGE
292 1 0.290000
293 2 0.290000
294 3 0.000000
295 4 0.000000
296 5 -0.290000
297 6 0.000000
298 7 0.000000
299 8 -0.290000
300
301 P A R T I A L C H A R G E S
302
303 IDX CHARGE
304 1 0.290000
305 2 0.290000
306 3 0.000000
307 4 0.000000
308 5 -0.290000
309 6 0.000000
310 7 0.000000
311 8 -0.290000
312
313 A T O M T Y P E S
314
315 IDX TYPE RING
316 1 c3 NO
317 2 c3 NO
318 3 h1 NO
319 4 h1 NO
320 5 c1 NO
321 6 h1 NO
322 7 h1 NO
323 8 c1 NO
324
325 F O R M A L C H A R G E S
326
327 IDX CHARGE
328 1 0.036009
329 2 0.036009
330 3 0.044101
331 4 0.044101
332 5 -0.124211
333 6 0.044101
```

334 7 0.044101
335 8 -0.124211

336

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

338

339 I D X C H A R G E

340 1 0.036009

341 2 0.036009

342 3 0.044101

343 4 0.044101

344 5 -0.124211

345 6 0.044101

346 7 0.044101

347 8 -0.124211

348

349 E N E R G Y

350

351

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

353

354	A T O M T Y P E S		FF	BOND	IDEAL	FORCE		
355	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
356	-----							
357	5	1	0	1.000	1.093	4.766	-0.093	3.578
358	5	1	0	1.000	1.093	4.766	-0.093	3.578
359	1	1	0	1.540	1.508	4.258	0.032	0.294
360	1	5	0	1.000	1.093	4.766	-0.093	3.578
361	1	12	0	1.670	1.773	2.974	-0.103	2.795
362	1	5	0	1.000	1.093	4.766	-0.093	3.578
363	1	12	0	1.670	1.773	2.974	-0.103	2.795

364 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

365

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

367

368	A T O M T Y P E S			FF	VALENCE	IDEAL	FORCE		
369	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
370	-----								
371	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
372	5	1	5	0	109.442	108.836	0.516	0.606	0.004
373	5	1	12	0	109.442	108.162	0.698	1.280	0.025
374	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
375	1	1	12	0	109.500	108.679	1.056	0.821	0.016
376	5	1	12	0	109.442	108.162	0.698	1.280	0.025
377	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
378	5	1	5	0	109.442	108.836	0.516	0.606	0.004
379	5	1	12	0	109.442	108.162	0.698	1.280	0.025
380	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
381	1	1	12	0	109.500	108.679	1.056	0.821	0.016
382	5	1	12	0	109.442	108.162	0.698	1.280	0.025

```

383      TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol
384
385  S T R E T C H   B E N D I N G
386
387  ATOM TYPES          FF      VALENCE      DELTA      FORCE CONSTANT
388    I      J      K      CLASS    ANGLE      ANGLE          I  J          J  K      ENERGY
389  -----
390    1      1      5        0    109.500     -1.049      0.227      0.070     -0.002
391    5      1      5        0    109.442      0.606      0.115      0.115     -0.033
392    5      1     12        0    109.442      1.280     -0.018      0.380     -0.121
393    1      1      5        0    109.500     -1.049      0.227      0.070     -0.002
394    1      1     12        0    109.500      0.821      0.176      0.386     -0.070
395    5      1     12        0    109.442      1.280     -0.018      0.380     -0.121
396    1      1      5        0    109.500     -1.049      0.227      0.070     -0.002
397    5      1      5        0    109.442      0.606      0.115      0.115     -0.033
398    5      1     12        0    109.442      1.280     -0.018      0.380     -0.121
399    1      1      5        0    109.500     -1.049      0.227      0.070     -0.002
400    1      1     12        0    109.500      0.821      0.176      0.386     -0.070
401    5      1     12        0    109.442      1.280     -0.018      0.380     -0.121
402      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
403
404  T O R S I O N A L
405
406  ATOM TYPES          FF      TORSION      FORCE CONSTANT
407    I      J      K      L      CLASS    ANGLE          V1   V2   V3      ENERGY
408  -----
409    5      1      1      5        0     20.000      0.284  -1.386  0.314      0.349
410    5      1      1      5        0    -100.000      0.284  -1.386  0.314     -0.991
411    5      1      1     12        0    140.000      0.678  -0.602  0.398      0.129
412    5      1      1      5        0    140.000      0.284  -1.386  0.314     -0.304
413    5      1      1      5        0     20.000      0.284  -1.386  0.314      0.349
414    5      1      1     12        0    -100.000      0.678  -0.602  0.398     -0.005
415   12      1      1      5        0    -100.000      0.678  -0.602  0.398     -0.005
416   12      1      1      5        0    140.000      0.678  -0.602  0.398      0.129
417   12      1      1     12        0     20.000      0.000   0.000  0.893      0.670
418      TOTAL TORSIONAL ENERGY =  0.31978 kcal/mol
419
420  O U T - O F - P L A N E   B E N D I N G
421
422  ATOM TYPES          FF      OOP      FORCE
423    I      J      K      L      CLASS    ANGLE    CONSTANT      ENERGY
424  -----
425      TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol
426
427  V A N   D E R   W A A L S
428
429  ATOM TYPES
430    I      J          Rij          R*IJ      EPSILON      ENERGY
431  -----

```



```

432      5      5      2.232      2.970      0.022      0.328
433      5      5      2.638      2.970      0.022      0.001
434      5     12      3.399      3.713      0.053     -0.028
435      5      5      2.831      2.970      0.022     -0.019
436      5      5      2.232      2.970      0.022      0.328
437      5     12      3.129      3.713      0.053      0.104
438     12      5      3.129      3.713      0.053      0.104
439     12      5      3.399      3.713      0.053     -0.028
440     12     12      2.711      4.089      0.276     16.993

```

441 TOTAL VAN DER WAALS ENERGY = 17.78153 kcal/mol

442
443 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

444
445 A T O M T Y P E S

```

446      I      J      Rij      Qi      Qj      ENERGY
447      -----
448     12     12      2.761     -0.290     -0.290      7.587

```

449 TOTAL ELECTROSTATIC ENERGY = 7.58721 kcal/mol

450
451 TOTAL ENERGY = 45.38946 kcal/mol

452
453 E N E R G Y

454
455
456 B O N D S T R E T C H I N G

```

457
458 A T O M T Y P E S      BOND      IDEAL      FORCE
459      I      J      LENGTH      LENGTH      CONSTANT      DELTA      ENERGY
460      -----
461     h1 c3      1.000      1.093      1406.346     -0.093      12.163
462     h1 c3      1.000      1.093      1406.346     -0.093      12.163
463     c3 c3      1.540      1.535      1269.019      0.005      0.032
464     c3 h1      1.000      1.093      1406.346     -0.093      12.163
465     c3 c1      1.670      1.786      1168.117     -0.116      15.718
466     c3 h1      1.000      1.093      1406.346     -0.093      12.163
467     c3 c1      1.670      1.786      1168.117     -0.116      15.718

```

468 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

469
470 A N G L E B E N D I N G

```

471
472 A T O M T Y P E S      VALENCE      IDEAL      FORCE
473      I      J      K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
474      -----
475     c3 c3 h1      109.500      110.070      194.100     -0.010      0.019
476     h1 c3 h1      109.442      109.550      164.039     -0.002      0.001
477     h1 c3 c1      109.442      105.930      183.005      0.061      0.688
478     c3 c3 h1      109.500      110.070      194.100     -0.010      0.019
479     c3 c3 c1      109.500      110.330      260.419     -0.014      0.055
480     h1 c3 c1      109.442      105.930      183.005      0.061      0.688

```

```

481  c3 c3 h1   109.500   110.070   194.100   -0.010   0.019
482  h1 c3 h1   109.442   109.550   164.039   -0.002   0.001
483  h1 c3 cl   109.442   105.930   183.005    0.061   0.688
484  c3 c3 h1   109.500   110.070   194.100   -0.010   0.019
485  c3 c3 cl   109.500   110.330   260.419   -0.014   0.055
486  h1 c3 cl   109.442   105.930   183.005    0.061   0.688
487      TOTAL ANGLE BENDING ENERGY =      2.938 kJ/mol
488
489  T O R S I O N A L
490
491  ----ATOM TYPES-----      FORCE      TORSION
492      I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
493  -----
494  h1 c3 c3 h1      0.651      0      20.000      3      0.977
495  h1 c3 c3 h1      0.651      0     -100.000      3      0.977
496  h1 c3 c3 cl      0.000      0      140.000      3      0.000
497  h1 c3 c3 h1      0.651      0      140.000      3      0.977
498  h1 c3 c3 h1      0.651      0      20.000      3      0.977
499  h1 c3 c3 cl      0.000      0     -100.000      3      0.000
500  cl c3 c3 h1      0.000      0     -100.000      3      0.000
501  cl c3 c3 h1      0.000      0      140.000      3      0.000
502  cl c3 c3 cl      0.000      0      20.000      3      0.000
503      TOTAL TORSIONAL ENERGY =      3.908 kJ/mol
504
505  I M P R O P E R   T O R S I O N A L
506
507  ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
508      I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
509  -----
510      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
511
512  V A N   D E R   W A A L S
513
514  ATOM TYPES
515      I      J      Rij      kij      ENERGY
516  -----
517  h1 h1      2.232      0.205
518  h1 h1      2.638     -0.029
519  h1 cl      3.399     -0.133
520  h1 h1      2.831     -0.032
521  h1 h1      2.232      0.205
522  h1 cl      3.129     -0.106
523  cl h1      3.129     -0.106
524  cl h1      3.399     -0.133
525  cl cl      2.711     33.340
526      TOTAL VAN DER WAALS ENERGY =      33.209 kJ/mol
527
528  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
529

```

```

530 ATOM TYPES
531 I J Rij 332.17*QiQj ENERGY
532 -----
533 h1 h1 2.232 1.352 0.606
534 h1 h1 2.638 1.352 0.513
535 h1 c1 3.399 -3.809 -1.121
536 h1 h1 2.831 1.352 0.478
537 h1 h1 2.232 1.352 0.606
538 h1 c1 3.129 -3.809 -1.217
539 c1 h1 3.129 -3.809 -1.217
540 c1 h1 3.399 -3.809 -1.121
541 c1 c1 2.711 10.728 3.958
542 TOTAL ELECTROSTATIC ENERGY = 1.484 kJ/mol
543
544 TOTAL ENERGY = 121.662 kJ/mol
545
546 A T O M T Y P E S
547
548 I D X T Y P E R I N G
549 1 1 N O
550 2 1 N O
551 3 5 N O
552 4 5 N O
553 5 12 N O
554 6 5 N O
555 7 5 N O
556 8 12 N O
557
558 F O R M A L C H A R G E S
559
560 I D X C H A R G E
561 1 0.000000
562 2 0.000000
563 3 0.000000
564 4 0.000000
565 5 0.000000
566 6 0.000000
567 7 0.000000
568 8 0.000000
569
570 P A R T I A L C H A R G E S
571
572 I D X C H A R G E
573 1 0.290000
574 2 0.290000
575 3 0.000000
576 4 0.000000
577 5 -0.290000
578 6 0.000000

```

```
579 7 0.000000
580 8 -0.290000
581
582 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 c1  NO
599 6 h1  NO
600 7 h1  NO
601 8 c1  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

630

631

632

633

634

635

636

637

638

639

640

641

642

643

644

645

646

647

648

649

650

651

652

653

654

655

656

657

658

659

660

661

662

663

664

665

666

667

668

669

670

671

672

673

674

675

676

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

```

677     TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
678
679 T O R S I O N A L
680
681 ATOM TYPES          FF      TORSION      FORCE CONSTANT
682   I    J    K    L    CLASS    ANGLE          V1    V2    V3      ENERGY
683 -----
684   5    1    1    5      0    40.000    0.284   -1.386    0.314   -0.243
685   5    1    1    5      0   -80.000    0.284   -1.386    0.314   -1.099
686   5    1    1   12      0   160.000    0.678   -0.602    0.398    0.050
687   5    1    1    5      0   160.000    0.284   -1.386    0.314   -0.075
688   5    1    1    5      0    40.000    0.284   -1.386    0.314   -0.243
689   5    1    1   12      0   -80.000    0.678   -0.602    0.398   -0.086
690  12    1    1    5      0   -80.000    0.678   -0.602    0.398   -0.086
691  12    1    1    5      0   160.000    0.678   -0.602    0.398    0.050
692  12    1    1   12      0    40.000    0.000    0.000    0.893    0.223
693     TOTAL TORSIONAL ENERGY = -1.51155 kcal/mol
694
695 O U T - O F - P L A N E   B E N D I N G
696
697 ATOM TYPES          FF      OOP      FORCE
698   I    J    K    L    CLASS    ANGLE    CONSTANT      ENERGY
699 -----
700     TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol
701
702 V A N   D E R   W A A L S
703
704 ATOM TYPES
705   I    J      Rij      R*IJ      EPSILON      ENERGY
706 -----
707   5    5      2.300    2.970      0.022      0.215
708   5    5      2.518    2.970      0.022      0.036
709   5   12      3.474    3.713      0.053     -0.041
710   5    5      2.885    2.970      0.022     -0.021
711   5    5      2.300    2.970      0.022      0.215
712   5   12      2.960    3.713      0.053      0.331
713  12    5      2.960    3.713      0.053      0.331
714  12    5      3.474    3.713      0.053     -0.041
715  12   12      2.865    4.089      0.276      9.664
716     TOTAL VAN DER WAALS ENERGY = 10.69051 kcal/mol
717
718 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
719
720 ATOM TYPES
721   I    J      Rij      Qi      Qj      ENERGY
722 -----
723  12   12      2.915    -0.290    -0.290      7.185
724     TOTAL ELECTROSTATIC ENERGY =  7.18544 kcal/mol
725

```

726 TOTAL ENERGY = 36.06534 kcal/mol

727

728 E N E R G Y

729

730

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

732

733 ATOM TYPES BOND IDEAL FORCE

734 I J LENGTH LENGTH CONSTANT DELTA ENERGY

735

736 h1 c3 1.000 1.093 1406.346 -0.093 12.163

737 h1 c3 1.000 1.093 1406.346 -0.093 12.163

738 h1 c3 1.000 1.093 1406.346 -0.093 12.163

739 c3 c3 1.540 1.535 1269.019 0.005 0.032

740 c3 h1 1.000 1.093 1406.346 -0.093 12.163

741 c3 c1 1.670 1.786 1168.117 -0.116 15.718

742 c3 c1 1.670 1.786 1168.117 -0.116 15.718

743 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

744

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

746

747 ATOM TYPES VALENCE IDEAL FORCE

748 I J K ANGLE ANGLE CONSTANT DELTA ENERGY

749

750 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

751 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

752 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

753 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

754 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

755 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

756 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

757 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

758 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

759 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

760 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

761 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

762 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

763

764 T O R S I O N A L

765

766 ----ATOM TYPES----- FORCE TORSION

767 I J K L CONSTANT s ANGLE n ENERGY

768

769 h1 c3 c3 h1 0.651 0 40.000 3 0.326

770 h1 c3 c3 h1 0.651 0 -80.000 3 0.326

771 h1 c3 c3 c1 0.000 0 160.000 3 0.000

772 h1 c3 c3 h1 0.651 0 160.000 3 0.326

773 h1 c3 c3 h1 0.651 0 40.000 3 0.326

774 h1 c3 c3 c1 0.000 0 -80.000 3 0.000

```

775 c1 c3 c3 h1      0.000      0    -80.000   3      0.000
776 c1 c3 c3 h1      0.000      0    160.000   3      0.000
777 c1 c3 c3 c1      0.000      0     40.000   3      0.000
778      TOTAL TORSIONAL ENERGY =      1.303 kJ/mol
779
780 I M P R O P E R   T O R S I O N A L
781
782 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
783   I    J    K    L      CONSTANT      s      ANGLE      n      ENERGY
784 -----
785      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
786
787 V A N   D E R   W A A L S
788
789 ATOM TYPES
790   I    J      Rij      kij      ENERGY
791 -----
792 h1 h1      2.300      0.109
793 h1 h1      2.518     -0.013
794 h1 c1      3.474     -0.129
795 h1 h1      2.885     -0.031
796 h1 h1      2.300      0.109
797 h1 c1      2.960      0.012
798 c1 h1      2.960      0.012
799 c1 h1      3.474     -0.129
800 c1 c1      2.865     15.169
801      TOTAL VAN DER WAALS ENERGY =     15.111 kJ/mol
802
803 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
804
805 ATOM TYPES
806   I    J      Rij      332.17*QiQj      ENERGY
807 -----
808 h1 h1      2.300      1.352      0.588
809 h1 h1      2.518      1.352      0.537
810 h1 c1      3.474     -3.809     -1.097
811 h1 h1      2.885      1.352      0.469
812 h1 h1      2.300      1.352      0.588
813 h1 c1      2.960     -3.809     -1.287
814 c1 h1      2.960     -3.809     -1.287
815 c1 h1      3.474     -3.809     -1.097
816 c1 c1      2.865     10.728      3.745
817      TOTAL ELECTROSTATIC ENERGY =      1.160 kJ/mol
818
819 TOTAL ENERGY =    100.634 kJ/mol
820
821 A T O M   T Y P E S
822
823 I D X   T Y P E   R I N G

```



```
824 1 1 NO
825 2 1 NO
826 3 5 NO
827 4 5 NO
828 5 12 NO
829 6 5 NO
830 7 5 NO
831 8 12 NO
832
833 F O R M A L C H A R G E S
834
835 IDX CHARGE
836 1 0.290000
837 2 0.290000
838 3 0.000000
839 4 0.000000
840 5 -0.290000
841 6 0.000000
842 7 0.000000
843 8 -0.290000
844
845 P A R T I A L C H A R G E S
846
847 IDX CHARGE
848 1 0.290000
849 2 0.290000
850 3 0.000000
851 4 0.000000
852 5 -0.290000
853 6 0.000000
854 7 0.000000
855 8 -0.290000
856
857 A T O M T Y P E S
858
859 IDX TYPE RING
860 1 c3 NO
861 2 c3 NO
862 3 h1 NO
863 4 h1 NO
864 5 c1 NO
865 6 h1 NO
866 7 h1 NO
867 8 c1 NO
868
869 F O R M A L C H A R G E S
870
871 IDX CHARGE
872 1 0.036009
```

873 2 0.036009
874 3 0.044101
875 4 0.044101
876 5 -0.124211
877 6 0.044101
878 7 0.044101
879 8 -0.124211

880

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

882

883 I D X C H A R G E

884 1 0.036009
885 2 0.036009
886 3 0.044101
887 4 0.044101
888 5 -0.124211
889 6 0.044101
890 7 0.044101
891 8 -0.124211

892

893 E N E R G Y

894

895

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

897

898	A T O M T Y P E S		FF	BOND	IDEAL	FORCE		
899	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
900	-----							
901	5	1	0	1.000	1.093	4.766	-0.093	3.578
902	5	1	0	1.000	1.093	4.766	-0.093	3.578
903	5	1	0	1.000	1.093	4.766	-0.093	3.578
904	1	1	0	1.540	1.508	4.258	0.032	0.294
905	1	5	0	1.000	1.093	4.766	-0.093	3.578
906	1	12	0	1.670	1.773	2.974	-0.103	2.795
907	1	12	0	1.670	1.773	2.974	-0.103	2.795

908 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

909

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

911

912	A T O M T Y P E S			FF	VALENCE	IDEAL	FORCE		
913	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
914	-----								
915	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
916	5	1	5	0	109.442	108.836	0.516	0.606	0.004
917	5	1	12	0	109.442	108.162	0.698	1.280	0.025
918	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
919	1	1	12	0	109.500	108.679	1.056	0.821	0.016
920	5	1	12	0	109.442	108.162	0.698	1.280	0.025
921	5	1	5	0	109.442	108.836	0.516	0.606	0.004

```

922 1 1 5 0 109.500 110.549 0.636 -1.049 0.015
923 5 1 12 0 109.442 108.162 0.698 1.280 0.025
924 1 1 5 0 109.500 110.549 0.636 -1.049 0.015
925 5 1 12 0 109.442 108.162 0.698 1.280 0.025
926 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

```

971 V A N   D E R   W A A L S
972
973 ATOM TYPES
974   I     J       Rij       R*IJ     EPSILON     ENERGY
975 -----
976   5     5       2.400     2.970     0.022       0.107
977   5     5       2.400     2.970     0.022       0.107
978   5    12       3.499     3.713     0.053      -0.044
979   5     5       2.903     2.970     0.022      -0.021
980   5     5       2.400     2.970     0.022       0.107
981   5    12       2.792     3.713     0.053       0.792
982  12     5       2.792     3.713     0.053       0.792
983  12     5       3.499     3.713     0.053      -0.044
984  12    12       3.087     4.089     0.276       3.947
985      TOTAL VAN DER WAALS ENERGY =   5.74158 kcal/mol
986
987 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
988
989 ATOM TYPES
990   I     J       Rij       Qi        Qj        ENERGY
991 -----
992  12    12       3.137    -0.290    -0.290       6.678
993      TOTAL ELECTROSTATIC ENERGY =   6.67788 kcal/mol
994
995 TOTAL ENERGY = 29.75490 kcal/mol
996
997 E N E R G Y
998
999
1000 B O N D   S T R E T C H I N G
1001
1002 ATOM TYPES  BOND      IDEAL      FORCE
1003   I     J    LENGTH   LENGTH   CONSTANT   DELTA     ENERGY
1004 -----
1005 h1 c3      1.000     1.093     1406.346    -0.093     12.163
1006 h1 c3      1.000     1.093     1406.346    -0.093     12.163
1007 h1 c3      1.000     1.093     1406.346    -0.093     12.163
1008 c3 c3      1.540     1.535     1269.019     0.005       0.032
1009 c3 h1      1.000     1.093     1406.346    -0.093     12.163
1010 c3 c1      1.670     1.786     1168.117    -0.116     15.718
1011 c3 c1      1.670     1.786     1168.117    -0.116     15.718
1012      TOTAL BOND STRETCHING ENERGY =   80.122 kJ/mol
1013
1014 A N G L E   B E N D I N G
1015
1016 ATOM TYPES      VALENCE      IDEAL      FORCE
1017   I     J     K     ANGLE     ANGLE     CONSTANT   DELTA     ENERGY
1018 -----
1019 c3 c3 h1    109.500    110.070      194.100    -0.010       0.019

```

1020	h1 c3 h1	109.442	109.550	164.039	-0.002	0.001
1021	h1 c3 c1	109.442	105.930	183.005	0.061	0.688
1022	c3 c3 h1	109.500	110.070	194.100	-0.010	0.019
1023	c3 c3 c1	109.500	110.330	260.419	-0.014	0.055
1024	h1 c3 c1	109.442	105.930	183.005	0.061	0.688
1025	h1 c3 h1	109.442	109.550	164.039	-0.002	0.001
1026	c3 c3 h1	109.500	110.070	194.100	-0.010	0.019
1027	h1 c3 c1	109.442	105.930	183.005	0.061	0.688
1028	c3 c3 h1	109.500	110.070	194.100	-0.010	0.019
1029	h1 c3 c1	109.442	105.930	183.005	0.061	0.688
1030	c3 c3 c1	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	
1038	h1	c3	c3	h1	0.651	0	60.000	3	0.000
1039	h1	c3	c3	h1	0.651	0	-60.000	3	0.000
1040	h1	c3	c3	c1	0.000	0	-180.000	3	0.000
1041	h1	c3	c3	h1	0.651	0	-180.000	3	0.000
1042	h1	c3	c3	h1	0.651	0	60.000	3	0.000
1043	h1	c3	c3	c1	0.000	0	-60.000	3	0.000
1044	c1	c3	c3	h1	0.000	0	-60.000	3	0.000
1045	c1	c3	c3	h1	0.000	0	180.000	3	0.000
1046	c1	c3	c3	c1	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
1061	h1	h1	2.400	0.030
1062	h1	h1	2.400	0.030
1063	h1	c1	3.499	-0.127
1064	h1	h1	2.903	-0.031
1065	h1	h1	2.400	0.030
1066	h1	c1	2.792	0.356
1067	c1	h1	2.792	0.356
1068	c1	h1	3.499	-0.127

```

1069  cl cl      3.087      4.588
1070      TOTAL VAN DER WAALS ENERGY =      5.105 kJ/mol
1071
1072  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
1122	6	0.000000
1123	7	0.000000
1124	8	-0.290000
1125		
1126	A T O M T Y P E S	
1127		
1128	IDX	TYPE RING
1129	1	c3 NO
1130	2	c3 NO
1131	3	h1 NO
1132	4	h1 NO
1133	5	cl NO
1134	6	h1 NO
1135	7	h1 NO
1136	8	cl NO
1137		
1138	F O R M A L C H A R G E S	
1139		
1140	IDX	CHARGE
1141	1	0.036009
1142	2	0.036009
1143	3	0.044101
1144	4	0.044101
1145	5	-0.124211
1146	6	0.044101
1147	7	0.044101
1148	8	-0.124211
1149		
1150	P A R T I A L C H A R G E S	
1151		
1152	IDX	CHARGE
1153	1	0.036009
1154	2	0.036009
1155	3	0.044101
1156	4	0.044101
1157	5	-0.124211
1158	6	0.044101
1159	7	0.044101
1160	8	-0.124211
1161		
1162	E N E R G Y	
1163		
1164		
1165	B O N D S T R E T C H I N G	
1166		

```

1167 ATOM TYPES      FF      BOND      IDEAL      FORCE
1168   I      J      CLASS  LENGTH      LENGTH      CONSTANT      DELTA      ENERGY
1169 -----
1170   5      1      0      1.000      1.093      4.766      -0.093      3.578
1171   5      1      0      1.000      1.093      4.766      -0.093      3.578
1172   5      1      0      1.000      1.093      4.766      -0.093      3.578
1173   1      1      0      1.540      1.508      4.258      0.032      0.294
1174   1      5      0      1.000      1.093      4.766      -0.093      3.578
1175   1     12      0      1.670      1.773      2.974      -0.103      2.795
1176   1     12      0      1.670      1.773      2.974      -0.103      2.795
1177      TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
1178
1179 A N G L E      B E N D I N G
1180
1181 ATOM TYPES      FF      VALENCE      IDEAL      FORCE
1182   I      J      K      CLASS  ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
1183 -----
1184   1      1      5      0     109.500     110.549      0.636      -1.049      0.015
1185   5      1      5      0     109.442     108.836      0.516      0.606      0.004
1186   5      1     12      0     109.442     108.162      0.698      1.280      0.025
1187   1      1      5      0     109.500     110.549      0.636      -1.049      0.015
1188   1      1     12      0     109.500     108.679      1.056      0.821      0.016
1189   5      1     12      0     109.442     108.162      0.698      1.280      0.025
1190   5      1      5      0     109.442     108.836      0.516      0.606      0.004
1191   1      1      5      0     109.500     110.549      0.636      -1.049      0.015
1192   5      1     12      0     109.442     108.162      0.698      1.280      0.025
1193   1      1      5      0     109.500     110.549      0.636      -1.049      0.015
1194   5      1     12      0     109.442     108.162      0.698      1.280      0.025
1195   1      1     12      0     109.500     108.679      1.056      0.821      0.016
1196      TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
1197
1198 S T R E T C H      B E N D I N G
1199
1200 ATOM TYPES      FF      VALENCE      DELTA      FORCE CONSTANT
1201   I      J      K      CLASS  ANGLE      ANGLE      I  J      J  K      ENERGY
1202 -----
1203   1      1      5      0     109.500     -1.049      0.227      0.070      -0.002
1204   5      1      5      0     109.442      0.606      0.115      0.115      -0.033
1205   5      1     12      0     109.442      1.280     -0.018      0.380      -0.121
1206   1      1      5      0     109.500     -1.049      0.227      0.070      -0.002
1207   1      1     12      0     109.500      0.821      0.176      0.386      -0.070
1208   5      1     12      0     109.442      1.280     -0.018      0.380      -0.121
1209   5      1      5      0     109.442      0.606      0.115      0.115      -0.033
1210   1      1      5      0     109.500     -1.049      0.227      0.070      -0.002
1211   5      1     12      0     109.442      1.280     -0.018      0.380      -0.121
1212   1      1      5      0     109.500     -1.049      0.227      0.070      -0.002
1213   5      1     12      0     109.442      1.280     -0.018      0.380      -0.121
1214   1      1     12      0     109.500      0.821      0.176      0.386      -0.070
1215      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

```



```

1216
1217 T O R S I O N A L
1218
1219 ATOM TYPES          FF      TORSION      FORCE CONSTANT
1220 I      J      K      L      CLASS      ANGLE      V1      V2      V3      ENERGY
1221 -----
1222 5      1      1      5      0      80.000      0.284      -1.386      0.314      -1.099
1223 5      1      1      5      0      -40.000      0.284      -1.386      0.314      -0.243
1224 5      1      1      12     0      -160.000      0.678      -0.602      0.398      0.050
1225 5      1      1      5      0      -160.000      0.284      -1.386      0.314      -0.075
1226 5      1      1      5      0      80.000      0.284      -1.386      0.314      -1.099
1227 5      1      1      12     0      -40.000      0.678      -0.602      0.398      0.449
1228 12     1      1      5      0      -40.000      0.678      -0.602      0.398      0.449
1229 12     1      1      5      0      -160.000      0.678      -0.602      0.398      0.050
1230 12     1      1      12     0      80.000      0.000      0.000      0.893      0.223
1231 TOTAL TORSIONAL ENERGY = -1.29534 kcal/mol
1232
1233 O U T - O F - P L A N E   B E N D I N G
1234
1235 ATOM TYPES          FF      OOP      FORCE
1236 I      J      K      L      CLASS      ANGLE      CONSTANT      ENERGY
1237 -----
1238 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
1239
1240 V A N   D E R   W A A L S
1241
1242 ATOM TYPES
1243 I      J      Rij      R*IJ      EPSILON      ENERGY
1244 -----
1245 5      5      2.518      2.970      0.022      0.036
1246 5      5      2.300      2.970      0.022      0.215
1247 5      12     3.474      3.713      0.053      -0.041
1248 5      5      2.885      2.970      0.022      -0.021
1249 5      5      2.518      2.970      0.022      0.036
1250 5      12     2.647      3.713      0.053      1.520
1251 12     5      2.647      3.713      0.053      1.520
1252 12     5      3.474      3.713      0.053      -0.041
1253 12     12     3.338      4.089      0.276      1.129
1254 TOTAL VAN DER WAALS ENERGY = 4.35500 kcal/mol
1255
1256 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
1257
1258 ATOM TYPES
1259 I      J      Rij      Qi      Qj      ENERGY
1260 -----
1261 12     12     3.388      -0.290      -0.290      6.182
1262 TOTAL ELECTROSTATIC ENERGY = 6.18170 kcal/mol
1263
1264 TOTAL ENERGY = 28.94230 kcal/mol

```

1265

1266 E N E R G Y

1267

1268

1269 B O N D S T R E T C H I N G

1270

1271 ATOM TYPES BOND IDEAL FORCE

1272 I J LENGTH LENGTH CONSTANT DELTA ENERGY

1273

1274 h1 c3 1.000 1.093 1406.346 -0.093 12.163

1275 h1 c3 1.000 1.093 1406.346 -0.093 12.163

1276 h1 c3 1.000 1.093 1406.346 -0.093 12.163

1277 c3 c3 1.540 1.535 1269.019 0.005 0.032

1278 c3 h1 1.000 1.093 1406.346 -0.093 12.163

1279 c3 c1 1.670 1.786 1168.117 -0.116 15.718

1280 c3 c1 1.670 1.786 1168.117 -0.116 15.718

1281 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

1282

1283 A N G L E B E N D I N G

1284

1285 ATOM TYPES VALENCE IDEAL FORCE

1286 I J K ANGLE ANGLE CONSTANT DELTA ENERGY

1287

1288 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

1289 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

1290 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

1291 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

1292 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

1293 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

1294 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

1295 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

1296 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

1297 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

1298 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

1299 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

1300 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

1301

1302 T O R S I O N A L

1303

1304 ----ATOM TYPES----- FORCE TORSION

1305 I J K L CONSTANT s ANGLE n ENERGY

1306

1307 h1 c3 c3 h1 0.651 0 80.000 3 0.326

1308 h1 c3 c3 h1 0.651 0 -40.000 3 0.326

1309 h1 c3 c3 c1 0.000 0 -160.000 3 0.000

1310 h1 c3 c3 h1 0.651 0 -160.000 3 0.326

1311 h1 c3 c3 h1 0.651 0 80.000 3 0.326

1312 h1 c3 c3 c1 0.000 0 -40.000 3 0.000

1313 c1 c3 c3 h1 0.000 0 -40.000 3 0.000

```

1314 c1 c3 c3 h1      0.000      0  -160.000  3      0.000
1315 c1 c3 c3 c1      0.000      0   80.000  3      0.000
1316      TOTAL TORSIONAL ENERGY =      1.303 kJ/mol
1317
1318 I M P R O P E R   T O R S I O N A L
1319
1320 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
1321 I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
1322 -----
1323      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
1324
1325 V A N   D E R   W A A L S
1326
1327 ATOM TYPES
1328 I      J      Rij      kij      ENERGY
1329 -----
1330 h1 h1      2.518      -0.013
1331 h1 h1      2.300      0.109
1332 h1 c1      3.474      -0.129
1333 h1 h1      2.885      -0.031
1334 h1 h1      2.518      -0.013
1335 h1 c1      2.647      1.083
1336 c1 h1      2.647      1.083
1337 c1 h1      3.474      -0.129
1338 c1 c1      3.338      0.738
1339      TOTAL VAN DER WAALS ENERGY =      2.701 kJ/mol
1340
1341 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
1342
1343 ATOM TYPES
1344 I      J      Rij      332.17*QiQj      ENERGY
1345 -----
1346 h1 h1      2.518      1.352      0.537
1347 h1 h1      2.300      1.352      0.588
1348 h1 c1      3.474      -3.809      -1.097
1349 h1 h1      2.885      1.352      0.469
1350 h1 h1      2.518      1.352      0.537
1351 h1 c1      2.647      -3.809      -1.439
1352 c1 h1      2.647      -3.809      -1.439
1353 c1 h1      3.474      -3.809      -1.097
1354 c1 c1      3.338      10.728      3.214
1355      TOTAL ELECTROSTATIC ENERGY =      0.273 kJ/mol
1356
1357 TOTAL ENERGY =      87.337 kJ/mol
1358
1359 A T O M   T Y P E S
1360
1361 IDX TYPE   RING
1362 1 1 NO

```

```
1363 2 1 NO
1364 3 5 NO
1365 4 5 NO
1366 5 12 NO
1367 6 5 NO
1368 7 5 NO
1369 8 12 NO
1370
1371 F O R M A L   C H A R G E S
1372
1373 IDX CHARGE
1374 1 0.000000
1375 2 0.000000
1376 3 0.000000
1377 4 0.000000
1378 5 0.000000
1379 6 0.000000
1380 7 0.000000
1381 8 0.000000
1382
1383 P A R T I A L   C H A R G E S
1384
1385 IDX CHARGE
1386 1 0.290000
1387 2 0.290000
1388 3 0.000000
1389 4 0.000000
1390 5 -0.290000
1391 6 0.000000
1392 7 0.000000
1393 8 -0.290000
1394
1395 S E T T I N G   U P   C A L C U L A T I O N S
1396
1397 SETTING UP BOND CALCULATIONS...
1398 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
1399 SETTING UP TORSION CALCULATIONS...
1400 SETTING UP OOP CALCULATIONS...
1401 SETTING UP VAN DER WAALS CALCULATIONS...
1402 SETTING UP ELECTROSTATIC CALCULATIONS...
1403
1404 A T O M   T Y P E S
1405
1406 IDX TYPE RING
1407 1 c3 NO
1408 2 c3 NO
1409 3 h1 NO
1410 4 h1 NO
1411 5 c1 NO
```

1412 6 h1 NO
1413 7 h1 NO
1414 8 cl NO

1415

1416 C H A R G E S

1417

1418 I D X C H A R G E

1419 1 0.036009
1420 2 0.036009
1421 3 0.044101
1422 4 0.044101
1423 5 -0.124211
1424 6 0.044101
1425 7 0.044101
1426 8 -0.124211

1427

1428 S E T T I N G U P C A L C U L A T I O N S

1429

1430 SETTING UP BOND CALCULATIONS...

1431 SETTING UP ANGLE CALCULATIONS...

1432 SETTING UP TORSION CALCULATIONS...

1433 SETTING UP IMPROPER TORSION CALCULATIONS...

1434 SETTING UP VAN DER WAALS CALCULATIONS...

1435 SETTING UP ELECTROSTATIC CALCULATIONS...

1436

1437 E N E R G Y

1438

1439

1440 B O N D S T R E T C H I N G

1441

1442	ATOM TYPES		FF	BOND	IDEAL	FORCE		
1443	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
1444	-----							
1445	5	1	0	1.000	1.093	4.766	-0.093	3.578
1446	5	1	0	1.000	1.093	4.766	-0.093	3.578
1447	1	1	0	1.540	1.508	4.258	0.032	0.294
1448	1	5	0	1.000	1.093	4.766	-0.093	3.578
1449	1	12	0	1.670	1.773	2.974	-0.103	2.795
1450	1	5	0	1.000	1.093	4.766	-0.093	3.578
1451	1	12	0	1.670	1.773	2.974	-0.103	2.795

1452 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

1453

1454 A N G L E B E N D I N G

1455

1456	ATOM TYPES			FF	VALENCE	IDEAL	FORCE		
1457	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
1458	-----								
1459	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
1460	5	1	5	0	109.442	108.836	0.516	0.606	0.004

1461	5	1	12	0	109.442	108.162	0.698	1.280	0.025
1462	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
1463	1	1	12	0	109.500	108.679	1.056	0.821	0.016
1464	5	1	12	0	109.442	108.162	0.698	1.280	0.025
1465	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
1466	5	1	5	0	109.442	108.836	0.516	0.606	0.004
1467	5	1	12	0	109.442	108.162	0.698	1.280	0.025
1468	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
1469	1	1	12	0	109.500	108.679	1.056	0.821	0.016
1470	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

1510	ATOM TYPES				FF	OOP	FORCE	
1511	I	J	K	L	CLASS	ANGLE	CONSTANT	ENERGY

1512 -----

1513 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol

1514

1515 V A N D E R W A A L S

1516

1517	ATOM TYPES						
1518	I	J	Rij	R*IJ	EPSILON	ENERGY	

1519 -----

1520	5	5	2.638	2.970	0.022	0.001	
1521	5	5	2.232	2.970	0.022	0.328	
1522	5	12	3.399	3.713	0.053	-0.028	
1523	5	5	2.831	2.970	0.022	-0.019	
1524	5	5	2.638	2.970	0.022	0.001	
1525	5	12	2.547	3.713	0.053	2.298	
1526	12	5	2.547	3.713	0.053	2.298	
1527	12	5	3.399	3.713	0.053	-0.028	
1528	12	12	3.587	4.089	0.276	0.100	

1529 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol

1530

1531 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

1532

1533	ATOM TYPES						
1534	I	J	Rij	Qi	Qj	ENERGY	

1535 -----

1536	12	12	3.637	-0.290	-0.290	5.759	
------	----	----	-------	--------	--------	-------	--

1537 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol

1538

1539 TOTAL ENERGY = 31.17064 kcal/mol

1540

1541 E N E R G Y

1542

1543

1544 B O N D S T R E T C H I N G

1545

1546	ATOM TYPES		BOND	IDEAL	FORCE		
1547	I	J	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY

1548 -----

1549	h1	c3	1.000	1.093	1406.346	-0.093	12.163
1550	h1	c3	1.000	1.093	1406.346	-0.093	12.163
1551	c3	c3	1.540	1.535	1269.019	0.005	0.032
1552	c3	h1	1.000	1.093	1406.346	-0.093	12.163
1553	c3	c1	1.670	1.786	1168.117	-0.116	15.718
1554	c3	h1	1.000	1.093	1406.346	-0.093	12.163
1555	c3	c1	1.670	1.786	1168.117	-0.116	15.718

1556 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

1557

1558 A N G L E B E N D I N G

```

1559
1560 ATOM TYPES          VALENCE          IDEAL          FORCE
1561   I      J      K          ANGLE          ANGLE          CONSTANT          DELTA          ENERGY
1562 -----
1563 c3 c3 h1    109.500    110.070        194.100        -0.010        0.019
1564 h1 c3 h1    109.442    109.550        164.039        -0.002        0.001
1565 h1 c3 c1    109.442    105.930        183.005         0.061        0.688
1566 c3 c3 h1    109.500    110.070        194.100        -0.010        0.019
1567 c3 c3 c1    109.500    110.330        260.419        -0.014        0.055
1568 h1 c3 c1    109.442    105.930        183.005         0.061        0.688
1569 c3 c3 h1    109.500    110.070        194.100        -0.010        0.019
1570 h1 c3 h1    109.442    109.550        164.039        -0.002        0.001
1571 h1 c3 c1    109.442    105.930        183.005         0.061        0.688
1572 c3 c3 h1    109.500    110.070        194.100        -0.010        0.019
1573 c3 c3 c1    109.500    110.330        260.419        -0.014        0.055
1574 h1 c3 c1    109.442    105.930        183.005         0.061        0.688
1575      TOTAL ANGLE BENDING ENERGY =      2.938 kJ/mol
1576
1577 T O R S I O N A L
1578
1579 ----ATOM TYPES-----      FORCE          TORSION
1580   I      J      K      L      CONSTANT      s          ANGLE      n          ENERGY
1581 -----
1582 h1 c3 c3 h1      0.651          0    -20.000    3          0.977
1583 h1 c3 c3 h1      0.651          0    100.000    3          0.977
1584 h1 c3 c3 c1      0.000          0   -140.000    3          0.000
1585 h1 c3 c3 h1      0.651          0    100.000    3          0.977
1586 h1 c3 c3 h1      0.651          0   -140.000    3          0.977
1587 h1 c3 c3 c1      0.000          0    -20.000    3          0.000
1588 c1 c3 c3 h1      0.000          0   -140.000    3          0.000
1589 c1 c3 c3 h1      0.000          0    -20.000    3          0.000
1590 c1 c3 c3 c1      0.000          0    100.000    3          0.000
1591      TOTAL TORSIONAL ENERGY =      3.908 kJ/mol
1592
1593 I M P R O P E R   T O R S I O N A L
1594
1595 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
1596   I      J      K      L      CONSTANT      s          ANGLE      n          ENERGY
1597 -----
1598      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
1599
1600 V A N   D E R   W A A L S
1601
1602 ATOM TYPES
1603   I      J          Rij          kij          ENERGY
1604 -----
1605 h1 h1          2.638    -0.029
1606 h1 h1          2.232     0.205
1607 h1 c1          3.399    -0.133

```



```

1608 h1 h1      2.831    -0.032
1609 h1 h1      2.638    -0.029
1610 h1 c1      2.547      2.064
1611 c1 h1      2.547      2.064
1612 c1 h1      3.399    -0.133
1613 c1 c1      3.587    -0.326
1614      TOTAL VAN DER WAALS ENERGY =      3.650 kJ/mol
1615
1616 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
1617
1618 ATOM TYPES
1619   I      J          Rij    332.17*QiQj  ENERGY
1620 -----
1621 h1 h1      2.638      1.352      0.513
1622 h1 h1      2.232      1.352      0.606
1623 h1 c1      3.399     -3.809     -1.121
1624 h1 h1      2.831      1.352      0.478
1625 h1 h1      2.638      1.352      0.513
1626 h1 c1      2.547     -3.809     -1.495
1627 c1 h1      2.547     -3.809     -1.495
1628 c1 h1      3.399     -3.809     -1.121
1629 c1 c1      3.587     10.728      2.991
1630      TOTAL ELECTROSTATIC ENERGY =     -0.132 kJ/mol
1631
1632 TOTAL ENERGY =      90.486 kJ/mol
1633
1634 A T O M   T Y P E S
1635
1636 IDX TYPE  RING
1637 1 1 NO
1638 2 1 NO
1639 3 5 NO
1640 4 5 NO
1641 5 12  NO
1642 6 5 NO
1643 7 5 NO
1644 8 12  NO
1645
1646 F O R M A L   C H A R G E S
1647
1648 IDX CHARGE
1649 1 0.290000
1650 2 0.290000
1651 3 0.000000
1652 4 0.000000
1653 5 -0.290000
1654 6 0.000000
1655 7 0.000000
1656 8 -0.290000

```

```
1657
1658 P A R T I A L   C H A R G E S
1659
1660 IDX CHARGE
1661 1 0.290000
1662 2 0.290000
1663 3 0.000000
1664 4 0.000000
1665 5 -0.290000
1666 6 0.000000
1667 7 0.000000
1668 8 -0.290000
1669
1670 A T O M   T Y P E S
1671
1672 IDX TYPE  RING
1673 1 c3  NO
1674 2 c3  NO
1675 3 h1  NO
1676 4 h1  NO
1677 5 c1  NO
1678 6 h1  NO
1679 7 h1  NO
1680 8 c1  NO
1681
1682 F O R M A L   C H A R G E S
1683
1684 IDX CHARGE
1685 1 0.036009
1686 2 0.036009
1687 3 0.044101
1688 4 0.044101
1689 5 -0.124211
1690 6 0.044101
1691 7 0.044101
1692 8 -0.124211
1693
1694 P A R T I A L   C H A R G E S
1695
1696 IDX CHARGE
1697 1 0.036009
1698 2 0.036009
1699 3 0.044101
1700 4 0.044101
1701 5 -0.124211
1702 6 0.044101
1703 7 0.044101
1704 8 -0.124211
1705
```

1706 E N E R G Y

1707

1708

1709 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

```

1759 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

1760

1761 T O R S I O N A L

1762

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

1775 TOTAL TORSIONAL ENERGY = 1.91150 kcal/mol

1776

1777 O U T - O F - P L A N E B E N D I N G

1778

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

1781

1782 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol

1783

1784 V A N D E R W A A L S

1785

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	

1798 TOTAL VAN DER WAALS ENERGY = 5.44875 kcal/mol

1799

1800 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

1801

ATOM TYPES						
I	J		Rij	Qi	Qj	ENERGY

1803

```

1804 -----
1805 12 12 3.856 -0.290 -0.290 5.432
1806 TOTAL ELECTROSTATIC ENERGY = 5.43239 kcal/mol
1807
1808 TOTAL ENERGY = 32.49359 kcal/mol
1809
1810 E N E R G Y
1811
1812
1813 B O N D S T R E T C H I N G
1814
1815 ATOM TYPES BOND IDEAL FORCE
1816 I J LENGTH LENGTH CONSTANT DELTA ENERGY
1817 -----
1818 h1 c3 1.000 1.093 1406.346 -0.093 12.163
1819 h1 c3 1.000 1.093 1406.346 -0.093 12.163
1820 c3 c3 1.540 1.535 1269.019 0.005 0.032
1821 c3 h1 1.000 1.093 1406.346 -0.093 12.163
1822 c3 c1 1.670 1.786 1168.117 -0.116 15.718
1823 c3 h1 1.000 1.093 1406.346 -0.093 12.163
1824 c3 c1 1.670 1.786 1168.117 -0.116 15.718
1825 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
1826
1827 A N G L E B E N D I N G
1828
1829 ATOM TYPES VALENCE IDEAL FORCE
1830 I J K ANGLE ANGLE CONSTANT DELTA ENERGY
1831 -----
1832 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
1833 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001
1834 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
1835 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
1836 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055
1837 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
1838 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
1839 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001
1840 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
1841 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
1842 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055
1843 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
1844 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
1845
1846 T O R S I O N A L
1847
1848 ----ATOM TYPES----- FORCE TORSION
1849 I J K L CONSTANT s ANGLE n ENERGY
1850 -----
1851 h1 c3 c3 h1 0.651 0 0.000 3 1.303
1852 h1 c3 c3 h1 0.651 0 120.000 3 1.303

```

```

1853 h1 c3 c3 c1      0.000      0  -120.000  3      0.000
1854 h1 c3 c3 h1      0.651      0   120.000  3      1.303
1855 h1 c3 c3 h1      0.651      0  -120.000  3      1.303
1856 h1 c3 c3 c1      0.000      0    0.000  3      0.000
1857 c1 c3 c3 h1      0.000      0  -120.000  3      0.000
1858 c1 c3 c3 h1      0.000      0   -0.000  3      0.000
1859 c1 c3 c3 c1      0.000      0   120.000  3      0.000
1860      TOTAL TORSIONAL ENERGY =      5.210 kJ/mol
1861
1862 I M P R O P E R   T O R S I O N A L
1863
1864 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
1865      I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
1866 -----
1867      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
1868
1869 V A N   D E R   W A A L S
1870
1871 ATOM TYPES
1872      I      J      Rij      kij      ENERGY
1873 -----
1874 h1 h1      2.746      -0.033
1875 h1 h1      2.208      0.251
1876 h1 c1      3.280      -0.134
1877 h1 h1      2.746      -0.033
1878 h1 h1      2.746      -0.033
1879 h1 c1      2.512      2.571
1880 c1 h1      2.512      2.571
1881 c1 h1      3.280      -0.134
1882 c1 c1      3.806      -0.542
1883      TOTAL VAN DER WAALS ENERGY =      4.485 kJ/mol
1884
1885 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
1886
1887 ATOM TYPES
1888      I      J      Rij      332.17*QiQj      ENERGY
1889 -----
1890 h1 h1      2.746      1.352      0.493
1891 h1 h1      2.208      1.352      0.613
1892 h1 c1      3.280      -3.809      -1.161
1893 h1 h1      2.746      1.352      0.493
1894 h1 h1      2.746      1.352      0.493
1895 h1 c1      2.512      -3.809      -1.516
1896 c1 h1      2.512      -3.809      -1.516
1897 c1 h1      3.280      -3.809      -1.161
1898 c1 c1      3.806      10.728      2.819
1899      TOTAL ELECTROSTATIC ENERGY =      -0.446 kJ/mol
1900
1901 TOTAL ENERGY =      92.310 kJ/mol

```

```
1902
1903 A T O M   T Y P E S
1904
1905 IDX TYPE  RING
1906 1 1 NO
1907 2 1 NO
1908 3 5 NO
1909 4 5 NO
1910 5 12  NO
1911 6 5 NO
1912 7 5 NO
1913 8 12  NO
1914
1915 F O R M A L   C H A R G E S
1916
1917 IDX CHARGE
1918 1 0.000000
1919 2 0.000000
1920 3 0.000000
1921 4 0.000000
1922 5 0.000000
1923 6 0.000000
1924 7 0.000000
1925 8 0.000000
1926
1927 P A R T I A L   C H A R G E S
1928
1929 IDX CHARGE
1930 1 0.290000
1931 2 0.290000
1932 3 0.000000
1933 4 0.000000
1934 5 -0.290000
1935 6 0.000000
1936 7 0.000000
1937 8 -0.290000
1938
1939 S E T T I N G   U P   C A L C U L A T I O N S
1940
1941 SETTING UP BOND CALCULATIONS...
1942 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
1943 SETTING UP TORSION CALCULATIONS...
1944 SETTING UP OOP CALCULATIONS...
1945 SETTING UP VAN DER WAALS CALCULATIONS...
1946 SETTING UP ELECTROSTATIC CALCULATIONS...
1947
1948 A T O M   T Y P E S
1949
1950 IDX TYPE  RING
```

1951 1 c3 NO
1952 2 c3 NO
1953 3 h1 NO
1954 4 h1 NO
1955 5 c1 NO
1956 6 h1 NO
1957 7 h1 NO
1958 8 c1 NO

1959

1960 C H A R G E S

1961

1962 IDX CHARGE

1963 1 0.036009

1964 2 0.036009

1965 3 0.044101

1966 4 0.044101

1967 5 -0.124211

1968 6 0.044101

1969 7 0.044101

1970 8 -0.124211

1971

1972 S E T T I N G U P C A L C U L A T I O N S

1973

1974 SETTING UP BOND CALCULATIONS...

1975 SETTING UP ANGLE CALCULATIONS...

1976 SETTING UP TORSION CALCULATIONS...

1977 SETTING UP IMPROPER TORSION CALCULATIONS...

1978 SETTING UP VAN DER WAALS CALCULATIONS...

1979 SETTING UP ELECTROSTATIC CALCULATIONS...

1980

1981 E N E R G Y

1982

1983

1984 B O N D S T R E T C H I N G

1985

1986	ATOM TYPES		FF	BOND	IDEAL	FORCE		
1987	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
1988	-----							
1989	5	1	0	1.000	1.093	4.766	-0.093	3.578
1990	5	1	0	1.000	1.093	4.766	-0.093	3.578
1991	1	1	0	1.540	1.508	4.258	0.032	0.294
1992	1	5	0	1.000	1.093	4.766	-0.093	3.578
1993	1	12	0	1.670	1.773	2.974	-0.103	2.795
1994	1	12	0	1.670	1.773	2.974	-0.103	2.795
1995	1	5	0	1.000	1.093	4.766	-0.093	3.578

1996 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

1997

1998 A N G L E B E N D I N G

1999

2000	ATOM TYPES			FF	VALENCE	IDEAL	FORCE		
2001	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
2002	-----								
2003	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2004	5	1	5	0	109.442	108.836	0.516	0.606	0.004
2005	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2006	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2007	1	1	12	0	109.500	108.679	1.056	0.821	0.016
2008	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2009	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2010	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2011	5	1	5	0	109.442	108.836	0.516	0.606	0.004
2012	1	1	12	0	109.500	108.679	1.056	0.821	0.016
2013	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2014	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2015	TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol								
2016									
2017	S T R E T C H B E N D I N G								
2018									
2019	ATOM TYPES			FF	VALENCE	DELTA	FORCE CONSTANT		
2020	I	J	K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY
2021	-----								
2022	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2023	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
2024	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2025	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2026	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
2027	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2028	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2029	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2030	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
2031	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
2032	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2033	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2034	TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol								
2035									
2036	T O R S I O N A L								
2037									
2038	ATOM TYPES			FF	TORSION	FORCE CONSTANT			
2039	I	J	K	L	CLASS	ANGLE	V1	V2	V3
2040	-----								
2041	5	1	1	5	0	20.000	0.284	-1.386	0.314
2042	5	1	1	12	0	-100.000	0.678	-0.602	0.398
2043	5	1	1	5	0	140.000	0.284	-1.386	0.314
2044	5	1	1	5	0	140.000	0.284	-1.386	0.314
2045	5	1	1	12	0	20.000	0.678	-0.602	0.398
2046	5	1	1	5	0	-100.000	0.284	-1.386	0.314
2047	12	1	1	5	0	-100.000	0.678	-0.602	0.398
2048	12	1	1	12	0	140.000	0.000	0.000	0.893

```

2049 12 1 1 5 0 20.000 0.678 -0.602 0.398 0.886
2050 TOTAL TORSIONAL ENERGY = 1.18015 kcal/mol
2051
2052 O U T - O F - P L A N E B E N D I N G
2053
2054 ATOM TYPES FF OOP FORCE
2055 I J K L CLASS ANGLE CONSTANT ENERGY
2056 -----
2057 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
2058
2059 V A N D E R W A A L S
2060
2061 ATOM TYPES
2062 I J RiJ R*IJ EPSILON ENERGY
2063 -----
2064 5 5 2.831 2.970 0.022 -0.019
2065 5 5 2.232 2.970 0.022 0.328
2066 5 12 3.129 3.713 0.053 0.104
2067 5 5 2.638 2.970 0.022 0.001
2068 5 5 2.831 2.970 0.022 -0.019
2069 5 12 2.547 3.713 0.053 2.298
2070 12 5 2.547 3.713 0.053 2.298
2071 12 5 3.129 3.713 0.053 0.104
2072 12 12 3.975 4.089 0.276 -0.269
2073 TOTAL VAN DER WAALS ENERGY = 4.82482 kcal/mol
2074
2075 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
2076
2077 ATOM TYPES
2078 I J RiJ Qi Qj ENERGY
2079 -----
2080 12 12 4.025 -0.290 -0.290 5.204
2081 TOTAL ELECTROSTATIC ENERGY = 5.20367 kcal/mol
2082
2083 TOTAL ENERGY = 30.90959 kcal/mol
2084
2085 E N E R G Y
2086
2087
2088 B O N D S T R E T C H I N G
2089
2090 ATOM TYPES BOND IDEAL FORCE
2091 I J LENGTH LENGTH CONSTANT DELTA ENERGY
2092 -----
2093 h1 c3 1.000 1.093 1406.346 -0.093 12.163
2094 h1 c3 1.000 1.093 1406.346 -0.093 12.163
2095 c3 c3 1.540 1.535 1269.019 0.005 0.032
2096 c3 h1 1.000 1.093 1406.346 -0.093 12.163
2097 c3 c1 1.670 1.786 1168.117 -0.116 15.718

```

```

2098 c3 c1      1.670      1.786      1168.117      -0.116      15.718
2099 c3 h1      1.000      1.093      1406.346      -0.093      12.163
2100      TOTAL BOND STRETCHING ENERGY =      80.122 kJ/mol
2101
2102 A N G L E    B E N D I N G
2103
2104 ATOM TYPES          VALENCE          IDEAL          FORCE
2105 I      J      K          ANGLE          ANGLE          CONSTANT          DELTA          ENERGY
2106 -----
2107 c3 c3 h1      109.500      110.070          194.100          -0.010          0.019
2108 h1 c3 h1      109.442      109.550          164.039          -0.002          0.001
2109 h1 c3 c1      109.442      105.930          183.005           0.061          0.688
2110 c3 c3 h1      109.500      110.070          194.100          -0.010          0.019
2111 c3 c3 c1      109.500      110.330          260.419          -0.014          0.055
2112 h1 c3 c1      109.442      105.930          183.005           0.061          0.688
2113 c3 c3 h1      109.500      110.070          194.100          -0.010          0.019
2114 h1 c3 c1      109.442      105.930          183.005           0.061          0.688
2115 h1 c3 h1      109.442      109.550          164.039          -0.002          0.001
2116 c3 c3 c1      109.500      110.330          260.419          -0.014          0.055
2117 c3 c3 h1      109.500      110.070          194.100          -0.010          0.019
2118 h1 c3 c1      109.442      105.930          183.005           0.061          0.688
2119      TOTAL ANGLE BENDING ENERGY =      2.938 kJ/mol
2120
2121 T O R S I O N A L
2122
2123 ----ATOM TYPES-----          FORCE          TORSION
2124 I      J      K      L          CONSTANT          s          ANGLE          n          ENERGY
2125 -----
2126 h1 c3 c3 h1          0.651           0      20.000      3          0.977
2127 h1 c3 c3 c1          0.000           0     -100.000      3          0.000
2128 h1 c3 c3 h1          0.651           0      140.000      3          0.977
2129 h1 c3 c3 h1          0.651           0      140.000      3          0.977
2130 h1 c3 c3 c1          0.000           0      20.000      3          0.000
2131 h1 c3 c3 h1          0.651           0     -100.000      3          0.977
2132 c1 c3 c3 h1          0.000           0     -100.000      3          0.000
2133 c1 c3 c3 c1          0.000           0      140.000      3          0.000
2134 c1 c3 c3 h1          0.000           0      20.000      3          0.000
2135      TOTAL TORSIONAL ENERGY =      3.908 kJ/mol
2136
2137 I M P R O P E R    T O R S I O N A L
2138
2139 ----ATOM TYPES-----          FORCE          IMPROPER_TORSION
2140 I      J      K      L          CONSTANT          s          ANGLE          n          ENERGY
2141 -----
2142      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
2143
2144 V A N    D E R    W A A L S
2145
2146 ATOM TYPES

```

```

2147   I      J      Rij      kij      ENERGY
2148   -----
2149   h1 h1      2.831     -0.032
2150   h1 h1      2.232      0.205
2151   h1 c1      3.129     -0.106
2152   h1 h1      2.638     -0.029
2153   h1 h1      2.831     -0.032
2154   h1 c1      2.547      2.064
2155   c1 h1      2.547      2.064
2156   c1 h1      3.129     -0.106
2157   c1 c1      3.975     -0.548
2158           TOTAL VAN DER WAALS ENERGY =      3.480 kJ/mol
2159
2160   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
2161
2162   ATOM TYPES
2163   I      J      Rij      332.17*QiQj      ENERGY
2164   -----
2165   h1 h1      2.831      1.352      0.478
2166   h1 h1      2.232      1.352      0.606
2167   h1 c1      3.129     -3.809     -1.217
2168   h1 h1      2.638      1.352      0.513
2169   h1 h1      2.831      1.352      0.478
2170   h1 c1      2.547     -3.809     -1.495
2171   c1 h1      2.547     -3.809     -1.495
2172   c1 h1      3.129     -3.809     -1.217
2173   c1 c1      3.975     10.728      2.699
2174           TOTAL ELECTROSTATIC ENERGY =     -0.652 kJ/mol
2175
2176   TOTAL ENERGY =      89.796 kJ/mol
2177
2178   A T O M   T Y P E S
2179
2180   IDX TYPE  RING
2181   1 1 NO
2182   2 1 NO
2183   3 5 NO
2184   4 5 NO
2185   5 12 NO
2186   6 5 NO
2187   7 5 NO
2188   8 12 NO
2189
2190   F O R M A L   C H A R G E S
2191
2192   IDX CHARGE
2193   1 0.000000
2194   2 0.000000
2195   3 0.000000

```

```
2196 4 0.000000
2197 5 0.000000
2198 6 0.000000
2199 7 0.000000
2200 8 0.000000
2201
2202 P A R T I A L   C H A R G E S
2203
2204 IDX CHARGE
2205 1 0.290000
2206 2 0.290000
2207 3 0.000000
2208 4 0.000000
2209 5 -0.290000
2210 6 0.000000
2211 7 0.000000
2212 8 -0.290000
2213
2214 S E T T I N G   U P   C A L C U L A T I O N S
2215
2216 SETTING UP BOND CALCULATIONS...
2217 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
2218 SETTING UP TORSION CALCULATIONS...
2219 SETTING UP OOP CALCULATIONS...
2220 SETTING UP VAN DER WAALS CALCULATIONS...
2221 SETTING UP ELECTROSTATIC CALCULATIONS...
2222
2223 A T O M   T Y P E S
2224
2225 IDX TYPE  RING
2226 1 c3  NO
2227 2 c3  NO
2228 3 h1  NO
2229 4 h1  NO
2230 5 c1  NO
2231 6 h1  NO
2232 7 h1  NO
2233 8 c1  NO
2234
2235 C H A R G E S
2236
2237 IDX CHARGE
2238 1 0.036009
2239 2 0.036009
2240 3 0.044101
2241 4 0.044101
2242 5 -0.124211
2243 6 0.044101
2244 7 0.044101
```

2245 8 -0.124211

2246

2247 S E T T I N G U P C A L C U L A T I O N S

2248

2249 SETTING UP BOND CALCULATIONS...

2250 SETTING UP ANGLE CALCULATIONS...

2251 SETTING UP TORSION CALCULATIONS...

2252 SETTING UP IMPROPER TORSION CALCULATIONS...

2253 SETTING UP VAN DER WAALS CALCULATIONS...

2254 SETTING UP ELECTROSTATIC CALCULATIONS...

2255

2256 E N E R G Y

2257

2258

2259 B O N D S T R E T C H I N G

2260

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	

2271 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

2272

2273 A N G L E B E N D I N G

2274

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	

2290 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

2291

2292 S T R E T C H B E N D I N G

2293

2294	ATOM TYPES			FF	VALENCE	DELTA	FORCE CONSTANT			
2295	I	J	K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY	
2296	-----									
2297	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
2298	5	1	5	0	109.442	0.606	0.115	0.115	-0.033	
2299	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
2300	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
2301	1	1	12	0	109.500	0.821	0.176	0.386	-0.070	
2302	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
2303	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
2304	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
2305	5	1	5	0	109.442	0.606	0.115	0.115	-0.033	
2306	1	1	12	0	109.500	0.821	0.176	0.386	-0.070	
2307	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
2308	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
2309	TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol									
2310										
2311	T O R S I O N A L									
2312										
2313	ATOM TYPES			FF	TORSION	FORCE CONSTANT				
2314	I	J	K	L	CLASS	ANGLE	V1	V2	V3	ENERGY
2315	-----									
2316	5	1	1	5	0	40.000	0.284	-1.386	0.314	-0.243
2317	5	1	1	12	0	-80.000	0.678	-0.602	0.398	-0.086
2318	5	1	1	5	0	160.000	0.284	-1.386	0.314	-0.075
2319	5	1	1	5	0	160.000	0.284	-1.386	0.314	-0.075
2320	5	1	1	12	0	40.000	0.678	-0.602	0.398	0.449
2321	5	1	1	5	0	-80.000	0.284	-1.386	0.314	-1.099
2322	12	1	1	5	0	-80.000	0.678	-0.602	0.398	-0.086
2323	12	1	1	12	0	160.000	0.000	0.000	0.893	0.223
2324	12	1	1	5	0	40.000	0.678	-0.602	0.398	0.449
2325	TOTAL TORSIONAL ENERGY = -0.54336 kcal/mol									
2326										
2327	O U T - O F - P L A N E B E N D I N G									
2328										
2329	ATOM TYPES			FF	OOP	FORCE				
2330	I	J	K	L	CLASS	ANGLE	CONSTANT	ENERGY		
2331	-----									
2332	TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol									
2333										
2334	V A N D E R W A A L S									
2335										
2336	ATOM TYPES									
2337	I	J	Rij		R*IJ	EPSILON	ENERGY			
2338	-----									
2339	5	5	2.885		2.970	0.022	-0.021			
2340	5	5	2.300		2.970	0.022	0.215			
2341	5	12	2.960		3.713	0.053	0.331			
2342	5	5	2.518		2.970	0.022	0.036			

```

2343      5      5      2.885      2.970      0.022      -0.021
2344      5     12      2.647      3.713      0.053      1.520
2345     12      5      2.647      3.713      0.053      1.520
2346     12      5      2.960      3.713      0.053      0.331
2347     12     12      4.082      4.089      0.276      -0.276
2348          TOTAL VAN DER WAALS ENERGY =   3.63663 kcal/mol
2349

```

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

2351

ATOM TYPES

```

2353      I      J      Rij      Qi      Qj      ENERGY
2354      -----

```

```

2355     12     12      4.132     -0.290     -0.290      5.069
2356          TOTAL ELECTROSTATIC ENERGY =   5.06915 kcal/mol
2357

```

2358 TOTAL ENERGY = 27.86335 kcal/mol

2359

E N E R G Y

2361

2362

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

2364

```

2365  ATOM TYPES  BOND      IDEAL      FORCE
2366      I      J  LENGTH  LENGTH  CONSTANT      DELTA      ENERGY
2367  -----

```

```

2368  h1 c3      1.000      1.093      1406.346      -0.093      12.163
2369  h1 c3      1.000      1.093      1406.346      -0.093      12.163
2370  c1 c3      1.670      1.786      1168.117      -0.116      15.718
2371  c3 c3      1.540      1.535      1269.019      0.005      0.032
2372  c3 h1      1.000      1.093      1406.346      -0.093      12.163
2373  c3 c1      1.670      1.786      1168.117      -0.116      15.718
2374  c3 h1      1.000      1.093      1406.346      -0.093      12.163

```

2375 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

2376

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

2378

```

2379  ATOM TYPES      VALENCE      IDEAL      FORCE
2380      I      J      K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
2381  -----

```

```

2382  c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
2383  h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
2384  h1 c3 c1      109.442      105.930      183.005      0.061      0.688
2385  c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
2386  c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
2387  h1 c3 c1      109.442      105.930      183.005      0.061      0.688
2388  h1 c3 c1      109.442      105.930      183.005      0.061      0.688
2389  c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
2390  h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
2391  c3 c3 c1      109.500      110.330      260.419      -0.014      0.055

```



```

2392 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
2393 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
2394 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
2395
2396 T O R S I O N A L
2397
2398 -----ATOM TYPES----- FORCE TORSION
2399 I J K L CONSTANT s ANGLE n ENERGY
2400 -----
2401 h1 c3 c3 h1 0.651 0 40.000 3 0.326
2402 h1 c3 c3 c1 0.000 0 -80.000 3 0.000
2403 h1 c3 c3 h1 0.651 0 160.000 3 0.326
2404 h1 c3 c3 h1 0.651 0 160.000 3 0.326
2405 h1 c3 c3 c1 0.000 0 40.000 3 0.000
2406 h1 c3 c3 h1 0.651 0 -80.000 3 0.326
2407 c1 c3 c3 h1 0.000 0 -80.000 3 0.000
2408 c1 c3 c3 c1 0.000 0 160.000 3 0.000
2409 c1 c3 c3 h1 0.000 0 40.000 3 0.000
2410 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
2411
2412 I M P R O P E R T O R S I O N A L
2413
2414 -----ATOM TYPES----- FORCE IMPROPER_TORSION
2415 I J K L CONSTANT s ANGLE n ENERGY
2416 -----
2417 TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2418
2419 V A N D E R W A A L S
2420
2421 ATOM TYPES
2422 I J Rij kij ENERGY
2423 -----
2424 h1 h1 2.885 -0.031
2425 h1 h1 2.300 0.109
2426 h1 c1 2.960 0.012
2427 h1 h1 2.518 -0.013
2428 h1 h1 2.885 -0.031
2429 h1 c1 2.647 1.083
2430 c1 h1 2.647 1.083
2431 c1 h1 2.960 0.012
2432 c1 c1 4.082 -0.522
2433 TOTAL VAN DER WAALS ENERGY = 1.704 kJ/mol
2434
2435 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
2436
2437 ATOM TYPES
2438 I J Rij 332.17*QiQj ENERGY
2439 -----
2440 h1 h1 2.885 1.352 0.469

```

```
2441 h1 h1      2.300      1.352      0.588
2442 h1 c1      2.960     -3.809     -1.287
2443 h1 h1      2.518      1.352      0.537
2444 h1 h1      2.885      1.352      0.469
2445 h1 c1      2.647     -3.809     -1.439
2446 c1 h1      2.647     -3.809     -1.439
2447 c1 h1      2.960     -3.809     -1.287
2448 c1 c1      4.082     10.728      2.628
2449      TOTAL ELECTROSTATIC ENERGY =    -0.761 kJ/mol
2450
2451      TOTAL ENERGY =    85.306 kJ/mol
2452
2453 A T O M      T Y P E S
2454
2455 I D X   T Y P E   R I N G
2456 1 1 NO
2457 2 1 NO
2458 3 5 NO
2459 4 5 NO
2460 5 12 NO
2461 6 5 NO
2462 7 5 NO
2463 8 12 NO
2464
2465 F O R M A L      C H A R G E S
2466
2467 I D X   C H A R G E
2468 1 0.000000
2469 2 0.000000
2470 3 0.000000
2471 4 0.000000
2472 5 0.000000
2473 6 0.000000
2474 7 0.000000
2475 8 0.000000
2476
2477 P A R T I A L      C H A R G E S
2478
2479 I D X   C H A R G E
2480 1 0.290000
2481 2 0.290000
2482 3 0.000000
2483 4 0.000000
2484 5 -0.290000
2485 6 0.000000
2486 7 0.000000
2487 8 -0.290000
2488
2489 S E T T I N G      U P      C A L C U L A T I O N S
```

```

2490
2491 SETTING UP BOND CALCULATIONS...
2492 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
2493 SETTING UP TORSION CALCULATIONS...
2494 SETTING UP OOP CALCULATIONS...
2495 SETTING UP VAN DER WAALS CALCULATIONS...
2496 SETTING UP ELECTROSTATIC CALCULATIONS...
2497
2498 A T O M   T Y P E S
2499
2500 IDX TYPE  RING
2501 1 c3  NO
2502 2 c3  NO
2503 3 h1  NO
2504 4 h1  NO
2505 5 c1  NO
2506 6 h1  NO
2507 7 h1  NO
2508 8 c1  NO
2509
2510 C H A R G E S
2511
2512 IDX CHARGE
2513 1 0.036009
2514 2 0.036009
2515 3 0.044101
2516 4 0.044101
2517 5 -0.124211
2518 6 0.044101
2519 7 0.044101
2520 8 -0.124211
2521
2522 S E T T I N G   U P   C A L C U L A T I O N S
2523
2524 SETTING UP BOND CALCULATIONS...
2525 SETTING UP ANGLE CALCULATIONS...
2526 SETTING UP TORSION CALCULATIONS...
2527 SETTING UP IMPROPER TORSION CALCULATIONS...
2528 SETTING UP VAN DER WAALS CALCULATIONS...
2529 SETTING UP ELECTROSTATIC CALCULATIONS...
2530
2531 E N E R G Y
2532
2533
2534 B O N D   S T R E T C H I N G
2535
2536 ATOM TYPES  FF  BOND  IDEAL  FORCE
2537 I    J    CLASS LENGTH  LENGTH  CONSTANT  DELTA  ENERGY
2538 -----

```

2539	5	1	0	1.000	1.093	4.766	-0.093	3.578	
2540	12	1	0	1.670	1.773	2.974	-0.103	2.795	
2541	5	1	0	1.000	1.093	4.766	-0.093	3.578	
2542	1	1	0	1.540	1.508	4.258	0.032	0.294	
2543	1	5	0	1.000	1.093	4.766	-0.093	3.578	
2544	1	12	0	1.670	1.773	2.974	-0.103	2.795	
2545	1	5	0	1.000	1.093	4.766	-0.093	3.578	
2546	TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol								
2547									
2548	A N G L E B E N D I N G								
2549									
2550	ATOM TYPES			FF	VALENCE	IDEAL	FORCE		
2551	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
2552	-----								
2553	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2554	5	1	5	0	109.442	108.836	0.516	0.606	0.004
2555	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2556	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2557	1	1	12	0	109.500	108.679	1.056	0.821	0.016
2558	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2559	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2560	1	1	12	0	109.500	108.679	1.056	0.821	0.016
2561	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2562	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2563	5	1	5	0	109.442	108.836	0.516	0.606	0.004
2564	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2565	TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol								
2566									
2567	S T R E T C H B E N D I N G								
2568									
2569	ATOM TYPES			FF	VALENCE	DELTA	FORCE CONSTANT		
2570	I	J	K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY
2571	-----								
2572	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2573	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
2574	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2575	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2576	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
2577	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2578	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2579	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
2580	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2581	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2582	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
2583	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2584	TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol								
2585									
2586	T O R S I O N A L								
2587									

```

2588 ATOM TYPES          FF      TORSION      FORCE CONSTANT
2589   I    J    K    L      CLASS    ANGLE          V1    V2    V3      ENERGY
2590 -----
2591   5    1    1   12        0   -60.000    0.678   -0.602    0.398    0.057
2592   5    1    1    5        0    60.000    0.284   -1.386    0.314   -0.827
2593   5    1    1    5        0  -180.000    0.284   -1.386    0.314    0.000
2594   5    1    1   12        0    60.000    0.678   -0.602    0.398    0.057
2595   5    1    1    5        0  -180.000    0.284   -1.386    0.314    0.000
2596   5    1    1    5        0   -60.000    0.284   -1.386    0.314   -0.826
2597  12    1    1   12        0   180.000    0.000    0.000    0.893    0.000
2598  12    1    1    5        0   -60.000    0.678   -0.602    0.398    0.057
2599  12    1    1    5        0    60.000    0.678   -0.602    0.398    0.057
2600      TOTAL TORSIONAL ENERGY = -1.42500 kcal/mol
2601
2602 O U T - O F - P L A N E   B E N D I N G
2603
2604 ATOM TYPES          FF      OOP      FORCE
2605   I    J    K    L      CLASS    ANGLE    CONSTANT      ENERGY
2606 -----
2607      TOTAL OUT-OF-PLANE BENDING ENERGY =  0.00000 kcal/mol
2608
2609 V A N   D E R   W A A L S
2610
2611 ATOM TYPES
2612   I    J          Rij          R*IJ      EPSILON      ENERGY
2613 -----
2614   5    5          2.903    2.970      0.022    -0.021
2615   5    5          2.400    2.970      0.022     0.107
2616   5   12          2.792    3.713      0.053     0.792
2617   5    5          2.400    2.970      0.022     0.107
2618   5    5          2.903    2.970      0.022    -0.021
2619   5   12          2.792    3.713      0.053     0.792
2620  12    5          2.792    3.713      0.053     0.792
2621  12    5          2.792    3.713      0.053     0.792
2622  12   12          4.118    4.089      0.276    -0.275
2623      TOTAL VAN DER WAALS ENERGY =  3.06216 kcal/mol
2624
2625 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
2626
2627 ATOM TYPES
2628   I    J          Rij          Qi          Qj          ENERGY
2629 -----
2630  12   12          4.168    -0.290    -0.290      5.025
2631      TOTAL ELECTROSTATIC ENERGY =  5.02482 kcal/mol
2632
2633 TOTAL ENERGY = 26.36292 kcal/mol
2634
2635 E N E R G Y
2636

```

2637

2638 B O N D S T R E T C H I N G

2639

ATOM	TYPES	BOND	IDEAL	FORCE		
I	J	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY

2642

h1	c3	1.000	1.093	1406.346	-0.093	12.163
----	----	-------	-------	----------	--------	--------

c1	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	c1	1.670	1.786	1168.117	-0.116	15.718
----	----	-------	-------	----------	--------	--------

c3	h1	1.000	1.093	1406.346	-0.093	12.163
----	----	-------	-------	----------	--------	--------

2650 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

2651

2652 A N G L E B E N D I N G

2653

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

2656

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	c1	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	c1	109.500	110.330	260.419	-0.014	0.055
----	----	----	---------	---------	---------	--------	-------

h1	c3	c1	109.442	105.930	183.005	0.061	0.688
----	----	----	---------	---------	---------	-------	-------

h1	c3	c1	109.442	105.930	183.005	0.061	0.688
----	----	----	---------	---------	---------	-------	-------

c3	c3	c1	109.500	110.330	260.419	-0.014	0.055
----	----	----	---------	---------	---------	--------	-------

h1	c3	c1	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
----	----	----	---------	---------	---------	--------	-------

2669 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

2670

2671 T O R S I O N A L

2672

ATOM	TYPES	FORCE	TORSION		
I	J	K	L	CONSTANT	s

2675

h1	c3	c3	c1	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	c1	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
----	----	----	----	-------	---	---------	---	-------

c1	c3	c3	c1	0.000	0	180.000	3	0.000
----	----	----	----	-------	---	---------	---	-------

c1	c3	c3	h1	0.000	0	-60.000	3	0.000
----	----	----	----	-------	---	---------	---	-------

c1	c3	c3	h1	0.000	0	60.000	3	0.000
----	----	----	----	-------	---	--------	---	-------

2685 TOTAL TORSIONAL ENERGY = 0.000 kJ/mol

```

2686
2687 I M P R O P E R   T O R S I O N A L
2688
2689 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
2690 I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
2691 -----
2692          TOTAL IMPROPER-TORSIONAL ENERGY =          0.000 kJ/mol
2693
2694 V A N   D E R   W A A L S
2695
2696 ATOM TYPES
2697 I      J      Rij      kij      ENERGY
2698 -----
2699 h1 h1      2.903      -0.031
2700 h1 h1      2.400      0.030
2701 h1 c1      2.792      0.356
2702 h1 h1      2.400      0.030
2703 h1 h1      2.903      -0.031
2704 h1 c1      2.792      0.356
2705 c1 h1      2.792      0.356
2706 c1 h1      2.792      0.356
2707 c1 c1      4.118      -0.510
2708          TOTAL VAN DER WAALS ENERGY =          0.910 kJ/mol
2709
2710 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
2711
2712 ATOM TYPES
2713 I      J      Rij      332.17*QiQj      ENERGY
2714 -----
2715 h1 h1      2.903      1.352      0.466
2716 h1 h1      2.400      1.352      0.563
2717 h1 c1      2.792      -3.809      -1.364
2718 h1 h1      2.400      1.352      0.563
2719 h1 h1      2.903      1.352      0.466
2720 h1 c1      2.792      -3.809      -1.364
2721 c1 h1      2.792      -3.809      -1.364
2722 c1 h1      2.792      -3.809      -1.364
2723 c1 c1      4.118      10.728      2.605
2724          TOTAL ELECTROSTATIC ENERGY =      -0.794 kJ/mol
2725
2726 TOTAL ENERGY =      83.176 kJ/mol
2727
2728 A T O M   T Y P E S
2729
2730 IDX TYPE   RING
2731 1 1 NO
2732 2 1 NO
2733 3 5 NO
2734 4 5 NO

```

```
2735 5 12 NO
2736 6 5 NO
2737 7 5 NO
2738 8 12 NO
2739
2740 F O R M A L C H A R G E S
2741
2742 IDX CHARGE
2743 1 0.000000
2744 2 0.000000
2745 3 0.000000
2746 4 0.000000
2747 5 0.000000
2748 6 0.000000
2749 7 0.000000
2750 8 0.000000
2751
2752 P A R T I A L C H A R G E S
2753
2754 IDX CHARGE
2755 1 0.290000
2756 2 0.290000
2757 3 0.000000
2758 4 0.000000
2759 5 -0.290000
2760 6 0.000000
2761 7 0.000000
2762 8 -0.290000
2763
2764 S E T T I N G U P C A L C U L A T I O N S
2765
2766 SETTING UP BOND CALCULATIONS...
2767 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
2768 SETTING UP TORSION CALCULATIONS...
2769 SETTING UP OOP CALCULATIONS...
2770 SETTING UP VAN DER WAALS CALCULATIONS...
2771 SETTING UP ELECTROSTATIC CALCULATIONS...
2772
2773 A T O M T Y P E S
2774
2775 IDX TYPE RING
2776 1 c3 NO
2777 2 c3 NO
2778 3 h1 NO
2779 4 h1 NO
2780 5 c1 NO
2781 6 h1 NO
2782 7 h1 NO
2783 8 c1 NO
```


2784

2785 C H A R G E S

2786

2787 IDX CHARGE

2788 1 0.036009

2789 2 0.036009

2790 3 0.044101

2791 4 0.044101

2792 5 -0.124211

2793 6 0.044101

2794 7 0.044101

2795 8 -0.124211

2796

2797 S E T T I N G U P C A L C U L A T I O N S

2798

2799 SETTING UP BOND CALCULATIONS...

2800 SETTING UP ANGLE CALCULATIONS...

2801 SETTING UP TORSION CALCULATIONS...

2802 SETTING UP IMPROPER TORSION CALCULATIONS...

2803 SETTING UP VAN DER WAALS CALCULATIONS...

2804 SETTING UP ELECTROSTATIC CALCULATIONS...

2805

2806 E N E R G Y

2807

2808

2809 B O N D S T R E T C H I N G

2810

ATOM TYPES		FF	BOND	IDEAL	FORCE			
I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY	

2813 -----

2814 12 1 0 1.670 1.773 2.974 -0.103 2.795

2815 5 1 0 1.000 1.093 4.766 -0.093 3.578

2816 5 1 0 1.000 1.093 4.766 -0.093 3.578

2817 1 1 0 1.540 1.508 4.258 0.032 0.294

2818 1 5 0 1.000 1.093 4.766 -0.093 3.578

2819 1 12 0 1.670 1.773 2.974 -0.103 2.795

2820 1 5 0 1.000 1.093 4.766 -0.093 3.578

2821 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

2822

2823 A N G L E B E N D I N G

2824

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

2827 -----

2828 1 1 5 0 109.500 110.549 0.636 -1.049 0.015

2829 5 1 5 0 109.442 108.836 0.516 0.606 0.004

2830 5 1 12 0 109.442 108.162 0.698 1.280 0.025

2831 1 1 5 0 109.500 110.549 0.636 -1.049 0.015

2832 1 1 12 0 109.500 108.679 1.056 0.821 0.016

2833	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2834	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2835	1	1	12	0	109.500	108.679	1.056	0.821	0.016
2836	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2837	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2838	5	1	5	0	109.442	108.836	0.516	0.606	0.004
2839	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

2882 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol

2883

2884 V A N D E R W A A L S

2885

2886 ATOM TYPES

I	J	R _{ij}	R*IJ	EPSILON	ENERGY
---	---	-----------------	------	---------	--------

2888 -----

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
----	----	-------	-------	-------	--------

2898 TOTAL VAN DER WAALS ENERGY = 3.63663 kcal/mol

2899

2900 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

2901

2902 ATOM TYPES

I	J	R _{ij}	Q _i	Q _j	ENERGY
---	---	-----------------	----------------	----------------	--------

2904 -----

12	12	4.132	-0.290	-0.290	5.069
----	----	-------	--------	--------	-------

2906 TOTAL ELECTROSTATIC ENERGY = 5.06915 kcal/mol

2907

2908 TOTAL ENERGY = 27.86335 kcal/mol

2909

2910 E N E R G Y

2911

2912

2913 B O N D S T R E T C H I N G

2914

ATOM TYPES	BOND	IDEAL	FORCE
------------	------	-------	-------

I	J	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
---	---	--------	--------	----------	-------	--------

2917 -----

c1	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	c1	1.670	1.786	1168.117	-0.116	15.718
----	----	-------	-------	----------	--------	--------

c3	h1	1.000	1.093	1406.346	-0.093	12.163
----	----	-------	-------	----------	--------	--------

2925 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

2926

2927 A N G L E B E N D I N G

2928

ATOM TYPES	VALENCE	IDEAL	FORCE
------------	---------	-------	-------

I	J	K	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
---	---	---	-------	-------	----------	-------	--------

```

2931 -----
2932 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
2933 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001
2934 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
2935 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
2936 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055
2937 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
2938 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
2939 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055
2940 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
2941 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
2942 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001
2943 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
2944 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
2945
2946 T O R S I O N A L
2947
2948 ----ATOM TYPES----- FORCE TORSION
2949 I J K L CONSTANT s ANGLE n ENERGY
2950 -----
2951 h1 c3 c3 c1 0.000 0 -40.000 3 0.000
2952 h1 c3 c3 h1 0.651 0 80.000 3 0.326
2953 h1 c3 c3 h1 0.651 0 -160.000 3 0.326
2954 h1 c3 c3 c1 0.000 0 80.000 3 0.000
2955 h1 c3 c3 h1 0.651 0 -160.000 3 0.326
2956 h1 c3 c3 h1 0.651 0 -40.000 3 0.326
2957 c1 c3 c3 c1 0.000 0 -160.000 3 0.000
2958 c1 c3 c3 h1 0.000 0 -40.000 3 0.000
2959 c1 c3 c3 h1 0.000 0 80.000 3 0.000
2960 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
2961
2962 I M P R O P E R T O R S I O N A L
2963
2964 ----ATOM TYPES----- FORCE IMPROPER_TORSION
2965 I J K L CONSTANT s ANGLE n ENERGY
2966 -----
2967 TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2968
2969 V A N D E R W A A L S
2970
2971 ATOM TYPES
2972 I J Rij kij ENERGY
2973 -----
2974 h1 h1 2.885 -0.031
2975 h1 h1 2.518 -0.013
2976 h1 c1 2.647 1.083
2977 h1 h1 2.300 0.109
2978 h1 h1 2.885 -0.031
2979 h1 c1 2.960 0.012

```

```

2980  cl h1      2.960      0.012
2981  cl h1      2.647      1.083
2982  cl cl      4.082     -0.522
2983      TOTAL VAN DER WAALS ENERGY =      1.704 kJ/mol
2984
2985  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
2986
2987  ATOM TYPES
2988      I      J           Rij    332.17*QiQj  ENERGY
2989  -----
2990  h1 h1      2.885      1.352      0.469
2991  h1 h1      2.518      1.352      0.537
2992  h1 cl      2.647     -3.809     -1.439
2993  h1 h1      2.300      1.352      0.588
2994  h1 h1      2.885      1.352      0.469
2995  h1 cl      2.960     -3.809     -1.287
2996  cl h1      2.960     -3.809     -1.287
2997  cl h1      2.647     -3.809     -1.439
2998  cl cl      4.082     10.728      2.628
2999      TOTAL ELECTROSTATIC ENERGY =     -0.761 kJ/mol
3000
3001  TOTAL ENERGY =      85.306 kJ/mol
3002
3003  A T O M   T Y P E S
3004
3005  IDX TYPE  RING
3006  1 1 NO
3007  2 1 NO
3008  3 5 NO
3009  4 5 NO
3010  5 12 NO
3011  6 5 NO
3012  7 5 NO
3013  8 12 NO
3014
3015  F O R M A L   C H A R G E S
3016
3017  IDX CHARGE
3018  1 0.000000
3019  2 0.000000
3020  3 0.000000
3021  4 0.000000
3022  5 0.000000
3023  6 0.000000
3024  7 0.000000
3025  8 0.000000
3026
3027  P A R T I A L   C H A R G E S
3028

```

```
3029  IDX CHARGE
3030  1  0.290000
3031  2  0.290000
3032  3  0.000000
3033  4  0.000000
3034  5 -0.290000
3035  6  0.000000
3036  7  0.000000
3037  8 -0.290000
3038
3039  S E T T I N G   U P   C A L C U L A T I O N S
3040
3041  SETTING UP BOND CALCULATIONS...
3042  SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
3043  SETTING UP TORSION CALCULATIONS...
3044  SETTING UP OOP CALCULATIONS...
3045  SETTING UP VAN DER WAALS CALCULATIONS...
3046  SETTING UP ELECTROSTATIC CALCULATIONS...
3047
3048  A T O M   T Y P E S
3049
3050  IDX TYPE  RING
3051  1  c3   NO
3052  2  c3   NO
3053  3  h1   NO
3054  4  h1   NO
3055  5  c1   NO
3056  6  h1   NO
3057  7  h1   NO
3058  8  c1   NO
3059
3060  C H A R G E S
3061
3062  IDX CHARGE
3063  1  0.036009
3064  2  0.036009
3065  3  0.044101
3066  4  0.044101
3067  5 -0.124211
3068  6  0.044101
3069  7  0.044101
3070  8 -0.124211
3071
3072  S E T T I N G   U P   C A L C U L A T I O N S
3073
3074  SETTING UP BOND CALCULATIONS...
3075  SETTING UP ANGLE CALCULATIONS...
3076  SETTING UP TORSION CALCULATIONS...
3077  SETTING UP IMPROPER TORSION CALCULATIONS...
```

3078 SETTING UP VAN DER WAALS CALCULATIONS...

3079 SETTING UP ELECTROSTATIC CALCULATIONS...

3080

3081 E N E R G Y

3082

3083

3084 B O N D S T R E T C H I N G

3085

ATOM TYPES		FF	BOND	IDEAL	FORCE			
I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY	

3088

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	
---	----	---	-------	-------	-------	--------	-------	--

3096 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

3097

3098 A N G L E B E N D I N G

3099

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

3102

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	
---	---	---	---	---------	---------	-------	-------	-------	--

3115 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

3116

3117 S T R E T C H B E N D I N G

3118

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

3121

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	
---	---	----	---	---------	-------	-------	-------	--------	--

3127	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
3128	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
3129	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
3130	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
3131	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
3132	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
3133	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	
3138	-----									
3139										
3140										
3141	12	1	1	5	0	-20.000	0.678	-0.602	0.398	0.886
3142	12	1	1	5	0	100.000	0.678	-0.602	0.398	-0.005
3143	12	1	1	12	0	-140.000	0.000	0.000	0.893	0.670
3144	5	1	1	5	0	100.000	0.284	-1.386	0.314	-0.991
3145	5	1	1	5	0	-140.000	0.284	-1.386	0.314	-0.304
3146	5	1	1	12	0	-20.000	0.678	-0.602	0.398	0.886
3147	5	1	1	5	0	-140.000	0.284	-1.386	0.314	-0.304
3148	5	1	1	5	0	-20.000	0.284	-1.386	0.314	0.349
3149	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		
3161								
3162								
3163								
3164	5	5	2.831	2.970	0.022	-0.019		
3165	5	5	2.638	2.970	0.022	0.001		
3166	5	12	2.547	3.713	0.053	2.298		
3167	5	5	2.232	2.970	0.022	0.328		
3168	5	5	2.831	2.970	0.022	-0.019		
3169	5	12	3.129	3.713	0.053	0.104		
3170	12	5	3.129	3.713	0.053	0.104		
3171	12	5	2.547	3.713	0.053	2.298		
3172	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


```

3176
3177 ATOM TYPES
3178   I      J      Rij      Qi      Qj      ENERGY
3179 -----
3180  12     12      4.025    -0.290   -0.290    5.204
3181      TOTAL ELECTROSTATIC ENERGY =  5.20367 kcal/mol
3182
3183 TOTAL ENERGY = 30.90959 kcal/mol
3184
3185 E N E R G Y
3186
3187
3188 B O N D   S T R E T C H I N G
3189
3190 ATOM TYPES  BOND      IDEAL      FORCE
3191   I      J  LENGTH    LENGTH    CONSTANT      DELTA      ENERGY
3192 -----
3193 c1 c3      1.670      1.786      1168.117      -0.116      15.718
3194 h1 c3      1.000      1.093      1406.346      -0.093      12.163
3195 c3 c3      1.540      1.535      1269.019       0.005       0.032
3196 c3 h1      1.000      1.093      1406.346      -0.093      12.163
3197 c3 h1      1.000      1.093      1406.346      -0.093      12.163
3198 c3 h1      1.000      1.093      1406.346      -0.093      12.163
3199 c3 c1      1.670      1.786      1168.117      -0.116      15.718
3200      TOTAL BOND STRETCHING ENERGY =  80.122 kJ/mol
3201
3202 A N G L E   B E N D I N G
3203
3204 ATOM TYPES      VALENCE      IDEAL      FORCE
3205   I      J  K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
3206 -----
3207 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3208 h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
3209 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3210 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3211 c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
3212 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3213 c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
3214 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3215 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3216 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3217 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3218 h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
3219      TOTAL ANGLE BENDING ENERGY =  2.938 kJ/mol
3220
3221 T O R S I O N A L
3222
3223 ----ATOM TYPES-----      FORCE      TORSION
3224   I      J      K      L  CONSTANT      s      ANGLE      n      ENERGY

```

```

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

```

```
3274      TOTAL ELECTROSTATIC ENERGY =    -0.652 kJ/mol
3275
3276      TOTAL ENERGY =      89.796 kJ/mol
3277
3278      A T O M      T Y P E S
3279
3280      IDX TYPE    RING
3281      1 1 NO
3282      2 1 NO
3283      3 5 NO
3284      4 5 NO
3285      5 12  NO
3286      6 5 NO
3287      7 5 NO
3288      8 12  NO
3289
3290      F O R M A L      C H A R G E S
3291
3292      IDX CHARGE
3293      1 0.290000
3294      2 0.290000
3295      3 0.000000
3296      4 0.000000
3297      5 -0.290000
3298      6 0.000000
3299      7 0.000000
3300      8 -0.290000
3301
3302      P A R T I A L      C H A R G E S
3303
3304      IDX CHARGE
3305      1 0.290000
3306      2 0.290000
3307      3 0.000000
3308      4 0.000000
3309      5 -0.290000
3310      6 0.000000
3311      7 0.000000
3312      8 -0.290000
3313
3314      A T O M      T Y P E S
3315
3316      IDX TYPE    RING
3317      1 c3  NO
3318      2 c3  NO
3319      3 h1  NO
3320      4 h1  NO
3321      5 c1  NO
3322      6 h1  NO
```

3323 7 h1 NO

3324 8 cl NO

3325

3326 F O R M A L C H A R G E S

3327

3328 I D X C H A R G E

3329 1 0.036009

3330 2 0.036009

3331 3 0.044101

3332 4 0.044101

3333 5 -0.124211

3334 6 0.044101

3335 7 0.044101

3336 8 -0.124211

3337

3338 P A R T I A L C H A R G E S

3339

3340 I D X C H A R G E

3341 1 0.036009

3342 2 0.036009

3343 3 0.044101

3344 4 0.044101

3345 5 -0.124211

3346 6 0.044101

3347 7 0.044101

3348 8 -0.124211

3349

3350 E N E R G Y

3351

3352

3353 B O N D S T R E T C H I N G

3354

3355	ATOM	TYPES	FF	BOND	IDEAL	FORCE		
3356	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY

3357 -----

3358	12	1	0	1.670	1.773	2.974	-0.103	2.795
------	----	---	---	-------	-------	-------	--------	-------

3359	5	1	0	1.000	1.093	4.766	-0.093	3.578
------	---	---	---	-------	-------	-------	--------	-------

3360	1	1	0	1.540	1.508	4.258	0.032	0.294
------	---	---	---	-------	-------	-------	-------	-------

3361	1	5	0	1.000	1.093	4.766	-0.093	3.578
------	---	---	---	-------	-------	-------	--------	-------

3362	1	5	0	1.000	1.093	4.766	-0.093	3.578
------	---	---	---	-------	-------	-------	--------	-------

3363	1	5	0	1.000	1.093	4.766	-0.093	3.578
------	---	---	---	-------	-------	-------	--------	-------

3364	1	12	0	1.670	1.773	2.974	-0.103	2.795
------	---	----	---	-------	-------	-------	--------	-------

3365 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

3366

3367 A N G L E B E N D I N G

3368

3369	ATOM	TYPES	FF	VALENCE	IDEAL	FORCE			
3370	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY

3371 -----

3372	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3373	5	1	5	0	109.442	108.836	0.516	0.606	0.004
3374	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3375	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3376	1	1	12	0	109.500	108.679	1.056	0.821	0.016
3377	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3378	1	1	12	0	109.500	108.679	1.056	0.821	0.016
3379	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3380	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3381	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3382	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3383	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

```

3421 O U T - O F - P L A N E   B E N D I N G
3422
3423 ATOM TYPES          FF          OOP          FORCE
3424 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 c1 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 c1        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

3474

I J K

ANGLE

ANGLE

CONSTANT

DELTA

ENERGY

3475

3476 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

3477 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

3478 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

3479 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

3480 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

3481 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

3482 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

3483 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

3484 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

3485 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

3486 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

3487 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

3488 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

3489

3490 T O R S I O N A L

3491

3492 ----ATOM TYPES-----

FORCE

TORSION

3493

I J K L

CONSTANT

s

ANGLE

n

ENERGY

3494

3495 c1 c3 c3 h1 0.000 0 0.000 3 0.000

3496 c1 c3 c3 h1 0.000 0 120.000 3 0.000

3497 c1 c3 c3 c1 0.000 0 -120.000 3 0.000

3498 h1 c3 c3 h1 0.651 0 120.000 3 1.303

3499 h1 c3 c3 h1 0.651 0 -120.000 3 1.303

3500 h1 c3 c3 c1 0.000 0 -0.000 3 0.000

3501 h1 c3 c3 h1 0.651 0 -120.000 3 1.303

3502 h1 c3 c3 h1 0.651 0 0.000 3 1.303

3503 h1 c3 c3 c1 0.000 0 120.000 3 0.000

3504 TOTAL TORSIONAL ENERGY = 5.210 kJ/mol

3505

3506 I M P R O P E R T O R S I O N A L

3507

3508 ----ATOM TYPES-----

FORCE

IMPROPER_TORSION

3509

I J K L

CONSTANT

s

ANGLE

n

ENERGY

3510

3511 TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol

3512

3513 V A N D E R W A A L S

3514

3515 ATOM TYPES

3516

I J

Rij

kij

ENERGY

3517

3518 h1 h1 2.746 -0.033

```

3519 h1 h1      2.746    -0.033
3520 h1 c1      2.512      2.571
3521 h1 h1      2.208      0.251
3522 h1 h1      2.746    -0.033
3523 h1 c1      3.280    -0.134
3524 c1 h1      3.280    -0.134
3525 c1 h1      2.512      2.571
3526 c1 c1      3.806    -0.542
3527      TOTAL VAN DER WAALS ENERGY =      4.485 kJ/mol
3528
3529 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
3530
3531 ATOM TYPES
3532   I      J          Rij    332.17*QiQj  ENERGY
3533 -----
3534 h1 h1      2.746      1.352      0.493
3535 h1 h1      2.746      1.352      0.493
3536 h1 c1      2.512     -3.809     -1.516
3537 h1 h1      2.208      1.352      0.613
3538 h1 h1      2.746      1.352      0.493
3539 h1 c1      3.280     -3.809     -1.161
3540 c1 h1      3.280     -3.809     -1.161
3541 c1 h1      2.512     -3.809     -1.516
3542 c1 c1      3.806     10.728      2.819
3543      TOTAL ELECTROSTATIC ENERGY =     -0.446 kJ/mol
3544
3545 TOTAL ENERGY =      92.310 kJ/mol
3546
3547 A T O M   T Y P E S
3548
3549 IDX TYPE  RING
3550 1 1 NO
3551 2 1 NO
3552 3 5 NO
3553 4 5 NO
3554 5 12  NO
3555 6 5 NO
3556 7 5 NO
3557 8 12  NO
3558
3559 F O R M A L   C H A R G E S
3560
3561 IDX CHARGE
3562 1 0.290000
3563 2 0.290000
3564 3 0.000000
3565 4 0.000000
3566 5 -0.290000
3567 6 0.000000

```



```
3568 7 0.000000
3569 8 -0.290000
3570
3571 P A R T I A L   C H A R G E S
3572
3573 IDX CHARGE
3574 1 0.290000
3575 2 0.290000
3576 3 0.000000
3577 4 0.000000
3578 5 -0.290000
3579 6 0.000000
3580 7 0.000000
3581 8 -0.290000
3582
3583 A T O M   T Y P E S
3584
3585 IDX TYPE  RING
3586 1 c3  NO
3587 2 c3  NO
3588 3 h1  NO
3589 4 h1  NO
3590 5 c1  NO
3591 6 h1  NO
3592 7 h1  NO
3593 8 c1  NO
3594
3595 F O R M A L   C H A R G E S
3596
3597 IDX CHARGE
3598 1 0.036009
3599 2 0.036009
3600 3 0.044101
3601 4 0.044101
3602 5 -0.124211
3603 6 0.044101
3604 7 0.044101
3605 8 -0.124211
3606
3607 P A R T I A L   C H A R G E S
3608
3609 IDX CHARGE
3610 1 0.036009
3611 2 0.036009
3612 3 0.044101
3613 4 0.044101
3614 5 -0.124211
3615 6 0.044101
3616 7 0.044101
```

3617 8 -0.124211

3618

3619 E N E R G Y

3620

3621

3622 B O N D S T R E T C H I N G

3623

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
---	----	---	-------	-------	-------	--------	-------

3634 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

3635

3636 A N G L E B E N D I N G

3637

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
---	---	---	---	---------	---------	-------	-------	-------

3653 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

3654

3655 S T R E T C H B E N D I N G

3656

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
---	---	----	---	---------	-------	--------	-------	--------

```

3666 1 1 12 0 109.500 0.821 0.176 0.386 -0.070
3667 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
3668 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
3669 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
3670 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
3671 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

```

3676 ATOM TYPES          FF      TORSION      FORCE CONSTANT
3677 I    J    K    L    CLASS    ANGLE      V1    V2    V3    ENERGY
3678 -----
3679 12    1    1    5      0    20.000    0.678   -0.602   0.398    0.886
3680 12    1    1    5      0   140.000    0.678   -0.602   0.398    0.129
3681 12    1    1   12      0  -100.000    0.000    0.000   0.893    0.670
3682  5    1    1    5      0   140.000    0.284   -1.386   0.314   -0.304
3683  5    1    1    5      0  -100.000    0.284   -1.386   0.314   -0.991
3684  5    1    1   12      0    20.000    0.678   -0.602   0.398    0.886
3685  5    1    1    5      0  -100.000    0.284   -1.386   0.314   -0.991
3686  5    1    1    5      0    20.000    0.284   -1.386   0.314    0.349
3687  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

```

3692 ATOM TYPES          FF      OOP      FORCE
3693 I    J    K    L    CLASS    ANGLE    CONSTANT    ENERGY
3694 -----

```

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

V A N D E R W A A L S

```

3699 ATOM TYPES
3700 I    J      Rij      R*IJ      EPSILON      ENERGY
3701 -----
3702  5    5      2.638    2.970    0.022    0.001
3703  5    5      2.831    2.970    0.022   -0.019
3704  5   12      2.547    3.713    0.053    2.298
3705  5    5      2.232    2.970    0.022    0.328
3706  5    5      2.638    2.970    0.022    0.001
3707  5   12      3.399    3.713    0.053   -0.028
3708 12    5      3.399    3.713    0.053   -0.028
3709 12    5      2.547    3.713    0.053    2.298
3710 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

```

3715 ATOM TYPES
3716   I      J      Rij      Qi      Qj      ENERGY
3717 -----
3718 12      12      3.637     -0.290    -0.290      5.759
3719      TOTAL ELECTROSTATIC ENERGY =  5.75922 kcal/mol
3720
3721 TOTAL ENERGY = 31.17064 kcal/mol
3722
3723 E N E R G Y
3724
3725
3726 B O N D   S T R E T C H I N G
3727
3728 ATOM TYPES  BOND      IDEAL      FORCE
3729   I      J      LENGTH  LENGTH    CONSTANT      DELTA      ENERGY
3730 -----
3731 c1 c3      1.670      1.786      1168.117      -0.116      15.718
3732 h1 c3      1.000      1.093      1406.346      -0.093      12.163
3733 c3 c3      1.540      1.535      1269.019       0.005       0.032
3734 c3 h1      1.000      1.093      1406.346      -0.093      12.163
3735 c3 h1      1.000      1.093      1406.346      -0.093      12.163
3736 c3 h1      1.000      1.093      1406.346      -0.093      12.163
3737 c3 c1      1.670      1.786      1168.117      -0.116      15.718
3738      TOTAL BOND STRETCHING ENERGY =  80.122 kJ/mol
3739
3740 A N G L E   B E N D I N G
3741
3742 ATOM TYPES      VALENCE      IDEAL      FORCE
3743   I      J      K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
3744 -----
3745 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3746 h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
3747 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3748 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3749 c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
3750 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3751 c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
3752 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3753 h1 c3 c1      109.442      105.930      183.005       0.061      0.688
3754 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3755 c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
3756 h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
3757      TOTAL ANGLE BENDING ENERGY =  2.938 kJ/mol
3758
3759 T O R S I O N A L
3760
3761 ----ATOM TYPES-----      FORCE      TORSION
3762   I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
3763 -----

```

```

3764 c1 c3 c3 h1      0.000      0      20.000  3      0.000
3765 c1 c3 c3 h1      0.000      0     140.000  3      0.000
3766 c1 c3 c3 c1      0.000      0    -100.000  3      0.000
3767 h1 c3 c3 h1      0.651      0     140.000  3      0.977
3768 h1 c3 c3 h1      0.651      0    -100.000  3      0.977
3769 h1 c3 c3 c1      0.000      0      20.000  3      0.000
3770 h1 c3 c3 h1      0.651      0    -100.000  3      0.977
3771 h1 c3 c3 h1      0.651      0      20.000  3      0.977
3772 h1 c3 c3 c1      0.000      0     140.000  3      0.000
3773      TOTAL TORSIONAL ENERGY =      3.908 kJ/mol
3774
3775 I M P R O P E R   T O R S I O N A L
3776
3777 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
3778   I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
3779 -----
3780      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
3781
3782 V A N   D E R   W A A L S
3783
3784 ATOM TYPES
3785   I      J      Rij      kij      ENERGY
3786 -----
3787 h1 h1      2.638      -0.029
3788 h1 h1      2.831      -0.032
3789 h1 c1      2.547      2.064
3790 h1 h1      2.232      0.205
3791 h1 h1      2.638      -0.029
3792 h1 c1      3.399      -0.133
3793 c1 h1      3.399      -0.133
3794 c1 h1      2.547      2.064
3795 c1 c1      3.587      -0.326
3796      TOTAL VAN DER WAALS ENERGY =      3.650 kJ/mol
3797
3798 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
3799
3800 ATOM TYPES
3801   I      J      Rij      332.17*QiQj      ENERGY
3802 -----
3803 h1 h1      2.638      1.352      0.513
3804 h1 h1      2.831      1.352      0.478
3805 h1 c1      2.547      -3.809      -1.495
3806 h1 h1      2.232      1.352      0.606
3807 h1 h1      2.638      1.352      0.513
3808 h1 c1      3.399      -3.809      -1.121
3809 c1 h1      3.399      -3.809      -1.121
3810 c1 h1      2.547      -3.809      -1.495
3811 c1 c1      3.587      10.728      2.991
3812      TOTAL ELECTROSTATIC ENERGY =      -0.132 kJ/mol

```

```
3813
3814 TOTAL ENERGY = 90.486 kJ/mol
3815
3816 A T O M   T Y P E S
3817
3818 I D X   T Y P E   R I N G
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 I D X   C H A R G E
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 I D X   C H A R G E
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
3866   3  h1    NO
3867   4  h1    NO
3868   5  c1    NO
3869   6  h1    NO
3870   7  h1    NO
3871   8  c1    NO
3872
3873   C H A R G E S
3874
3875   IDX CHARGE
3876   1  0.036009
3877   2  0.036009
3878   3  0.044101
3879   4  0.044101
3880   5 -0.124211
3881   6  0.044101
3882   7  0.044101
3883   8 -0.124211
3884
3885   S E T T I N G   U P   C A L C U L A T I O N S
3886
3887   SETTING UP BOND CALCULATIONS...
3888   SETTING UP ANGLE CALCULATIONS...
3889   SETTING UP TORSION CALCULATIONS...
3890   SETTING UP IMPROPER TORSION CALCULATIONS...
3891   SETTING UP VAN DER WAALS CALCULATIONS...
3892   SETTING UP ELECTROSTATIC CALCULATIONS...
3893
3894   E N E R G Y
3895
3896
3897   B O N D   S T R E T C H I N G
3898
3899   ATOM TYPES      FF      BOND      IDEAL      FORCE
3900   I      J      CLASS  LENGTH      LENGTH      CONSTANT      DELTA      ENERGY
3901   -----
3902   12      1      0      1.670      1.773      2.974      -0.103      2.795
3903   5       1      0      1.000      1.093      4.766      -0.093      3.578
3904   5       1      0      1.000      1.093      4.766      -0.093      3.578
3905   1       1      0      1.540      1.508      4.258      0.032      0.294
3906   1       5      0      1.000      1.093      4.766      -0.093      3.578
3907   1      12      0      1.670      1.773      2.974      -0.103      2.795
3908   1       5      0      1.000      1.093      4.766      -0.093      3.578
3909   TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
3910

```

```

3911 A N G L E   B E N D I N G
3912
3913 ATOM TYPES          FF      VALENCE      IDEAL      FORCE
3914 I      J      K      CLASS      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
3915 -----
3916 1      1      5      0      109.500      110.549      0.636      -1.049      0.015
3917 5      1      5      0      109.442      108.836      0.516      0.606      0.004
3918 5      1      12     0      109.442      108.162      0.698      1.280      0.025
3919 1      1      5      0      109.500      110.549      0.636      -1.049      0.015
3920 1      1      12     0      109.500      108.679      1.056      0.821      0.016
3921 5      1      12     0      109.442      108.162      0.698      1.280      0.025
3922 5      1      12     0      109.442      108.162      0.698      1.280      0.025
3923 1      1      12     0      109.500      108.679      1.056      0.821      0.016
3924 5      1      12     0      109.442      108.162      0.698      1.280      0.025
3925 1      1      5      0      109.500      110.549      0.636      -1.049      0.015
3926 5      1      5      0      109.442      108.836      0.516      0.606      0.004
3927 1      1      5      0      109.500      110.549      0.636      -1.049      0.015
3928      TOTAL ANGLE BENDING ENERGY =  0.20058 kcal/mol
3929
3930 S T R E T C H   B E N D I N G
3931
3932 ATOM TYPES          FF      VALENCE      DELTA      FORCE CONSTANT
3933 I      J      K      CLASS      ANGLE      ANGLE      I  J      J  K      ENERGY
3934 -----
3935 1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
3936 5      1      5      0      109.442      0.606      0.115      0.115      -0.033
3937 5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
3938 1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
3939 1      1      12     0      109.500      0.821      0.176      0.386      -0.070
3940 5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
3941 5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
3942 1      1      12     0      109.500      0.821      0.176      0.386      -0.070
3943 5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
3944 1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
3945 5      1      5      0      109.442      0.606      0.115      0.115      -0.033
3946 1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
3947      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
3948
3949 T O R S I O N A L
3950
3951 ATOM TYPES          FF      TORSION      FORCE CONSTANT
3952 I      J      K      L      CLASS      ANGLE      V1  V2  V3      ENERGY
3953 -----
3954 5      1      1      12     0      40.000      0.678  -0.602  0.398      0.449
3955 5      1      1      5      0      -80.000      0.284  -1.386  0.314     -1.099
3956 5      1      1      5      0      160.000      0.284  -1.386  0.314     -0.075
3957 5      1      1      12     0      160.000      0.678  -0.602  0.398      0.050
3958 5      1      1      5      0      40.000      0.284  -1.386  0.314     -0.243
3959 5      1      1      5      0      -80.000      0.284  -1.386  0.314     -1.099

```



```

3960 12 1 1 12 0 -80.000 0.000 0.000 0.893 0.223
3961 12 1 1 5 0 160.000 0.678 -0.602 0.398 0.050
3962 12 1 1 5 0 40.000 0.678 -0.602 0.398 0.449
3963 TOTAL TORSIONAL ENERGY = -1.29534 kcal/mol
3964
3965 O U T - O F - P L A N E B E N D I N G
3966
3967 ATOM TYPES FF OOP FORCE
3968 I J K L CLASS ANGLE CONSTANT ENERGY
3969 -----
3970 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
3971
3972 V A N D E R W A A L S
3973
3974 ATOM TYPES
3975 I J RiJ R*IJ EPSILON ENERGY
3976 -----
3977 5 5 2.518 2.970 0.022 0.036
3978 5 5 2.885 2.970 0.022 -0.021
3979 5 12 2.647 3.713 0.053 1.520
3980 5 5 2.300 2.970 0.022 0.215
3981 5 5 2.518 2.970 0.022 0.036
3982 5 12 3.474 3.713 0.053 -0.041
3983 12 5 3.474 3.713 0.053 -0.041
3984 12 5 2.647 3.713 0.053 1.520
3985 12 12 3.338 4.089 0.276 1.129
3986 TOTAL VAN DER WAALS ENERGY = 4.35500 kcal/mol
3987
3988 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
3989
3990 ATOM TYPES
3991 I J RiJ Qi Qj ENERGY
3992 -----
3993 12 12 3.388 -0.290 -0.290 6.182
3994 TOTAL ELECTROSTATIC ENERGY = 6.18170 kcal/mol
3995
3996 TOTAL ENERGY = 28.94230 kcal/mol
3997
3998 E N E R G Y
3999
4000
4001 B O N D S T R E T C H I N G
4002
4003 ATOM TYPES BOND IDEAL FORCE
4004 I J LENGTH LENGTH CONSTANT DELTA ENERGY
4005 -----
4006 c1 c3 1.670 1.786 1168.117 -0.116 15.718
4007 h1 c3 1.000 1.093 1406.346 -0.093 12.163
4008 h1 c3 1.000 1.093 1406.346 -0.093 12.163

```

```

4009  c3 c3      1.540      1.535      1269.019      0.005      0.032
4010  c3 h1      1.000      1.093      1406.346      -0.093      12.163
4011  c3 c1      1.670      1.786      1168.117      -0.116      15.718
4012  c3 h1      1.000      1.093      1406.346      -0.093      12.163
4013      TOTAL BOND STRETCHING ENERGY =      80.122 kJ/mol
4014
4015  A N G L E    B E N D I N G
4016
4017  ATOM TYPES      VALENCE      IDEAL      FORCE
4018      I      J      K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
4019  -----
4020  c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
4021  h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
4022  h1 c3 c1      109.442      105.930      183.005      0.061      0.688
4023  c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
4024  c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
4025  h1 c3 c1      109.442      105.930      183.005      0.061      0.688
4026  h1 c3 c1      109.442      105.930      183.005      0.061      0.688
4027  c3 c3 c1      109.500      110.330      260.419      -0.014      0.055
4028  h1 c3 c1      109.442      105.930      183.005      0.061      0.688
4029  c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
4030  h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
4031  c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
4032      TOTAL ANGLE BENDING ENERGY =      2.938 kJ/mol
4033
4034  T O R S I O N A L
4035
4036  ----ATOM TYPES-----      FORCE      TORSION
4037      I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
4038  -----
4039  h1 c3 c3 c1      0.000      0      40.000      3      0.000
4040  h1 c3 c3 h1      0.651      0      -80.000      3      0.326
4041  h1 c3 c3 h1      0.651      0      160.000      3      0.326
4042  h1 c3 c3 c1      0.000      0      160.000      3      0.000
4043  h1 c3 c3 h1      0.651      0      40.000      3      0.326
4044  h1 c3 c3 h1      0.651      0      -80.000      3      0.326
4045  c1 c3 c3 c1      0.000      0      -80.000      3      0.000
4046  c1 c3 c3 h1      0.000      0      160.000      3      0.000
4047  c1 c3 c3 h1      0.000      0      40.000      3      0.000
4048      TOTAL TORSIONAL ENERGY =      1.303 kJ/mol
4049
4050  I M P R O P E R    T O R S I O N A L
4051
4052  ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
4053      I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
4054  -----
4055      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
4056
4057  V A N    D E R    W A A L S

```

```

4058
4059 ATOM TYPES
4060   I      J          Rij      kij      ENERGY
4061 -----
4062 h1 h1      2.518      -0.013
4063 h1 h1      2.885      -0.031
4064 h1 c1      2.647       1.083
4065 h1 h1      2.300       0.109
4066 h1 h1      2.518      -0.013
4067 h1 c1      3.474      -0.129
4068 c1 h1      3.474      -0.129
4069 c1 h1      2.647       1.083
4070 c1 c1      3.338       0.738
4071      TOTAL VAN DER WAALS ENERGY =      2.701 kJ/mol
4072
4073 E L E C T R O S T A T I C   I N T E R A C T I O N S
4074
4075 ATOM TYPES
4076   I      J          Rij      332.17*QiQj  ENERGY
4077 -----
4078 h1 h1      2.518       1.352      0.537
4079 h1 h1      2.885       1.352      0.469
4080 h1 c1      2.647      -3.809     -1.439
4081 h1 h1      2.300       1.352      0.588
4082 h1 h1      2.518       1.352      0.537
4083 h1 c1      3.474      -3.809     -1.097
4084 c1 h1      3.474      -3.809     -1.097
4085 c1 h1      2.647      -3.809     -1.439
4086 c1 c1      3.338     10.728      3.214
4087      TOTAL ELECTROSTATIC ENERGY =      0.273 kJ/mol
4088
4089 TOTAL ENERGY =      87.337 kJ/mol
4090
4091 A T O M   T Y P E S
4092
4093 IDX TYPE  RING
4094 1 1 NO
4095 2 1 NO
4096 3 5 NO
4097 4 5 NO
4098 5 12 NO
4099 6 5 NO
4100 7 5 NO
4101 8 12 NO
4102
4103 F O R M A L   C H A R G E S
4104
4105 IDX CHARGE
4106 1 0.000000

```

```
4107 2 0.000000
4108 3 0.000000
4109 4 0.000000
4110 5 0.000000
4111 6 0.000000
4112 7 0.000000
4113 8 0.000000
4114
4115 P A R T I A L   C H A R G E S
4116
4117 IDX CHARGE
4118 1 0.290000
4119 2 0.290000
4120 3 0.000000
4121 4 0.000000
4122 5 -0.290000
4123 6 0.000000
4124 7 0.000000
4125 8 -0.290000
4126
4127 S E T T I N G   U P   C A L C U L A T I O N S
4128
4129 SETTING UP BOND CALCULATIONS...
4130 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4131 SETTING UP TORSION CALCULATIONS...
4132 SETTING UP OOP CALCULATIONS...
4133 SETTING UP VAN DER WAALS CALCULATIONS...
4134 SETTING UP ELECTROSTATIC CALCULATIONS...
4135
4136 A T O M   T Y P E S
4137
4138 IDX TYPE  RING
4139 1 c3  NO
4140 2 c3  NO
4141 3 h1  NO
4142 4 h1  NO
4143 5 c1  NO
4144 6 h1  NO
4145 7 h1  NO
4146 8 c1  NO
4147
4148 C H A R G E S
4149
4150 IDX CHARGE
4151 1 0.036009
4152 2 0.036009
4153 3 0.044101
4154 4 0.044101
4155 5 -0.124211
```

4156 6 0.044101
4157 7 0.044101
4158 8 -0.124211

4159

4160 S E T T I N G U P C A L C U L A T I O N S

4161

4162 SETTING UP BOND CALCULATIONS...

4163 SETTING UP ANGLE CALCULATIONS...

4164 SETTING UP TORSION CALCULATIONS...

4165 SETTING UP IMPROPER TORSION CALCULATIONS...

4166 SETTING UP VAN DER WAALS CALCULATIONS...

4167 SETTING UP ELECTROSTATIC CALCULATIONS...

4168

4169 E N E R G Y

4170

4171

4172 B O N D S T R E T C H I N G

4173

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	

4184 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

4185

4186 A N G L E B E N D I N G

4187

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	

4203 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

4204

```

4205 S T R E T C H   B E N D I N G
4206
4207 ATOM TYPES          FF      VALENCE      DELTA      FORCE CONSTANT
4208 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
4258     12       5          3.499      3.713      0.053     -0.044
4259     12       5          2.792      3.713      0.053      0.792
4260     12      12          3.087      4.089      0.276      3.947

```

```

4261          TOTAL VAN DER WAALS ENERGY =  5.74158 kcal/mol

```

```

4262

```

```

4263  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

```

```

4264

```

```

4265  ATOM TYPES

```

```

4266      I      J          Rij          Qi          Qj          ENERGY

```

```

4267  -----

```

```

4268     12     12          3.137     -0.290     -0.290          6.678

```

```

4269          TOTAL ELECTROSTATIC ENERGY =  6.67788 kcal/mol

```

```

4270

```

```

4271  TOTAL ENERGY = 29.75490 kcal/mol

```

```

4272

```

```

4273  E N E R G Y

```

```

4274

```

```

4275

```

```

4276  B O N D   S T R E T C H I N G

```

```

4277

```

```

4278  ATOM TYPES  BOND          IDEAL          FORCE

```

```

4279      I      J      LENGTH      LENGTH      CONSTANT      DELTA      ENERGY

```

```

4280  -----

```

```

4281     h1 c3          1.000          1.093      1406.346      -0.093      12.163

```

```

4282     c1 c3          1.670          1.786      1168.117      -0.116      15.718

```

```

4283     h1 c3          1.000          1.093      1406.346      -0.093      12.163

```

```

4284     c3 c3          1.540          1.535      1269.019          0.005          0.032

```

```

4285     c3 h1          1.000          1.093      1406.346      -0.093      12.163

```

```

4286     c3 c1          1.670          1.786      1168.117      -0.116      15.718

```

```

4287     c3 h1          1.000          1.093      1406.346      -0.093      12.163

```

```

4288          TOTAL BOND STRETCHING ENERGY =  80.122 kJ/mol

```

```

4289

```

```

4290  A N G L E   B E N D I N G

```

```

4291

```

```

4292  ATOM TYPES          VALENCE          IDEAL          FORCE

```

```

4293      I      J      K          ANGLE          ANGLE          CONSTANT          DELTA          ENERGY

```

```

4294  -----

```

```

4295     c3 c3 h1      109.500      110.070          194.100      -0.010          0.019

```

```

4296     h1 c3 h1      109.442      109.550          164.039      -0.002          0.001

```

```

4297     h1 c3 c1      109.442      105.930          183.005          0.061          0.688

```

```

4298     c3 c3 h1      109.500      110.070          194.100      -0.010          0.019

```

```

4299     c3 c3 c1      109.500      110.330          260.419      -0.014          0.055

```

```

4300     h1 c3 c1      109.442      105.930          183.005          0.061          0.688

```

```

4301     h1 c3 c1      109.442      105.930          183.005          0.061          0.688

```

```

4302     c3 c3 c1      109.500      110.330          260.419      -0.014          0.055

```

```

4303 h1 c3 c1 109.442 105.930 183.005 0.061 0.688
4304 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
4305 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001
4306 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
4307 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
4308
4309 T O R S I O N A L
4310
4311 ----ATOM TYPES----- FORCE TORSION
4312 I J K L CONSTANT s ANGLE n ENERGY
4313 -----
4314 h1 c3 c3 c1 0.000 0 60.000 3 0.000
4315 h1 c3 c3 h1 0.651 0 -60.000 3 0.000
4316 h1 c3 c3 h1 0.651 0 -180.000 3 0.000
4317 h1 c3 c3 c1 0.000 0 -180.000 3 0.000
4318 h1 c3 c3 h1 0.651 0 60.000 3 0.000
4319 h1 c3 c3 h1 0.651 0 -60.000 3 0.000
4320 c1 c3 c3 c1 0.000 0 -60.000 3 0.000
4321 c1 c3 c3 h1 0.000 0 180.000 3 0.000
4322 c1 c3 c3 h1 0.000 0 60.000 3 0.000
4323 TOTAL TORSIONAL ENERGY = 0.000 kJ/mol
4324
4325 I M P R O P E R T O R S I O N A L
4326
4327 ----ATOM TYPES----- FORCE IMPROPER_TORSION
4328 I J K L CONSTANT s ANGLE n ENERGY
4329 -----
4330 TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
4331
4332 V A N D E R W A A L S
4333
4334 ATOM TYPES
4335 I J Rij kij ENERGY
4336 -----
4337 h1 h1 2.400 0.030
4338 h1 h1 2.903 -0.031
4339 h1 c1 2.792 0.356
4340 h1 h1 2.400 0.030
4341 h1 h1 2.400 0.030
4342 h1 c1 3.499 -0.127
4343 c1 h1 3.499 -0.127
4344 c1 h1 2.792 0.356
4345 c1 c1 3.087 4.588
4346 TOTAL VAN DER WAALS ENERGY = 5.105 kJ/mol
4347
4348 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
4349
4350 ATOM TYPES
4351 I J Rij 332.17*QiQj ENERGY

```



```

4352 -----
4353 h1 h1      2.400      1.352      0.563
4354 h1 h1      2.903      1.352      0.466
4355 h1 c1      2.792     -3.809     -1.364
4356 h1 h1      2.400      1.352      0.563
4357 h1 h1      2.400      1.352      0.563
4358 h1 c1      3.499     -3.809     -1.089
4359 c1 h1      3.499     -3.809     -1.089
4360 c1 h1      2.792     -3.809     -1.364
4361 c1 c1      3.087     10.728      3.476
4362      TOTAL ELECTROSTATIC ENERGY =      0.726 kJ/mol
4363
4364 TOTAL ENERGY =      88.891 kJ/mol
4365
4366 A T O M      T Y P E S
4367
4368 IDX TYPE  RING
4369 1 1 NO
4370 2 1 NO
4371 3 5 NO
4372 4 5 NO
4373 5 12  NO
4374 6 5 NO
4375 7 5 NO
4376 8 12  NO
4377
4378 F O R M A L      C H A R G E S
4379
4380 IDX CHARGE
4381 1 0.000000
4382 2 0.000000
4383 3 0.000000
4384 4 0.000000
4385 5 0.000000
4386 6 0.000000
4387 7 0.000000
4388 8 0.000000
4389
4390 P A R T I A L      C H A R G E S
4391
4392 IDX CHARGE
4393 1 0.290000
4394 2 0.290000
4395 3 0.000000
4396 4 0.000000
4397 5 -0.290000
4398 6 0.000000
4399 7 0.000000
4400 8 -0.290000

```

4401
4402 S E T T I N G U P C A L C U L A T I O N S
4403
4404 SETTING UP BOND CALCULATIONS...
4405 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4406 SETTING UP TORSION CALCULATIONS...
4407 SETTING UP OOP CALCULATIONS...
4408 SETTING UP VAN DER WAALS CALCULATIONS...
4409 SETTING UP ELECTROSTATIC CALCULATIONS...

4410
4411 A T O M T Y P E S
4412

4413 I D X T Y P E R I N G
4414 1 c3 N O
4415 2 c3 N O
4416 3 h1 N O
4417 4 h1 N O
4418 5 c1 N O
4419 6 h1 N O
4420 7 h1 N O
4421 8 c1 N O

4422
4423 C H A R G E S
4424

4425 I D X C H A R G E
4426 1 0.036009
4427 2 0.036009
4428 3 0.044101
4429 4 0.044101
4430 5 -0.124211
4431 6 0.044101
4432 7 0.044101
4433 8 -0.124211

4434
4435 S E T T I N G U P C A L C U L A T I O N S
4436

4437 SETTING UP BOND CALCULATIONS...
4438 SETTING UP ANGLE CALCULATIONS...
4439 SETTING UP TORSION CALCULATIONS...
4440 SETTING UP IMPROPER TORSION CALCULATIONS...
4441 SETTING UP VAN DER WAALS CALCULATIONS...
4442 SETTING UP ELECTROSTATIC CALCULATIONS...

4443
4444 E N E R G Y
4445

4446
4447 B O N D S T R E T C H I N G
4448

4449 A T O M T Y P E S F F B O N D I D E A L F O R C E

```

4450      I      J      CLASS  LENGTH      LENGTH      CONSTANT      DELTA      ENERGY
4451      -----
4452      5      1      0      1.000      1.093      4.766      -0.093      3.578
4453      5      1      0      1.000      1.093      4.766      -0.093      3.578
4454      12     1      0      1.670      1.773      2.974      -0.103      2.795
4455      1      1      0      1.540      1.508      4.258      0.032      0.294
4456      1      5      0      1.000      1.093      4.766      -0.093      3.578
4457      1      12     0      1.670      1.773      2.974      -0.103      2.795
4458      1      5      0      1.000      1.093      4.766      -0.093      3.578
4459      TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
4460
4461      A N G L E      B E N D I N G
4462
4463      ATOM TYPES      FF      VALENCE      IDEAL      FORCE
4464      I      J      K      CLASS      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
4465      -----
4466      1      1      5      0      109.500      110.549      0.636      -1.049      0.015
4467      5      1      5      0      109.442      108.836      0.516      0.606      0.004
4468      5      1      12     0      109.442      108.162      0.698      1.280      0.025
4469      1      1      5      0      109.500      110.549      0.636      -1.049      0.015
4470      1      1      12     0      109.500      108.679      1.056      0.821      0.016
4471      5      1      12     0      109.442      108.162      0.698      1.280      0.025
4472      5      1      12     0      109.442      108.162      0.698      1.280      0.025
4473      1      1      5      0      109.500      110.549      0.636      -1.049      0.015
4474      5      1      5      0      109.442      108.836      0.516      0.606      0.004
4475      1      1      12     0      109.500      108.679      1.056      0.821      0.016
4476      5      1      12     0      109.442      108.162      0.698      1.280      0.025
4477      1      1      5      0      109.500      110.549      0.636      -1.049      0.015
4478      TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
4479
4480      S T R E T C H      B E N D I N G
4481
4482      ATOM TYPES      FF      VALENCE      DELTA      FORCE CONSTANT
4483      I      J      K      CLASS      ANGLE      ANGLE      I J      J K      ENERGY
4484      -----
4485      1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
4486      5      1      5      0      109.442      0.606      0.115      0.115      -0.033
4487      5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
4488      1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
4489      1      1      12     0      109.500      0.821      0.176      0.386      -0.070
4490      5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
4491      5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
4492      1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
4493      5      1      5      0      109.442      0.606      0.115      0.115      -0.033
4494      1      1      12     0      109.500      0.821      0.176      0.386      -0.070
4495      5      1      12     0      109.442      1.280      -0.018      0.380      -0.121
4496      1      1      5      0      109.500      -1.049      0.227      0.070      -0.002
4497      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
4498

```

```

4499 T O R S I O N A L
4500
4501 ATOM TYPES          FF      TORSION      FORCE CONSTANT
4502 I      J      K      L      CLASS      ANGLE      V1      V2      V3      ENERGY
4503 -----
4504 5      1      1      5      0      -40.000      0.284      -1.386      0.314      -0.243
4505 5      1      1      12     0      80.000      0.678      -0.602      0.398      -0.086
4506 5      1      1      5      0     -160.000      0.284      -1.386      0.314      -0.075
4507 5      1      1      5      0      80.000      0.284      -1.386      0.314      -1.099
4508 5      1      1      12     0     -160.000      0.678      -0.602      0.398      0.050
4509 5      1      1      5      0     -40.000      0.284      -1.386      0.314      -0.243
4510 12     1      1      5      0     -160.000      0.678      -0.602      0.398      0.050
4511 12     1      1      12     0     -40.000      0.000      0.000      0.893      0.223
4512 12     1      1      5      0      80.000      0.678      -0.602      0.398      -0.086
4513      TOTAL TORSIONAL ENERGY = -1.51155 kcal/mol
4514
4515 O U T - O F - P L A N E   B E N D I N G
4516
4517 ATOM TYPES          FF      OOP      FORCE
4518 I      J      K      L      CLASS      ANGLE      CONSTANT      ENERGY
4519 -----
4520      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
4521
4522 V A N   D E R   W A A L S
4523
4524 ATOM TYPES
4525 I      J      Rij      R*IJ      EPSILON      ENERGY
4526 -----
4527 5      5      2.300      2.970      0.022      0.215
4528 5      5      2.885      2.970      0.022      -0.021
4529 5     12      2.960      3.713      0.053      0.331
4530 5      5      2.518      2.970      0.022      0.036
4531 5      5      2.300      2.970      0.022      0.215
4532 5     12      3.474      3.713      0.053      -0.041
4533 12     5      3.474      3.713      0.053      -0.041
4534 12     5      2.960      3.713      0.053      0.331
4535 12    12      2.865      4.089      0.276      9.664
4536      TOTAL VAN DER WAALS ENERGY = 10.69051 kcal/mol
4537
4538 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
4539
4540 ATOM TYPES
4541 I      J      Rij      Qi      Qj      ENERGY
4542 -----
4543 12    12      2.915     -0.290     -0.290      7.185
4544      TOTAL ELECTROSTATIC ENERGY = 7.18544 kcal/mol
4545
4546 TOTAL ENERGY = 36.06534 kcal/mol
4547

```

4548 E N E R G Y

4549

4550

4551 B O N D S T R E T C H I N G

4552

4553 ATOM TYPES BOND IDEAL FORCE

4554 I J LENGTH LENGTH CONSTANT DELTA ENERGY

4555

4556 h1 c3 1.000 1.093 1406.346 -0.093 12.163

4557 h1 c3 1.000 1.093 1406.346 -0.093 12.163

4558 c1 c3 1.670 1.786 1168.117 -0.116 15.718

4559 c3 c3 1.540 1.535 1269.019 0.005 0.032

4560 c3 h1 1.000 1.093 1406.346 -0.093 12.163

4561 c3 c1 1.670 1.786 1168.117 -0.116 15.718

4562 c3 h1 1.000 1.093 1406.346 -0.093 12.163

4563 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

4564

4565 A N G L E B E N D I N G

4566

4567 ATOM TYPES VALENCE IDEAL FORCE

4568 I J K ANGLE ANGLE CONSTANT DELTA ENERGY

4569

4570 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

4571 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

4572 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

4573 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

4574 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

4575 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

4576 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

4577 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

4578 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

4579 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

4580 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

4581 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

4582 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

4583

4584 T O R S I O N A L

4585

4586 ----ATOM TYPES----- FORCE TORSION

4587 I J K L CONSTANT s ANGLE n ENERGY

4588

4589 h1 c3 c3 h1 0.651 0 -40.000 3 0.326

4590 h1 c3 c3 c1 0.000 0 80.000 3 0.000

4591 h1 c3 c3 h1 0.651 0 -160.000 3 0.326

4592 h1 c3 c3 h1 0.651 0 80.000 3 0.326

4593 h1 c3 c3 c1 0.000 0 -160.000 3 0.000

4594 h1 c3 c3 h1 0.651 0 -40.000 3 0.326

4595 c1 c3 c3 h1 0.000 0 -160.000 3 0.000

4596 c1 c3 c3 c1 0.000 0 -40.000 3 0.000

```

4597 c1 c3 c3 h1      0.000      0      80.000  3      0.000
4598      TOTAL TORSIONAL ENERGY =      1.303 kJ/mol
4599
4600 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 c1      2.960      0.012
4615 h1 h1      2.518     -0.013
4616 h1 h1      2.300      0.109
4617 h1 c1      3.474     -0.129
4618 c1 h1      3.474     -0.129
4619 c1 h1      2.960      0.012
4620 c1 c1      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 c1      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 c1      3.474     -3.809     -1.097
4634 c1 h1      3.474     -3.809     -1.097
4635 c1 h1      2.960     -3.809     -1.287
4636 c1 c1      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
4650 7 5 NO
4651 8 12 NO
4652
4653 F O R M A L C H A R G E S
4654
4655 I D X C H A R G E
4656 1 0.000000
4657 2 0.000000
4658 3 0.000000
4659 4 0.000000
4660 5 0.000000
4661 6 0.000000
4662 7 0.000000
4663 8 0.000000
4664
4665 P A R T I A L C H A R G E S
4666
4667 I D X C H A R G E
4668 1 0.290000
4669 2 0.290000
4670 3 0.000000
4671 4 0.000000
4672 5 -0.290000
4673 6 0.000000
4674 7 0.000000
4675 8 -0.290000
4676
4677 S E T T I N G U P C A L C U L A T I O N S
4678
4679 S E T T I N G U P B O N D C A L C U L A T I O N S . . .
4680 S E T T I N G U P A N G L E & S T R E T C H - B E N D C A L C U L A T I O N S . . .
4681 S E T T I N G U P T O R S I O N C A L C U L A T I O N S . . .
4682 S E T T I N G U P O O P C A L C U L A T I O N S . . .
4683 S E T T I N G U P V A N D E R W A A L S C A L C U L A T I O N S . . .
4684 S E T T I N G U P E L E C T R O S T A T I C C A L C U L A T I O N S . . .
4685
4686 A T O M T Y P E S
4687
4688 I D X T Y P E R I N G
4689 1 c3 NO
4690 2 c3 NO
4691 3 h1 NO
4692 4 h1 NO
4693 5 c1 NO
4694 6 h1 NO
```

4695 7 h1 NO

4696 8 cl NO

4697

4698 C H A R G E S

4699

4700 IDX CHARGE

4701 1 0.036009

4702 2 0.036009

4703 3 0.044101

4704 4 0.044101

4705 5 -0.124211

4706 6 0.044101

4707 7 0.044101

4708 8 -0.124211

4709

4710 S E T T I N G U P C A L C U L A T I O N S

4711

4712 SETTING UP BOND CALCULATIONS...

4713 SETTING UP ANGLE CALCULATIONS...

4714 SETTING UP TORSION CALCULATIONS...

4715 SETTING UP IMPROPER TORSION CALCULATIONS...

4716 SETTING UP VAN DER WAALS CALCULATIONS...

4717 SETTING UP ELECTROSTATIC CALCULATIONS...

4718

4719 E N E R G Y

4720

4721

4722 B O N D S T R E T C H I N G

4723

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	

4734 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

4735

4736 A N G L E B E N D I N G

4737

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	

4744	1	1	5	0	109.500	110.549	0.636	-1.049	0.015	
4745	1	1	12	0	109.500	108.679	1.056	0.821	0.016	
4746	5	1	12	0	109.442	108.162	0.698	1.280	0.025	
4747	1	1	5	0	109.500	110.549	0.636	-1.049	0.015	
4748	5	1	12	0	109.442	108.162	0.698	1.280	0.025	
4749	5	1	5	0	109.442	108.836	0.516	0.606	0.004	
4750	1	1	12	0	109.500	108.679	1.056	0.821	0.016	
4751	1	1	5	0	109.500	110.549	0.636	-1.049	0.015	
4752	5	1	12	0	109.442	108.162	0.698	1.280	0.025	
4753	TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol									
4754										
4755	S T R E T C H B E N D I N G									
4756										
4757	ATOM TYPES			FF	VALENCE	DELTA	FORCE CONSTANT			
4758	I	J	K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY	
4759	-----									
4760	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
4761	5	1	5	0	109.442	0.606	0.115	0.115	-0.033	
4762	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
4763	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
4764	1	1	12	0	109.500	0.821	0.176	0.386	-0.070	
4765	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
4766	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
4767	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
4768	5	1	5	0	109.442	0.606	0.115	0.115	-0.033	
4769	1	1	12	0	109.500	0.821	0.176	0.386	-0.070	
4770	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002	
4771	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121	
4772	TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol									
4773										
4774	T O R S I O N A L									
4775										
4776	ATOM TYPES				FF	TORSION	FORCE CONSTANT			
4777	I	J	K	L	CLASS	ANGLE	V1	V2	V3	ENERGY
4778	-----									
4779	5	1	1	5	0	-20.000	0.284	-1.386	0.314	0.349
4780	5	1	1	12	0	100.000	0.678	-0.602	0.398	-0.005
4781	5	1	1	5	0	-140.000	0.284	-1.386	0.314	-0.304
4782	5	1	1	5	0	100.000	0.284	-1.386	0.314	-0.991
4783	5	1	1	12	0	-140.000	0.678	-0.602	0.398	0.129
4784	5	1	1	5	0	-20.000	0.284	-1.386	0.314	0.349
4785	12	1	1	5	0	-140.000	0.678	-0.602	0.398	0.129
4786	12	1	1	12	0	-20.000	0.000	0.000	0.893	0.670
4787	12	1	1	5	0	100.000	0.678	-0.602	0.398	-0.005
4788	TOTAL TORSIONAL ENERGY = 0.31978 kcal/mol									
4789										
4790	O U T - O F - P L A N E B E N D I N G									
4791										
4792	ATOM TYPES				FF	OOP	FORCE			

4793 I J K L CLASS ANGLE CONSTANT ENERGY

4794 -----

4795 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol

4796

4797 V A N D E R W A A L S

4798

4799 ATOM TYPES

4800 I J RiJ R*IJ EPSILON ENERGY

4801 -----

4802 5 5 2.232 2.970 0.022 0.328

4803 5 5 2.831 2.970 0.022 -0.019

4804 5 12 3.129 3.713 0.053 0.104

4805 5 5 2.638 2.970 0.022 0.001

4806 5 5 2.232 2.970 0.022 0.328

4807 5 12 3.399 3.713 0.053 -0.028

4808 12 5 3.399 3.713 0.053 -0.028

4809 12 5 3.129 3.713 0.053 0.104

4810 12 12 2.711 4.089 0.276 16.993

4811 TOTAL VAN DER WAALS ENERGY = 17.78153 kcal/mol

4812

4813 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

4814

4815 ATOM TYPES

4816 I J RiJ Qi Qj ENERGY

4817 -----

4818 12 12 2.761 -0.290 -0.290 7.587

4819 TOTAL ELECTROSTATIC ENERGY = 7.58721 kcal/mol

4820

4821 TOTAL ENERGY = 45.38946 kcal/mol

4822

4823 E N E R G Y

4824

4825

4826 B O N D S T R E T C H I N G

4827

4828 ATOM TYPES BOND IDEAL FORCE

4829 I J LENGTH LENGTH CONSTANT DELTA ENERGY

4830 -----

4831 h1 c3 1.000 1.093 1406.346 -0.093 12.163

4832 h1 c3 1.000 1.093 1406.346 -0.093 12.163

4833 c3 c3 1.540 1.535 1269.019 0.005 0.032

4834 c3 h1 1.000 1.093 1406.346 -0.093 12.163

4835 c3 c1 1.670 1.786 1168.117 -0.116 15.718

4836 c3 c1 1.670 1.786 1168.117 -0.116 15.718

4837 c3 h1 1.000 1.093 1406.346 -0.093 12.163

4838 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

4839

4840 A N G L E B E N D I N G

4841

```

4842 ATOM TYPES          VALENCE      IDEAL      FORCE
4843   I    J    K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
4844 -----
4845 c3 c3 h1    109.500    110.070      194.100      -0.010      0.019
4846 h1 c3 h1    109.442    109.550      164.039      -0.002      0.001
4847 h1 c3 c1    109.442    105.930      183.005       0.061      0.688
4848 c3 c3 h1    109.500    110.070      194.100      -0.010      0.019
4849 c3 c3 c1    109.500    110.330      260.419      -0.014      0.055
4850 h1 c3 c1    109.442    105.930      183.005       0.061      0.688
4851 c3 c3 h1    109.500    110.070      194.100      -0.010      0.019
4852 h1 c3 c1    109.442    105.930      183.005       0.061      0.688
4853 h1 c3 h1    109.442    109.550      164.039      -0.002      0.001
4854 c3 c3 c1    109.500    110.330      260.419      -0.014      0.055
4855 c3 c3 h1    109.500    110.070      194.100      -0.010      0.019
4856 h1 c3 c1    109.442    105.930      183.005       0.061      0.688
4857     TOTAL ANGLE BENDING ENERGY =      2.938 kJ/mol
4858
4859 T O R S I O N A L
4860
4861 ----ATOM TYPES-----      FORCE      TORSION
4862   I    J    K    L      CONSTANT      s      ANGLE      n      ENERGY
4863 -----
4864 h1 c3 c3 h1      0.651      0    -20.000    3      0.977
4865 h1 c3 c3 c1      0.000      0    100.000    3      0.000
4866 h1 c3 c3 h1      0.651      0   -140.000    3      0.977
4867 h1 c3 c3 h1      0.651      0    100.000    3      0.977
4868 h1 c3 c3 c1      0.000      0   -140.000    3      0.000
4869 h1 c3 c3 h1      0.651      0    -20.000    3      0.977
4870 c1 c3 c3 h1      0.000      0   -140.000    3      0.000
4871 c1 c3 c3 c1      0.000      0    -20.000    3      0.000
4872 c1 c3 c3 h1      0.000      0    100.000    3      0.000
4873     TOTAL TORSIONAL ENERGY =      3.908 kJ/mol
4874
4875 I M P R O P E R   T O R S I O N A L
4876
4877 ----ATOM TYPES-----      FORCE      IMPROPER_TORSION
4878   I    J    K    L      CONSTANT      s      ANGLE      n      ENERGY
4879 -----
4880     TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
4881
4882 V A N   D E R   W A A L S
4883
4884 ATOM TYPES
4885   I    J      Rij      kij      ENERGY
4886 -----
4887 h1 h1      2.232      0.205
4888 h1 h1      2.831     -0.032
4889 h1 c1      3.129     -0.106
4890 h1 h1      2.638     -0.029

```

```

4891 h1 h1      2.232      0.205
4892 h1 c1      3.399     -0.133
4893 c1 h1      3.399     -0.133
4894 c1 h1      3.129     -0.106
4895 c1 c1      2.711     33.340
4896      TOTAL VAN DER WAALS ENERGY =      33.209 kJ/mol
4897
4898 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
4899
4900 ATOM TYPES
4901   I      J              Rij      332.17*QiQj      ENERGY
4902 -----
4903 h1 h1      2.232      1.352      0.606
4904 h1 h1      2.831      1.352      0.478
4905 h1 c1      3.129     -3.809     -1.217
4906 h1 h1      2.638      1.352      0.513
4907 h1 h1      2.232      1.352      0.606
4908 h1 c1      3.399     -3.809     -1.121
4909 c1 h1      3.399     -3.809     -1.121
4910 c1 h1      3.129     -3.809     -1.217
4911 c1 c1      2.711     10.728      3.958
4912      TOTAL ELECTROSTATIC ENERGY =      1.484 kJ/mol
4913
4914 TOTAL ENERGY = 121.662 kJ/mol
4915
4916 A T O M      T Y P E S
4917
4918 IDX TYPE  RING
4919 1 1 NO
4920 2 1 NO
4921 3 5 NO
4922 4 5 NO
4923 5 12 NO
4924 6 5 NO
4925 7 5 NO
4926 8 12 NO
4927
4928 F O R M A L      C H A R G E S
4929
4930 IDX CHARGE
4931 1 0.000000
4932 2 0.000000
4933 3 0.000000
4934 4 0.000000
4935 5 0.000000
4936 6 0.000000
4937 7 0.000000
4938 8 0.000000
4939

```

```
4940 P A R T I A L   C H A R G E S
4941
4942 IDX CHARGE
4943 1 0.290000
4944 2 0.290000
4945 3 0.000000
4946 4 0.000000
4947 5 -0.290000
4948 6 0.000000
4949 7 0.000000
4950 8 -0.290000
4951
4952 S E T T I N G   U P   C A L C U L A T I O N S
4953
4954 SETTING UP BOND CALCULATIONS...
4955 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4956 SETTING UP TORSION CALCULATIONS...
4957 SETTING UP OOP CALCULATIONS...
4958 SETTING UP VAN DER WAALS CALCULATIONS...
4959 SETTING UP ELECTROSTATIC CALCULATIONS...
4960
4961 A T O M   T Y P E S
4962
4963 IDX TYPE   RING
4964 1 c3   NO
4965 2 c3   NO
4966 3 h1   NO
4967 4 h1   NO
4968 5 c1   NO
4969 6 h1   NO
4970 7 h1   NO
4971 8 c1   NO
4972
4973 C H A R G E S
4974
4975 IDX CHARGE
4976 1 0.036009
4977 2 0.036009
4978 3 0.044101
4979 4 0.044101
4980 5 -0.124211
4981 6 0.044101
4982 7 0.044101
4983 8 -0.124211
4984
4985 S E T T I N G   U P   C A L C U L A T I O N S
4986
4987 SETTING UP BOND CALCULATIONS...
4988 SETTING UP ANGLE CALCULATIONS...
```

4989 SETTING UP TORSION CALCULATIONS...

4990 SETTING UP IMPROPER TORSION CALCULATIONS...

4991 SETTING UP VAN DER WAALS CALCULATIONS...

4992 SETTING UP ELECTROSTATIC CALCULATIONS...

4993

4994 E N E R G Y

4995

4996

4997 B O N D S T R E T C H I N G

4998

ATOM TYPES	FF	BOND	IDEAL	FORCE				
I J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY		
5000								
5001								
5002	5 1	0	1.000	1.093	4.766	-0.093	3.578	
5003	5 1	0	1.000	1.093	4.766	-0.093	3.578	
5004	1 1	0	1.540	1.508	4.258	0.032	0.294	
5005	1 5	0	1.000	1.093	4.766	-0.093	3.578	
5006	1 12	0	1.670	1.773	2.974	-0.103	2.795	
5007	1 5	0	1.000	1.093	4.766	-0.093	3.578	
5008	1 12	0	1.670	1.773	2.974	-0.103	2.795	
5009	TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol							

5010

5011 A N G L E B E N D I N G

5012

ATOM TYPES	FF	VALENCE	IDEAL	FORCE				
I J K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY		
5013								
5014								
5015								
5016	1 1 5	0	109.500	110.549	0.636	-1.049	0.015	
5017	5 1 5	0	109.442	108.836	0.516	0.606	0.004	
5018	5 1 12	0	109.442	108.162	0.698	1.280	0.025	
5019	1 1 5	0	109.500	110.549	0.636	-1.049	0.015	
5020	1 1 12	0	109.500	108.679	1.056	0.821	0.016	
5021	5 1 12	0	109.442	108.162	0.698	1.280	0.025	
5022	1 1 5	0	109.500	110.549	0.636	-1.049	0.015	
5023	5 1 5	0	109.442	108.836	0.516	0.606	0.004	
5024	5 1 12	0	109.442	108.162	0.698	1.280	0.025	
5025	1 1 5	0	109.500	110.549	0.636	-1.049	0.015	
5026	1 1 12	0	109.500	108.679	1.056	0.821	0.016	
5027	5 1 12	0	109.442	108.162	0.698	1.280	0.025	
5028	TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol							

5029

5030 S T R E T C H B E N D I N G

5031

ATOM TYPES	FF	VALENCE	DELTA	FORCE	CONSTANT			
I J K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY		
5032								
5033								
5034								
5035	1 1 5	0	109.500	-1.049	0.227	0.070	-0.002	
5036	5 1 5	0	109.442	0.606	0.115	0.115	-0.033	
5037	5 1 12	0	109.442	1.280	-0.018	0.380	-0.121	

5038	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
5039	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5040	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
5041	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
5042	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
5043	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
5044	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
5045	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5046	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
5053	-----					
5054	5	1	1	5	0	0.000 0.284 -1.386 0.314 0.598
5055	5	1	1	5	0	-120.000 0.284 -1.386 0.314 -0.655
5056	5	1	1	12	0	120.000 0.678 -0.602 0.398 0.116
5057	5	1	1	5	0	120.000 0.284 -1.386 0.314 -0.655
5058	5	1	1	5	0	0.000 0.284 -1.386 0.314 0.598
5059	5	1	1	12	0	-120.000 0.678 -0.602 0.398 0.116
5060	12	1	1	5	0	-120.000 0.678 -0.602 0.398 0.116
5061	12	1	1	5	0	120.000 0.678 -0.602 0.398 0.116
5062	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		Rij	R*IJ	EPSILON	ENERGY
I J					
5076	-----				
5077	5	5	2.208	2.970	0.022 0.377
5078	5	5	2.746	2.970	0.022 -0.014
5079	5	12	3.280	3.713	0.053 0.009
5080	5	5	2.746	2.970	0.022 -0.014
5081	5	5	2.208	2.970	0.022 0.377
5082	5	12	3.280	3.713	0.053 0.009
5083	12	5	3.280	3.713	0.053 0.009
5084	12	5	3.280	3.713	0.053 0.009
5085	12	12	2.655	4.089	0.276 20.655

TOTAL VAN DER WAALS ENERGY = 21.41512 kcal/mol

5087

5088 E L E C T R O S T A T I C I N T E R A C T I O N S

5089

5090 A T O M T Y P E S

5091 I J R_{ij} Q_i Q_j E N E R G Y

5092 -----

5093 12 12 2.705 -0.290 -0.290 7.743

5094 TOTAL ELECTROSTATIC ENERGY = 7.74347 kcal/mol

5095

5096 TOTAL ENERGY = 50.10353 kcal/mol

5097

5098 E N E R G Y

5099

5100

5101 B O N D S T R E T C H I N G

5102

5103 A T O M T Y P E S B O N D I D E A L F O R C E

5104 I J L E N G T H L E N G T H C O N S T A N T D E L T A E N E R G Y

5105 -----

5106 h1 c3 1.000 1.093 1406.346 -0.093 12.163

5107 h1 c3 1.000 1.093 1406.346 -0.093 12.163

5108 c3 c3 1.540 1.535 1269.019 0.005 0.032

5109 c3 h1 1.000 1.093 1406.346 -0.093 12.163

5110 c3 c1 1.670 1.786 1168.117 -0.116 15.718

5111 c3 h1 1.000 1.093 1406.346 -0.093 12.163

5112 c3 c1 1.670 1.786 1168.117 -0.116 15.718

5113 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

5114

5115 A N G L E B E N D I N G

5116

5117 A T O M T Y P E S V A L E N C E I D E A L F O R C E

5118 I J K A N G L E A N G L E C O N S T A N T D E L T A E N E R G Y

5119 -----

5120 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

5121 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

5122 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

5123 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

5124 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

5125 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

5126 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

5127 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001

5128 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

5129 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019

5130 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055

5131 h1 c3 c1 109.442 105.930 183.005 0.061 0.688

5132 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

5133

5134 T O R S I O N A L

5135


```

5136 -----ATOM TYPES-----      FORCE      TORSION
5137      I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
5138 -----
5139 h1 c3 c3 h1      0.651      0      0.000      3      1.303
5140 h1 c3 c3 h1      0.651      0     -120.000      3      1.303
5141 h1 c3 c3 c1      0.000      0      120.000      3      0.000
5142 h1 c3 c3 h1      0.651      0      120.000      3      1.303
5143 h1 c3 c3 h1      0.651      0      0.000      3      1.303
5144 h1 c3 c3 c1      0.000      0     -120.000      3      0.000
5145 c1 c3 c3 h1      0.000      0     -120.000      3      0.000
5146 c1 c3 c3 h1      0.000      0      120.000      3      0.000
5147 c1 c3 c3 c1      0.000      0      -0.000      3      0.000
5148      TOTAL TORSIONAL ENERGY =      5.210 kJ/mol
5149
5150 I M P R O P E R      T O R S I O N A L
5151
5152 -----ATOM TYPES-----      FORCE      IMPROPER_TORSION
5153      I      J      K      L      CONSTANT      s      ANGLE      n      ENERGY
5154 -----
5155      TOTAL IMPROPER-TORSIONAL ENERGY =      0.000 kJ/mol
5156
5157 V A N      D E R      W A A L S
5158
5159 ATOM TYPES
5160      I      J      Rij      kij      ENERGY
5161 -----
5162 h1 h1      2.208      0.251
5163 h1 h1      2.746     -0.033
5164 h1 c1      3.280     -0.134
5165 h1 h1      2.746     -0.033
5166 h1 h1      2.208      0.251
5167 h1 c1      3.280     -0.134
5168 c1 h1      3.280     -0.134
5169 c1 h1      3.280     -0.134
5170 c1 c1      2.655     44.245
5171      TOTAL VAN DER WAALS ENERGY =      44.146 kJ/mol
5172
5173 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
5174
5175 ATOM TYPES
5176      I      J      Rij      332.17*QiQj      ENERGY
5177 -----
5178 h1 h1      2.208      1.352      0.613
5179 h1 h1      2.746      1.352      0.493
5180 h1 c1      3.280     -3.809     -1.161
5181 h1 h1      2.746      1.352      0.493
5182 h1 h1      2.208      1.352      0.613
5183 h1 c1      3.280     -3.809     -1.161
5184 c1 h1      3.280     -3.809     -1.161

```

```
5185 | cl h1      3.280    -3.809    -1.161
5186 | cl cl      2.655    10.728     4.041
5187 |          TOTAL ELECTROSTATIC ENERGY =      1.607 kJ/mol
5188 |
5189 | TOTAL ENERGY =  134.023 kJ/mol
```