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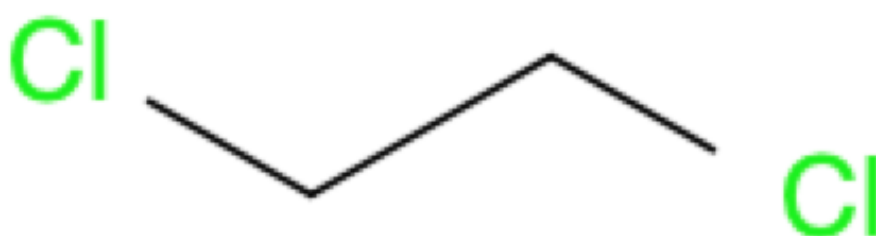
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BIM2005: Homework I

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

Preparation

- Structure of $C_2H_4Cl_2$ (For reference)



- Headers are added to 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 Cl 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 Cl 2 1.67 1 109.5 5 0.0
```

Procedure

Details of implementation could be found in the GitHub repository [zcorn2017/BIM2005-HWK1](https://github.com/zcorn2017/BIM2005-HWK1) (github.com).

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

1. We [added the headers to the code manually](#) for it to be recognised by [OpenBabel](#)
2. We modify the code in order to change $\tau(Cl^8 - C^2 - C^1 - Cl^5)$ by $20 \times N^\circ$. (As the reference plane, which is the 2 – 1 – 5 plane, is the same for the last three definitions of atoms, we only need to change the dihedral angles of the last three lines by an increment of 20° .)
3. We convert the code from the .gzmat format to the .xyz. one via [the Python bindings to the OpenBabel C++ library](#).
4. During the conversion, we use the python bindings to set up the force fields for MMFF94 and GAFF respectively, then calculating the energy, where the analysis process is recorded (See [Appendix I](#)).
5. The energy are stored in lists for further analysis.
6. We repeat the steps 2-5 for $N = 0 \dots 18$, 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](#).
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

```

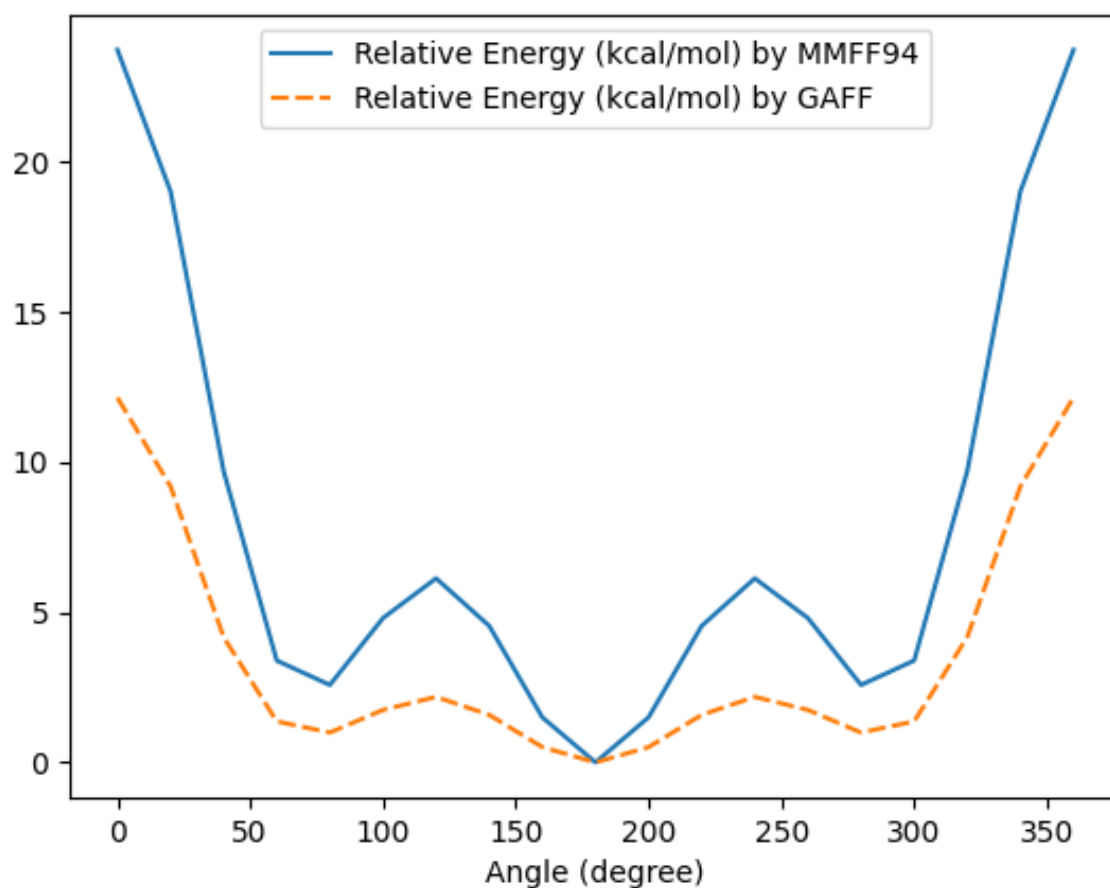
1  8
2  ./CODE/C2H4Cl2_360_degrees.gzmat
3  C      0.00000      0.00000      0.00000
4  C      1.54000      0.00000      0.00000
5  H     -0.33381      0.00000     -0.94264
6  H     -0.33381     -0.81635      0.47132
7  Cl     -0.55746      1.36331      0.78711
8  H      1.87381      0.00000     -0.94264
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  gzmat_code = ""
14  #
15
16  C2H4Cl2
17
```

```

18  O 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
manipulate
34      atom_counter = 0
35
36      # .xyz code after conversion
37      code_aft_cnv = ""
38      for line in gzmat_code.split("\n"):
39          words = line.split()
40
41          # if the line is empty, do not make modifications
42          if len(words) == 0:
43              pass
44
45          # if the title is met, rename the title to mark it with the torsion angle
46          elif line.startswith("C2H4Cl2"):
47              words.append(str(20 * n))
48              words.append("degrees")
49              code_aft_cnv = code_aft_cnv + "-".join(words) + "\n"
50              continue
51
52          elif words[0].isalpha() and len(words[0]) in [1, 2]:
53              atom_counter = atom_counter + 1
54
55              if atom_counter in [6, 7, 8]:
56
57                  words[-1] = str(float(words[-1]) + 20 * n)
58                  if float(words[-1]) >= 360:
59                      words[-1] = str(float(words[-1]) - 360)
60
61              code_aft_cnv = code_aft_cnv + " ".join(words) + "\n"
62              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
144 data_in_KJ_df = pd.DataFrame(data_in_KJ_dict, index=[angle for angle in range(0,
145     380, 20)])
146
147 data_in_Kcal_df.to_csv("./DATA/data_in_Kcal.csv")
148 data_in_KJ_df.to_csv("./DATA/data_in_KJ.csv")
149
150 data_dict = {
151     "Absolute Energy (kcal/mol) by MMFF94":
152     np.round(MMFF94_abs_energy_in_Kcal_vec.tolist(), 3),
153     "Absolute Energy (kcal/mol) by GAFF":
154     np.round(GAFF_abs_energy_in_Kcal_vec.tolist(), 3),
155     "Relative Energy (kcal/mol) by MMFF94":
156     np.round(MMFF94_rel_energy_in_Kcal_vec.tolist(), 3),
157     "Relative Energy (kcal/mol) by GAFF":
158     np.round(GAFF_rel_energy_in_Kcal_vec.tolist(), 3),
159     "Absolute Energy (kJ/mol) by MMFF94":
160     np.round(MMFF94_abs_energy_in_KJ_vec.tolist(), 3),
161     "Absolute Energy (kJ/mol) by GAFF":
162     np.round(GAFF_abs_energy_in_KJ_vec.tolist(), 3),

```

```

151     "Relative Energy (kJ/mol) by MMFF94":
152     np.round(MMFF94_rel_energy_in_KJ_vec.tolist(), 3),
153     "Relative Energy (kJ/mol) by GAFF":
154     np.round(GAFF_rel_energy_in_KJ_vec.tolist(), 3)
155 }
156
157 data_df = pd.DataFrame(data_dict, index=[angle for angle in range(0, 380, 20)])
158 data_df.index.name = "Angle (degree)"
159 data_df.to_csv("./DATA/data.csv")
160
161 # Plot the lineplot of relative energy in kcal/mol with respect to angle in
162 degrees
163 lineplot_df = data_df.loc[:, ["Relative Energy (kcal/mol) by MMFF94", "Relative
164                               Energy (kcal/mol) by GAFF"]]
165 sns.lineplot(data=lineplot_df)
166
167 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```")
17
18 # Redirect the output to the file writing object.
19 with open("XYZ_GAMAT_SUMMARY.md", "w") as sys.stdout:
20     for angle in range(0, 380, 20):
21         mkdoc_heading(f"Torsion Angle at {angle}$\degree$", level= 4)
22
23         print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.gzmat\n")
24         with open(f"./CODE/C2H4Cl2_{angle}_degrees.gzmat", "r") as gzmat:
25             wrap_code(gzmat.read(), lang="gzmat")
26
27         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 I D X T Y P E R I N G

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 I D X C H A R G E

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
95      TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
96
97  A N G L E      B E N D I N G
98
99  ATOM TYPES      FF      VALENCE      IDEAL      FORCE
100  I      J      K      CLASS      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
101  -----
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
114      TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
115
116  S T R E T C H      B E N D I N G
117
118  ATOM TYPES      FF      VALENCE      DELTA      FORCE CONSTANT
119  I      J      K      CLASS      ANGLE      ANGLE      I J      J K      ENERGY
120  -----
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
133      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
134
135  T O R S I O N A L
136
137  ATOM TYPES      FF      TORSION      FORCE CONSTANT
138  I      J      K      L      CLASS      ANGLE      V1      V2      V3      ENERGY
139  -----
140      5      1      1      5      0      0.000      0.284      -1.386      0.314      0.598
141      5      1      1      5      0     -120.000      0.284      -1.386      0.314      -0.655

```

142	5	1	1	12	0	120.000	0.678	-0.602	0.398	0.116
143	5	1	1	5	0	120.000	0.284	-1.386	0.314	-0.654
144	5	1	1	5	0	0.000	0.284	-1.386	0.314	0.598
145	5	1	1	12	0	-120.000	0.678	-0.602	0.398	0.116
146	12	1	1	5	0	-120.000	0.678	-0.602	0.398	0.116
147	12	1	1	5	0	120.000	0.678	-0.602	0.398	0.116
148	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	R _{ij}	R*IJ	EPSILON	ENERGY

163	5	5	2.208	2.970	0.022	0.377
164	5	5	2.746	2.970	0.022	-0.014
165	5	12	3.280	3.713	0.053	0.009
166	5	5	2.746	2.970	0.022	-0.014
167	5	5	2.208	2.970	0.022	0.377
168	5	12	3.280	3.713	0.053	0.009
169	12	5	3.280	3.713	0.053	0.009
170	12	5	3.280	3.713	0.053	0.009
171	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	R _{ij}	Q _i	Q _j	ENERGY

179	12	12	2.705	-0.290	-0.290	7.743
-----	----	----	-------	--------	--------	-------

TOTAL ELECTROSTATIC ENERGY = 7.74347 kcal/mol

TOTAL ENERGY = 50.10353 kcal/mol

E N E R G Y

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

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

```

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

```

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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 IDX CHARGE

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

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

364 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

365

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

367

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

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

```

TOTAL VAN DER WAALS ENERGY = 17.78153 kcal/mol

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

A T O M T Y P E S

I	J	Rij	Qi	Qj	ENERGY
---	---	-----	----	----	--------

12	12	2.761	-0.290	-0.290	7.587
----	----	-------	--------	--------	-------

TOTAL ELECTROSTATIC ENERGY = 7.58721 kcal/mol

TOTAL ENERGY = 45.38946 kcal/mol

E N E R G Y

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

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

h1	c3	1.000	1.093	1406.346	-0.093	12.163
h1	c3	1.000	1.093	1406.346	-0.093	12.163
c3	c3	1.540	1.535	1269.019	0.005	0.032
c3	h1	1.000	1.093	1406.346	-0.093	12.163
c3	c1	1.670	1.786	1168.117	-0.116	15.718
c3	h1	1.000	1.093	1406.346	-0.093	12.163
c3	c1	1.670	1.786	1168.117	-0.116	15.718

TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol

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

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

c3	c3	h1	109.500	110.070	194.100	-0.010	0.019
h1	c3	h1	109.442	109.550	164.039	-0.002	0.001
h1	c3	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
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

```

485 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055
486 h1 c3 c1 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 c1 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 c1 0.000 0 -100.000 3 0.000
500 c1 c3 c3 h1 0.000 0 -100.000 3 0.000
501 c1 c3 c3 h1 0.000 0 140.000 3 0.000
502 c1 c3 c3 c1 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 c1 3.399 -0.133
520 h1 h1 2.831 -0.032
521 h1 h1 2.232 0.205
522 h1 c1 3.129 -0.106
523 c1 h1 3.129 -0.106
524 c1 h1 3.399 -0.133
525 c1 c1 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

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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 NO
550 2 1 NO
551 3 5 NO
552 4 5 NO
553 5 12 NO
554 6 5 NO
555 7 5 NO
556 8 12 NO
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
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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   I D X   T Y P E   R I N G
594   1  c3   N O
595   2  c3   N O
596   3  h1   N O
597   4  h1   N O
598   5  c1   N O
599   6  h1   N O
600   7  h1   N O
601   8  c1   N O
602
603 C H A R G E S
604
605   I D X   C H A R G E
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   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
630   I       J       C L A S S   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
631   -----

```

```

632 5 1 0 1.000 1.093 4.766 -0.093 3.578
633 5 1 0 1.000 1.093 4.766 -0.093 3.578
634 5 1 0 1.000 1.093 4.766 -0.093 3.578
635 1 1 0 1.540 1.508 4.258 0.032 0.294
636 1 5 0 1.000 1.093 4.766 -0.093 3.578
637 1 12 0 1.670 1.773 2.974 -0.103 2.795
638 1 12 0 1.670 1.773 2.974 -0.103 2.795
639 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
640
641 A N G L E B E N D I N G
642
643 ATOM TYPES FF VALENCE IDEAL FORCE
644 I J K CLASS ANGLE ANGLE CONSTANT DELTA ENERGY
645 -----
646 1 1 5 0 109.500 110.549 0.636 -1.049 0.015
647 5 1 5 0 109.442 108.836 0.516 0.606 0.004
648 5 1 12 0 109.442 108.162 0.698 1.280 0.025
649 1 1 5 0 109.500 110.549 0.636 -1.049 0.015
650 1 1 12 0 109.500 108.679 1.056 0.821 0.016
651 5 1 12 0 109.442 108.162 0.698 1.280 0.025
652 5 1 5 0 109.442 108.836 0.516 0.606 0.004
653 1 1 5 0 109.500 110.549 0.636 -1.049 0.015
654 5 1 12 0 109.442 108.162 0.698 1.280 0.025
655 1 1 5 0 109.500 110.549 0.636 -1.049 0.015
656 5 1 12 0 109.442 108.162 0.698 1.280 0.025
657 1 1 12 0 109.500 108.679 1.056 0.821 0.016
658 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
659
660 S T R E T C H B E N D I N G
661
662 ATOM TYPES FF VALENCE DELTA FORCE CONSTANT
663 I J K CLASS ANGLE ANGLE I J J K ENERGY
664 -----
665 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
666 5 1 5 0 109.442 0.606 0.115 0.115 -0.033
667 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
668 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
669 1 1 12 0 109.500 0.821 0.176 0.386 -0.070
670 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
671 5 1 5 0 109.442 0.606 0.115 0.115 -0.033
672 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
673 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
674 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
675 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
676 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

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```

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
749							ENERGY

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
768						ANGLE

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


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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 IDX TYPE  RING
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

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

908 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

909

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

911

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

926 1 1 12 0 109.500 108.679 1.056 0.821 0.016

927 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol

928

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

930

931 ATOM TYPES FF VALENCE DELTA FORCE CONSTANT

932 I J K CLASS ANGLE ANGLE I J J K ENERGY

933 -----

934 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002

935 5 1 5 0 109.442 0.606 0.115 0.115 -0.033

936 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121

937 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002

938 1 1 12 0 109.500 0.821 0.176 0.386 -0.070

939 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121

940 5 1 5 0 109.442 0.606 0.115 0.115 -0.033

941 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002

942 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121

943 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002

944 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121

945 1 1 12 0 109.500 0.821 0.176 0.386 -0.070

946 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

947

948 T O R S I O N A L

949

950 ATOM TYPES FF TORSION FORCE CONSTANT

951 I J K L CLASS ANGLE V1 V2 V3 ENERGY

952 -----

953 5 1 1 5 0 60.000 0.284 -1.386 0.314 -0.827

954 5 1 1 5 0 -60.000 0.284 -1.386 0.314 -0.826

955 5 1 1 12 0 -180.000 0.678 -0.602 0.398 0.000

956 5 1 1 5 0 -180.000 0.284 -1.386 0.314 0.000

957 5 1 1 5 0 60.000 0.284 -1.386 0.314 -0.827

958 5 1 1 12 0 -60.000 0.678 -0.602 0.398 0.057

959 12 1 1 5 0 -60.000 0.678 -0.602 0.398 0.057

960 12 1 1 5 0 180.000 0.678 -0.602 0.398 0.000

961 12 1 1 12 0 60.000 0.000 0.000 0.893 0.000

962 TOTAL TORSIONAL ENERGY = -2.36550 kcal/mol

963

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

965

966 ATOM TYPES FF OOP FORCE

967 I J K L CLASS ANGLE CONSTANT ENERGY

968 -----

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

970

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

```

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

```

990 I J Ri j Qi Qj ENERGY
991 -----
992 12 12 3.137 -0.290 -0.290 6.678
993 TOTAL ELECTROSTATIC ENERGY = 6.67788 kcal/mol
994

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TOTAL ENERGY = 29.75490 kcal/mol

E N E R G Y

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

```

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

```

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

```

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
1031 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
1032
1033 T O R S I O N A L
1034
1035 ----ATOM TYPES----- FORCE TORSION
1036 I J K L CONSTANT s ANGLE n ENERGY
1037 -----
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
1047 TOTAL TORSIONAL ENERGY = 0.000 kJ/mol
1048
1049 I M P R O P E R T O R S I O N A L
1050
1051 ----ATOM TYPES----- FORCE IMPROPER_TORSION
1052 I J K L CONSTANT s ANGLE n ENERGY
1053 -----
1054 TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
1055
1056 V A N D E R W A A L S
1057
1058 ATOM TYPES
1059 I J Rij kij ENERGY
1060 -----
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 c1 c1 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 c1      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 c1      2.792     -3.809     -1.364
1083 c1 h1      2.792     -3.809     -1.364
1084 c1 h1      3.499     -3.809     -1.089
1085 c1 c1      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 I D X   T Y P E   R I N G
1129 1 c3   N O
1130 2 c3   N O
1131 3 h1   N O
1132 4 h1   N O
1133 5 c1   N O
1134 6 h1   N O
1135 7 h1   N O
1136 8 c1   N O
1137
1138 F O R M A L   C H A R G E S
1139
1140 I D X   C H A R G E
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 I D X   C H A R G E
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 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
1168 I     J     C L A S S   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
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

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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

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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	-----						
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1274	h1	c3	1.000	1.093	1406.346	-0.093	12.163
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1275	h1	c3	1.000	1.093	1406.346	-0.093	12.163
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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
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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
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1280	c3	c1	1.670	1.786	1168.117	-0.116	15.718
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1281	TOTAL BOND STRETCHING ENERGY =					80.122	kJ/mol
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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	-----							
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1288	c3	c3	h1	109.500	110.070	194.100	-0.010	0.019
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1289	h1	c3	h1	109.442	109.550	164.039	-0.002	0.001
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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
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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	-----								
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1307	h1	c3	c3	h1	0.651	0	80.000	3	0.326
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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
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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
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1315	c1	c3	c3	c1	0.000	0	80.000	3	0.000
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1316	TOTAL TORSIONAL ENERGY =					1.303	kJ/mol
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1317

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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

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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 I D X   C H A R G E
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 I D X   C H A R G E
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 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 . . .
1398 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 . . .
1399 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 . . .
1400 S E T T I N G   U P   O O P   C A L C U L A T I O N S . . .
1401 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 . . .
1402 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 . . .
1403
1404 A T O M   T Y P E S
1405
1406 I D X   T Y P E   R I N G
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 c1 NO
1415
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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

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

1452 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

1453

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

1455

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

```

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

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

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

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1612  cl h1      3.399   -0.133
1613  cl cl      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 cl      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 cl      2.547     -3.809     -1.495
1627  cl h1      2.547     -3.809     -1.495
1628  cl h1      3.399     -3.809     -1.121
1629  cl cl      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	cl NO
1678	6	h1 NO
1679	7	h1 NO
1680	8	cl 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			
I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY	

1712

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TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol

1722

1723

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

1724

1725

1726

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

1727

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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

1745

1746

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

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1759      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
1760
1761  T O R S I O N A L
1762
1763  ATOM TYPES          FF      TORSION      FORCE CONSTANT
1764    I    J    K    L    CLASS    ANGLE          V1    V2    V3      ENERGY
1765  -----
1766    5    1    1    5      0      0.000    0.284   -1.386    0.314    0.598
1767    5    1    1    5      0     120.000    0.284   -1.386    0.314   -0.654
1768    5    1    1   12      0    -120.000    0.678   -0.602    0.398    0.116
1769    5    1    1    5      0     120.000    0.284   -1.386    0.314   -0.655
1770    5    1    1    5      0    -120.000    0.284   -1.386    0.314   -0.655
1771    5    1    1   12      0      0.000    0.678   -0.602    0.398    1.076
1772   12    1    1    5      0    -120.000    0.678   -0.602    0.398    0.116
1773   12    1    1    5      0     -0.000    0.678   -0.602    0.398    1.076
1774   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
1779  ATOM TYPES          FF      OOP      FORCE
1780    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
1786  ATOM TYPES
1787    I    J      Rij      R*IJ      EPSILON      ENERGY
1788  -----
1789    5    5      2.746      2.970      0.022     -0.014
1790    5    5      2.208      2.970      0.022      0.377
1791    5   12      3.280      3.713      0.053      0.009
1792    5    5      2.746      2.970      0.022     -0.014
1793    5    5      2.746      2.970      0.022     -0.014
1794    5   12      2.512      3.713      0.053      2.649
1795   12    5      2.512      3.713      0.053      2.649
1796   12    5      3.280      3.713      0.053      0.009
1797   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
1802  ATOM TYPES
1803    I    J      Rij      Qi      Qj      ENERGY
1804  -----
1805   12   12      3.856     -0.290     -0.290      5.432
1806      TOTAL ELECTROSTATIC ENERGY =  5.43239 kcal/mol
1807

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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

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

1817 -----

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

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

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

1831 -----

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

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

1844 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

1845

1846 T O R S I O N A L

1847

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

1850 -----

h1	c3	c3	h1	0.651	0	0.000	3	1.303
----	----	----	----	-------	---	-------	---	-------

h1	c3	c3	h1	0.651	0	120.000	3	1.303
----	----	----	----	-------	---	---------	---	-------

h1	c3	c3	c1	0.000	0	-120.000	3	0.000
----	----	----	----	-------	---	----------	---	-------

h1	c3	c3	h1	0.651	0	120.000	3	1.303
----	----	----	----	-------	---	---------	---	-------

h1	c3	c3	h1	0.651	0	-120.000	3	1.303
----	----	----	----	-------	---	----------	---	-------

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

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1857 cl c3 c3 h1      0.000      0  -120.000  3      0.000
1858 cl c3 c3 h1      0.000      0   -0.000  3      0.000
1859 cl c3 c3 cl      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 cl      3.280      -0.134
1877 h1 h1      2.746      -0.033
1878 h1 h1      2.746      -0.033
1879 h1 cl      2.512      2.571
1880 cl h1      2.512      2.571
1881 cl h1      3.280      -0.134
1882 cl cl      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 cl      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 cl      2.512      -3.809      -1.516
1896 cl h1      2.512      -3.809      -1.516
1897 cl h1      3.280      -3.809      -1.161
1898 cl cl      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
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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	ENERGY
2040	-----									
2041	5	1	1	5	0	20.000	0.284	-1.386	0.314	0.349
2042	5	1	1	12	0	-100.000	0.678	-0.602	0.398	-0.005
2043	5	1	1	5	0	140.000	0.284	-1.386	0.314	-0.304
2044	5	1	1	5	0	140.000	0.284	-1.386	0.314	-0.304
2045	5	1	1	12	0	20.000	0.678	-0.602	0.398	0.886
2046	5	1	1	5	0	-100.000	0.284	-1.386	0.314	-0.991
2047	12	1	1	5	0	-100.000	0.678	-0.602	0.398	-0.005
2048	12	1	1	12	0	140.000	0.000	0.000	0.893	0.670
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 Ri j 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 Ri j 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

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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

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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
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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

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

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

TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

T O R S I O N A L

ATOM TYPES	FF	TORSION	FORCE CONSTANT			
I J K L	CLASS	ANGLE	V1	V2	V3	ENERGY

5 1 1 5	0	40.000	0.284	-1.386	0.314	-0.243
5 1 1 12	0	-80.000	0.678	-0.602	0.398	-0.086
5 1 1 5	0	160.000	0.284	-1.386	0.314	-0.075
5 1 1 5	0	160.000	0.284	-1.386	0.314	-0.075
5 1 1 12	0	40.000	0.678	-0.602	0.398	0.449
5 1 1 5	0	-80.000	0.284	-1.386	0.314	-1.099
12 1 1 5	0	-80.000	0.678	-0.602	0.398	-0.086
12 1 1 12	0	160.000	0.000	0.000	0.893	0.223
12 1 1 5	0	40.000	0.678	-0.602	0.398	0.449

TOTAL TORSIONAL ENERGY = -0.54336 kcal/mol

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

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

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

V A N D E R W A A L S

ATOM TYPES					
I J	Rij	R*IJ	EPSILON	ENERGY	

5 5	2.885	2.970	0.022	-0.021	
5 5	2.300	2.970	0.022	0.215	
5 12	2.960	3.713	0.053	0.331	
5 5	2.518	2.970	0.022	0.036	
5 5	2.885	2.970	0.022	-0.021	
5 12	2.647	3.713	0.053	1.520	
12 5	2.647	3.713	0.053	1.520	
12 5	2.960	3.713	0.053	0.331	

2347 12 12 4.082 4.089 0.276 -0.276

2348 TOTAL VAN DER WAALS ENERGY = 3.63663 kcal/mol

2349

2350 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

2352 ATOM TYPES

2353 I J Ri j 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

2360 E N E R G Y

2361

2362

2363 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

2377 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

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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

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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 IDX TYPE  RING
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 IDX CHARGE
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 IDX CHARGE
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...

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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 I D X   T Y P E   R I N G
2501 1  c3   N O
2502 2  c3   N O
2503 3  h1   N O
2504 4  h1   N O
2505 5  c1   N O
2506 6  h1   N O
2507 7  h1   N O
2508 8  c1   N O
2509
2510 C H A R G E S
2511
2512 I D X   C H A R G E
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 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
2537 I       J       C L A S S   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
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

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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

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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
2640  ATOM TYPES  BOND      IDEAL      FORCE

```

2641	I	J	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
2642	-----						
2643	h1	c3	1.000	1.093	1406.346	-0.093	12.163
2644	c1	c3	1.670	1.786	1168.117	-0.116	15.718
2645	h1	c3	1.000	1.093	1406.346	-0.093	12.163
2646	c3	c3	1.540	1.535	1269.019	0.005	0.032
2647	c3	h1	1.000	1.093	1406.346	-0.093	12.163
2648	c3	c1	1.670	1.786	1168.117	-0.116	15.718
2649	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							
2654	ATOM TYPES		VALENCE	IDEAL	FORCE		
2655	I	J	K	ANGLE	ANGLE	CONSTANT	DELTA ENERGY
2656	-----						
2657	c3	c3	h1	109.500	110.070	194.100	-0.010 0.019
2658	h1	c3	h1	109.442	109.550	164.039	-0.002 0.001
2659	h1	c3	c1	109.442	105.930	183.005	0.061 0.688
2660	c3	c3	h1	109.500	110.070	194.100	-0.010 0.019
2661	c3	c3	c1	109.500	110.330	260.419	-0.014 0.055
2662	h1	c3	c1	109.442	105.930	183.005	0.061 0.688
2663	h1	c3	c1	109.442	105.930	183.005	0.061 0.688
2664	c3	c3	c1	109.500	110.330	260.419	-0.014 0.055
2665	h1	c3	c1	109.442	105.930	183.005	0.061 0.688
2666	c3	c3	h1	109.500	110.070	194.100	-0.010 0.019
2667	h1	c3	h1	109.442	109.550	164.039	-0.002 0.001
2668	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							
2673	----ATOM TYPES-----			FORCE	TORSION		
2674	I	J	K	L	CONSTANT	s	ANGLE n ENERGY
2675	-----						
2676	h1	c3	c3	c1	0.000	0	-60.000 3 0.000
2677	h1	c3	c3	h1	0.651	0	60.000 3 0.000
2678	h1	c3	c3	h1	0.651	0	-180.000 3 0.000
2679	h1	c3	c3	c1	0.000	0	60.000 3 0.000
2680	h1	c3	c3	h1	0.651	0	-180.000 3 0.000
2681	h1	c3	c3	h1	0.651	0	-60.000 3 0.000
2682	c1	c3	c3	c1	0.000	0	180.000 3 0.000
2683	c1	c3	c3	h1	0.000	0	-60.000 3 0.000
2684	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		

	I	J	K	L	CONSTANT	s	ANGLE	n	ENERGY
2690									
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	cl		2.792	0.356				
2702	h1	h1		2.400	0.030				
2703	h1	h1		2.903	-0.031				
2704	h1	cl		2.792	0.356				
2705	cl	h1		2.792	0.356				
2706	cl	h1		2.792	0.356				
2707	cl	cl		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	cl		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	cl		2.792	-3.809	-1.364			
2721	cl	h1		2.792	-3.809	-1.364			
2722	cl	h1		2.792	-3.809	-1.364			
2723	cl	cl		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						


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2739
2740 F O R M A L   C H A R G E S
2741
2742   I D X   C H A R G E
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   I D X   C H A R G E
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   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 . . .
2767   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 . . .
2768   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 . . .
2769   S E T T I N G   U P   O O P   C A L C U L A T I O N S . . .
2770   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 . . .
2771   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 . . .
2772
2773 A T O M   T Y P E S
2774
2775   I D X   T Y P E   R I N G
2776   1  c3   N O
2777   2  c3   N O
2778   3  h1   N O
2779   4  h1   N O
2780   5  c1   N O
2781   6  h1   N O
2782   7  h1   N O
2783   8  c1   N O
2784
2785 C H A R G E S
2786
2787   I D X   C H A R G E
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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
2811 ATOM TYPES      FF      BOND      IDEAL      FORCE
2812  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
2825 ATOM TYPES      FF      VALENCE      IDEAL      FORCE
2826  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

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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
2840 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
2841
2842 S T R E T C H B E N D I N G
2843
2844 ATOM TYPES FF VALENCE DELTA FORCE CONSTANT
2845 I J K CLASS ANGLE ANGLE I J J K ENERGY
2846 -----
2847 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
2848 5 1 5 0 109.442 0.606 0.115 0.115 -0.033
2849 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
2850 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
2851 1 1 12 0 109.500 0.821 0.176 0.386 -0.070
2852 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
2853 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
2854 1 1 12 0 109.500 0.821 0.176 0.386 -0.070
2855 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121
2856 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
2857 5 1 5 0 109.442 0.606 0.115 0.115 -0.033
2858 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002
2859 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
2860
2861 T O R S I O N A L
2862
2863 ATOM TYPES FF TORSION FORCE CONSTANT
2864 I J K L CLASS ANGLE V1 V2 V3 ENERGY
2865 -----
2866 5 1 1 12 0 -40.000 0.678 -0.602 0.398 0.449
2867 5 1 1 5 0 80.000 0.284 -1.386 0.314 -1.099
2868 5 1 1 5 0 -160.000 0.284 -1.386 0.314 -0.075
2869 5 1 1 12 0 80.000 0.678 -0.602 0.398 -0.086
2870 5 1 1 5 0 -160.000 0.284 -1.386 0.314 -0.075
2871 5 1 1 5 0 -40.000 0.284 -1.386 0.314 -0.243
2872 12 1 1 12 0 -160.000 0.000 0.000 0.893 0.223
2873 12 1 1 5 0 -40.000 0.678 -0.602 0.398 0.449
2874 12 1 1 5 0 80.000 0.678 -0.602 0.398 -0.086
2875 TOTAL TORSIONAL ENERGY = -0.54336 kcal/mol
2876
2877 O U T - O F - P L A N E B E N D I N G
2878
2879 ATOM TYPES FF OOP FORCE
2880 I J K L CLASS ANGLE CONSTANT ENERGY
2881 -----
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

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2886 ATOM TYPES
2887   I      J      Rij      R*IJ      EPSILON      ENERGY
2888 -----
2889   5      5      2.885      2.970      0.022      -0.021
2890   5      5      2.518      2.970      0.022      0.036
2891   5     12      2.647      3.713      0.053      1.520
2892   5      5      2.300      2.970      0.022      0.215
2893   5      5      2.885      2.970      0.022      -0.021
2894   5     12      2.960      3.713      0.053      0.331
2895  12      5      2.960      3.713      0.053      0.331
2896  12      5      2.647      3.713      0.053      1.520
2897  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
2903   I      J      Rij      Qi      Qj      ENERGY
2904 -----
2905  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
2915 ATOM TYPES  BOND      IDEAL      FORCE
2916   I      J  LENGTH  LENGTH  CONSTANT      DELTA      ENERGY
2917 -----
2918 c1 c3      1.670      1.786      1168.117      -0.116      15.718
2919 h1 c3      1.000      1.093      1406.346      -0.093      12.163
2920 h1 c3      1.000      1.093      1406.346      -0.093      12.163
2921 c3 c3      1.540      1.535      1269.019      0.005      0.032
2922 c3 h1      1.000      1.093      1406.346      -0.093      12.163
2923 c3 c1      1.670      1.786      1168.117      -0.116      15.718
2924 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
2929 ATOM TYPES      VALENCE      IDEAL      FORCE
2930   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

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2935 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019
2936 c3 c3 cl 109.500 110.330 260.419 -0.014 0.055
2937 h1 c3 cl 109.442 105.930 183.005 0.061 0.688
2938 h1 c3 cl 109.442 105.930 183.005 0.061 0.688
2939 c3 c3 cl 109.500 110.330 260.419 -0.014 0.055
2940 h1 c3 cl 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 cl 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 cl 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 cl c3 c3 cl 0.000 0 -160.000 3 0.000
2958 cl c3 c3 h1 0.000 0 -40.000 3 0.000
2959 cl 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 cl 2.647 1.083
2977 h1 h1 2.300 0.109
2978 h1 h1 2.885 -0.031
2979 h1 cl 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 c1      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 c1      2.960     -3.809     -1.287
2996 c1 h1      2.960     -3.809     -1.287
2997 c1 h1      2.647     -3.809     -1.439
2998 c1 c1      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

3086	ATOM TYPES			FF	BOND	IDEAL	FORCE		
3087	I	J		CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
3088	-----								
3089	12	1		0	1.670	1.773	2.974	-0.103	2.795
3090	5	1		0	1.000	1.093	4.766	-0.093	3.578
3091	1	1		0	1.540	1.508	4.258	0.032	0.294
3092	1	5		0	1.000	1.093	4.766	-0.093	3.578
3093	1	5		0	1.000	1.093	4.766	-0.093	3.578
3094	1	5		0	1.000	1.093	4.766	-0.093	3.578
3095	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

3100	ATOM TYPES			FF	VALENCE	IDEAL	FORCE		
3101	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
3102	-----								
3103	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3104	5	1	5	0	109.442	108.836	0.516	0.606	0.004
3105	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3106	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3107	1	1	12	0	109.500	108.679	1.056	0.821	0.016
3108	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3109	1	1	12	0	109.500	108.679	1.056	0.821	0.016
3110	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3111	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3112	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3113	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3114	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

3119	ATOM TYPES			FF	VALENCE	DELTA	FORCE CONSTANT		
3120	I	J	K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY
3121	-----								
3122	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
3123	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
3124	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
3125	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
3126	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

3134 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol

3136 T O R S I O N A L

3137
3138 ATOM TYPES FF TORSION FORCE CONSTANT
3139 I J K L CLASS ANGLE V1 V2 V3 ENERGY
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

3150 TOTAL TORSIONAL ENERGY = 1.18015 kcal/mol

3152 O U T - O F - P L A N E B E N D I N G

3153
3154 ATOM TYPES FF OOP FORCE
3155 I J K L CLASS ANGLE CONSTANT ENERGY

3156 -----
3157 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol

3159 V A N D E R W A A L S

3160
3161 ATOM TYPES
3162 I J Rij R*IJ EPSILON ENERGY
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

3173 TOTAL VAN DER WAALS ENERGY = 4.82482 kcal/mol

3175 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	c1	c3	c3	h1	0.000	0	-20.000	3	0.000
3227	c1	c3	c3	h1	0.000	0	100.000	3	0.000
3228	c1	c3	c3	c1	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 c1      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 c1      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 c1      2.547      2.064
3252 h1 h1      2.232      0.205
3253 h1 h1      2.831      -0.032
3254 h1 c1      3.129      -0.106
3255 c1 h1      3.129      -0.106
3256 c1 h1      2.547      2.064
3257 c1 c1      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 c1      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 c1      3.129      -3.809      -1.217
3271 c1 h1      3.129      -3.809      -1.217
3272 c1 h1      2.547      -3.809      -1.495
3273 c1 c1      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 I D X   T Y P E   R I N G
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 I D X   C H A R G E
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 I D X   C H A R G E
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 I D X   T Y P E   R I N G
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 c1 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

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

3365 T O T A L B O N D S T R E T C H I N G E N E R G Y = 20.19629 kcal/mol

3366

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

3368

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

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

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

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

3425 -----
3426 TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
3427

3428 V A N D E R W A A L S

3429

3430 ATOM TYPES

3431 I J Rij R*IJ EPSILON ENERGY

3432 -----

3433 5 5 2.746 2.970 0.022 -0.014

3434 5 5 2.746 2.970 0.022 -0.014

3435 5 12 2.512 3.713 0.053 2.649

3436 5 5 2.208 2.970 0.022 0.377

3437 5 5 2.746 2.970 0.022 -0.014

3438 5 12 3.280 3.713 0.053 0.009

3439 12 5 3.280 3.713 0.053 0.009

3440 12 5 2.512 3.713 0.053 2.649

3441 12 12 3.806 4.089 0.276 -0.201

3442 TOTAL VAN DER WAALS ENERGY = 5.44875 kcal/mol

3443

3444 E L E C T R O S T A T I C I N T E R A C T I O N S

3445

3446 ATOM TYPES

3447 I J Rij Qi Qj ENERGY

3448 -----

3449 12 12 3.856 -0.290 -0.290 5.432

3450 TOTAL ELECTROSTATIC ENERGY = 5.43239 kcal/mol

3451

3452 TOTAL ENERGY = 32.49359 kcal/mol

3453

3454 E N E R G Y

3455

3456

3457 B O N D S T R E T C H I N G

3458

3459 ATOM TYPES BOND IDEAL FORCE

3460 I J LENGTH LENGTH CONSTANT DELTA ENERGY

3461 -----

3462 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

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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

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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

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3572
3573   I D X   C H A R G E
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   I D X   T Y P E   R I N G
3586   1   c3   N O
3587   2   c3   N O
3588   3   h1   N O
3589   4   h1   N O
3590   5   c1   N O
3591   6   h1   N O
3592   7   h1   N O
3593   8   c1   N O
3594
3595   F O R M A L       C H A R G E S
3596
3597   I D X   C H A R G E
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   I D X   C H A R G E
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
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3621

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

3623

3624	ATOM TYPES		FF	BOND	IDEAL	FORCE		
3625	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
3626	-----							
3627	12	1	0	1.670	1.773	2.974	-0.103	2.795
3628	5	1	0	1.000	1.093	4.766	-0.093	3.578
3629	1	1	0	1.540	1.508	4.258	0.032	0.294
3630	1	5	0	1.000	1.093	4.766	-0.093	3.578
3631	1	5	0	1.000	1.093	4.766	-0.093	3.578
3632	1	5	0	1.000	1.093	4.766	-0.093	3.578
3633	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

3638	ATOM TYPES			FF	VALENCE	IDEAL	FORCE		
3639	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
3640	-----								
3641	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3642	5	1	5	0	109.442	108.836	0.516	0.606	0.004
3643	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3644	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3645	1	1	12	0	109.500	108.679	1.056	0.821	0.016
3646	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3647	1	1	12	0	109.500	108.679	1.056	0.821	0.016
3648	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3649	5	1	12	0	109.442	108.162	0.698	1.280	0.025
3650	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3651	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
3652	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

3657	ATOM TYPES			FF	VALENCE	DELTA	FORCE CONSTANT		
3658	I	J	K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY
3659	-----								
3660	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
3661	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
3662	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
3663	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
3664	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
3665	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

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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
3672      TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
3673
3674      T O R S I O N A L
3675
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
3688      TOTAL TORSIONAL ENERGY = 0.76131 kcal/mol
3689
3690      O U T - O F - P L A N E      B E N D I N G
3691
3692      ATOM TYPES              FF      OOP      FORCE
3693      I      J      K      L      CLASS      ANGLE      CONSTANT      ENERGY
3694      -----
3695      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
3696
3697      V A N      D E R      W A A L S
3698
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
3711      TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol
3712
3713      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
3714
3715      ATOM TYPES
3716      I      J      Rij      Qi      Qj      ENERGY
3717      -----
3718      12      12      3.637      -0.290      -0.290      5.759

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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

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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      Ri j      ki j      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      Ri j      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

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3817
3818   IDX TYPE   RING
3819   1 1 NO
3820   2 1 NO
3821   3 5 NO
3822   4 5 NO
3823   5 12 NO
3824   6 5 NO
3825   7 5 NO
3826   8 12 NO
3827
3828   F O R M A L   C H A R G E S
3829
3830   IDX CHARGE
3831   1 0.000000
3832   2 0.000000
3833   3 0.000000
3834   4 0.000000
3835   5 0.000000
3836   6 0.000000
3837   7 0.000000
3838   8 0.000000
3839
3840   P A R T I A L   C H A R G E S
3841
3842   IDX CHARGE
3843   1 0.290000
3844   2 0.290000
3845   3 0.000000
3846   4 0.000000
3847   5 -0.290000
3848   6 0.000000
3849   7 0.000000
3850   8 -0.290000
3851
3852   S E T T I N G   U P   C A L C U L A T I O N S
3853
3854   SETTING UP BOND CALCULATIONS...
3855   SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
3856   SETTING UP TORSION CALCULATIONS...
3857   SETTING UP OOP CALCULATIONS...
3858   SETTING UP VAN DER WAALS CALCULATIONS...
3859   SETTING UP ELECTROSTATIC CALCULATIONS...
3860
3861   A T O M   T Y P E S
3862
3863   IDX TYPE   RING
3864   1 c3 NO
3865   2 c3 NO
```

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


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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

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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

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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

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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

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3996 TOTAL ENERGY = 28.94230 kcal/mol
3997

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3998 E N E R G Y
3999

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4000

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4001 B O N D   S T R E T C H I N G
4002

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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

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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  -----

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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

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```
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 I D X   C H A R G E
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 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 . . .
4130 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 . . .
4131 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 . . .
4132 S E T T I N G   U P   O O P   C A L C U L A T I O N S . . .
4133 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 . . .
4134 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 . . .
4135
4136 A T O M   T Y P E S
4137
4138 I D X   T Y P E   R I N G
4139 1 c3   N O
4140 2 c3   N O
4141 3 h1   N O
4142 4 h1   N O
4143 5 c1   N O
4144 6 h1   N O
4145 7 h1   N O
4146 8 c1   N O
4147
4148 C H A R G E S
4149
4150 I D X   C H A R G E
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

4174	ATOM TYPES		FF	BOND	IDEAL	FORCE		
4175	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
4176	-----							
4177	5	1	0	1.000	1.093	4.766	-0.093	3.578
4178	12	1	0	1.670	1.773	2.974	-0.103	2.795
4179	5	1	0	1.000	1.093	4.766	-0.093	3.578
4180	1	1	0	1.540	1.508	4.258	0.032	0.294
4181	1	5	0	1.000	1.093	4.766	-0.093	3.578
4182	1	12	0	1.670	1.773	2.974	-0.103	2.795
4183	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

4188	ATOM TYPES			FF	VALENCE	IDEAL	FORCE		
4189	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
4190	-----								
4191	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
4192	5	1	5	0	109.442	108.836	0.516	0.606	0.004
4193	5	1	12	0	109.442	108.162	0.698	1.280	0.025
4194	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
4195	1	1	12	0	109.500	108.679	1.056	0.821	0.016
4196	5	1	12	0	109.442	108.162	0.698	1.280	0.025
4197	5	1	12	0	109.442	108.162	0.698	1.280	0.025
4198	1	1	12	0	109.500	108.679	1.056	0.821	0.016
4199	5	1	12	0	109.442	108.162	0.698	1.280	0.025
4200	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
4201	5	1	5	0	109.442	108.836	0.516	0.606	0.004
4202	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

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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

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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

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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...

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4405  SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4406  SETTING UP TORSION CALCULATIONS...
4407  SETTING UP OOP CALCULATIONS...
4408  SETTING UP VAN DER WAALS CALCULATIONS...
4409  SETTING UP ELECTROSTATIC CALCULATIONS...
4410
4411  A T O M   T Y P E S
4412
4413  IDX TYPE  RING
4414  1 c3   NO
4415  2 c3   NO
4416  3 h1   NO
4417  4 h1   NO
4418  5 c1   NO
4419  6 h1   NO
4420  7 h1   NO
4421  8 c1   NO
4422
4423  C H A R G E S
4424
4425  IDX CHARGE
4426  1 0.036009
4427  2 0.036009
4428  3 0.044101
4429  4 0.044101
4430  5 -0.124211
4431  6 0.044101
4432  7 0.044101
4433  8 -0.124211
4434
4435  S E T T I N G   U P   C A L C U L A T I O N S
4436
4437  SETTING UP BOND CALCULATIONS...
4438  SETTING UP ANGLE CALCULATIONS...
4439  SETTING UP TORSION CALCULATIONS...
4440  SETTING UP IMPROPER TORSION CALCULATIONS...
4441  SETTING UP VAN DER WAALS CALCULATIONS...
4442  SETTING UP ELECTROSTATIC CALCULATIONS...
4443
4444  E N E R G Y
4445
4446
4447  B O N D   S T R E T C H I N G
4448
4449  ATOM TYPES      FF      BOND      IDEAL      FORCE
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

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4552

4553

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

4554

4555

4556

h1	c3	1.000	1.093	1406.346	-0.093	12.163
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4557

h1	c3	1.000	1.093	1406.346	-0.093	12.163
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4558

c1	c3	1.670	1.786	1168.117	-0.116	15.718
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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		
I	J	K	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY

4568

4569

4570

c3	c3	h1	109.500	110.070	194.100	-0.010	0.019
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4571

h1	c3	h1	109.442	109.550	164.039	-0.002	0.001
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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			
I	J	K	L	CONSTANT	s	ANGLE	n	ENERGY

4587

4588

4589

h1	c3	c3	h1	0.651	0	-40.000	3	0.326
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4590

h1	c3	c3	c1	0.000	0	80.000	3	0.000
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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
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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

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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

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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 IDX CHARGE
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 IDX CHARGE
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 SETTING UP BOND CALCULATIONS...
4680 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4681 SETTING UP TORSION CALCULATIONS...
4682 SETTING UP OOP CALCULATIONS...
4683 SETTING UP VAN DER WAALS CALCULATIONS...
4684 SETTING UP ELECTROSTATIC CALCULATIONS...
4685
4686 A T O M T Y P E S
4687
4688 IDX TYPE RING
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 c1 NO
4697
4698 C H A R G E S
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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
4724   ATOM TYPES      FF      BOND      IDEAL      FORCE
4725   I      J      CLASS  LENGTH      LENGTH      CONSTANT      DELTA      ENERGY
4726   -----
4727   5      1      0      1.000      1.093      4.766      -0.093      3.578
4728   5      1      0      1.000      1.093      4.766      -0.093      3.578
4729   1      1      0      1.540      1.508      4.258      0.032      0.294
4730   1      5      0      1.000      1.093      4.766      -0.093      3.578
4731   1     12      0      1.670      1.773      2.974      -0.103      2.795
4732   1     12      0      1.670      1.773      2.974      -0.103      2.795
4733   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
4738   ATOM TYPES      FF      VALENCE      IDEAL      FORCE
4739   I      J      K      CLASS  ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
4740   -----
4741   1      1      5      0     109.500     110.549      0.636      -1.049      0.015
4742   5      1      5      0     109.442     108.836      0.516      0.606      0.004
4743   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

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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

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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

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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

```

TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol

T O R S I O N A L

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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

```

TOTAL TORSIONAL ENERGY = 3.908 kJ/mol

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

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4877 ----ATOM TYPES----- FORCE      IMPROPER_TORSION
4878 I    J    K    L    CONSTANT      s      ANGLE    n    ENERGY
4879 -----

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TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol

V A N D E R W A A L S

A T O M T Y P E S

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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

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4895  cl cl      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 cl      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 cl      3.399     -3.809     -1.121
4909  cl h1      3.399     -3.809     -1.121
4910  cl h1      3.129     -3.809     -1.217
4911  cl cl      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

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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...
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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

4999	ATOM TYPES		FF	BOND	IDEAL	FORCE		
5000	I	J	CLASS	LENGTH	LENGTH	CONSTANT	DELTA	ENERGY
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

5013	ATOM TYPES			FF	VALENCE	IDEAL	FORCE		
5014	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
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

5032	ATOM TYPES			FF	VALENCE	DELTA	FORCE CONSTANT		
5033	I	J	K	CLASS	ANGLE	ANGLE	I J	J K	ENERGY
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

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					
I J	Rij	R*IJ	EPSILON	ENERGY	

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

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


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5091      I      J      Rij      Qi      Qj      ENERGY
5092      -----
5093      12      12      2.705      -0.290      -0.290      7.743
5094      TOTAL ELECTROSTATIC ENERGY = 7.74347 kcal/mol
5095
5096      TOTAL ENERGY = 50.10353 kcal/mol
5097
5098      E N E R G Y
5099
5100
5101      B O N D      S T R E T C H I N G
5102
5103      ATOM TYPES      BOND      IDEAL      FORCE
5104      I      J      LENGTH      LENGTH      CONSTANT      DELTA      ENERGY
5105      -----
5106      h1 c3      1.000      1.093      1406.346      -0.093      12.163
5107      h1 c3      1.000      1.093      1406.346      -0.093      12.163
5108      c3 c3      1.540      1.535      1269.019      0.005      0.032
5109      c3 h1      1.000      1.093      1406.346      -0.093      12.163
5110      c3 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      ATOM TYPES      VALENCE      IDEAL      FORCE
5118      I      J      K      ANGLE      ANGLE      CONSTANT      DELTA      ENERGY
5119      -----
5120      c3 c3 h1      109.500      110.070      194.100      -0.010      0.019
5121      h1 c3 h1      109.442      109.550      164.039      -0.002      0.001
5122      h1 c3 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

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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 c1 h1      3.280     -3.809     -1.161
5186 c1 c1      2.655     10.728      4.041
5187      TOTAL ELECTROSTATIC ENERGY =      1.607 kJ/mol
5188

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5189 | TOTAL ENERGY = 134.023 kJ/mol