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BIM2005: Homework I

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

Preparation

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

```
1
 2
 3
    C2H4C12
 4
5
   0 1
 6
 7
    C 1 1.54
 8
      н 1 1.0 2 109.5
9
      H 1 1.0 2 109.5 3 120.0
     Cl 1 1.67 2 109.5 4 120.0
10
      H 2 1.0 1 109.5 5 -120.0
11
      H 2 1.0 1 109.5 5 120.0
12
      Cl 2 1.67 1 109.5 5 0.0
13
```

Procedure

Details of implementation could be found in the GitHub repository <u>zcorn2017/BIM2001-HWK1</u> (github.com).

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

- 1. We <u>added the headers to the code manually</u> for it to be recognised by <u>OpenBabel</u>
- 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 <u>the Python bindings to the OpenBabel C++ library</u>.
- 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 <u>Appendix I</u>).
- 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 <u>Pandas</u> and it could be found in <u>Results</u> II.
- 10. A lineplot of relative energy in kcal/mol with respect to angle in degrees is displayed by [Seaborn] [https://seaborn.pydata.org/]. For details, please refer to Result III

GitHub Repo File Hierarchy

```
- C2H4Cl2 100 degrees.gzmat
 6
          - C2H4Cl2 100 degrees.xyz
 8
          - C2H4Cl2 120 degrees.gzmat
9
        ─ C2H4Cl2 120 degrees.xyz
10
          — C2H4Cl2_140_degrees.gzmat
          - C2H4Cl2 140 degrees.xyz
11
        C2H4Cl2_160_degrees.gzmat
12
          - C2H4Cl2_160_degrees.xyz
13
        — C2H4Cl2 180 degrees.gzmat
14
          — C2H4Cl2_180_degrees.xyz
15
          — C2H4Cl2 200 degrees.gzmat
16
17
        — C2H4Cl2 200 degrees.xyz
18
          — C2H4Cl2_20_degrees.gzmat
          - C2H4Cl2 20 degrees.xyz
19
          — C2H4Cl2 220 degrees.gzmat
2.0
          - C2H4Cl2_220_degrees.xyz
2.1
        — C2H4Cl2 240 degrees.gzmat
2.2
23
         — C2H4Cl2_240_degrees.xyz
          — C2H4Cl2 260 degrees.gzmat
24
25
        - C2H4Cl2 260 degrees.xyz
        C2H4Cl2_280_degrees.gzmat
26
          - C2H4Cl2 280 degrees.xyz
27
          — C2H4Cl2 300 degrees.gzmat
28
         — C2H4Cl2 300 degrees.xyz
2.9
30
         — C2H4Cl2 320 degrees.gzmat
31
        — C2H4Cl2_320_degrees.xyz
        — C2H4Cl2 340 degrees.gzmat
32
33
        — C2H4Cl2_340_degrees.xyz
          — C2H4Cl2_360_degrees.gzmat
34
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
          — C2H4Cl2_80_degrees.gzmat
40
        C2H4Cl2 80 degrees.xyz
41
     — DATA
                                        // .csv table file containing all the energy
42
    data
        — data.csv
43
          data in KJ.csv
44
        data in Kcal.csv
45
      - README.md
                                       // This file you are in
46
     - XYZ GAMAT SUMMARY.md
                                       // (Not Important)
47
    - code2mkdoc.py
                                        // The script used to facilitate the processing
48
    of the documentation
     — file tree.txt
                                      // The file tree (Not Important)
49
    └─ requirements.txt
50
                                      // All the requirements in my environment to run
    this script and some of them are redundant for you
    - rel_energy.png
                                      // Lineplot of the relative energy in kcal/mol
```

```
52 Lorsion_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 $0\,^\circ$

• ./CODE/C2H4Cl2_0_degrees.gzmat

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

./CODE/C2H4Cl2_0_degrees.xyz

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

Torsion Angle at $20\,^\circ$

• ./CODE/C2H4Cl2_20_degrees.gzmat

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

• ./CODE/C2H4Cl2_20_degrees.xyz

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

Torsion Angle at $40\,^\circ$

• ./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
```

./CODE/C2H4Cl2_40_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 40 degrees.gzmat
   С
             0.00000
                          0.00000
3
                                        0.00000
4
   C
            1.54000
                          0.00000
                                        0.00000
5
            -0.33381
                          0.00000
   H
                                       -0.94264
                         -0.81635
            -0.33381
                                        0.47132
6
7
           -0.55746
                          1.36331
                                        0.78711
   Cl
            1.87381
                          0.60592
                                       -0.72211
8
   Η
                        -0.92832
9
            1.87381
                                       -0.16369
            2.09746
10
  Cl
                          0.53841
                                        1.47927
11
```

Torsion Angle at $60\,^\circ$

• ./CODE/C2H4Cl2_60_degrees.gzmat

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

• ./CODE/C2H4Cl2_60_degrees.xyz

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

Torsion Angle at $80\,^\circ$

• ./CODE/C2H4Cl2_80_degrees.gzmat

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

• ./CODE/C2H4Cl2_80_degrees.xyz

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

Torsion Angle at $100\,^\circ$

• ./CODE/C2H4Cl2_100_degrees.gzmat

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

• ./CODE/C2H4Cl2_100_degrees.xyz

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

Torsion Angle at $120\,^\circ$

• ./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
```

./CODE/C2H4Cl2_120_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 120 degrees.gzmat
   C
             0.00000
                         0.00000
3
                                        0.00000
4
   C
            1.54000
                          0.00000
                                        0.00000
            -0.33381
                          0.00000
5
   H
                                       -0.94264
            -0.33381
                        -0.81635
                                        0.47132
6
7
           -0.55746
                         1.36331
                                        0.78711
   Cl
            1.87381
                          0.81635
                                        0.47132
8
   Η
                          0.00000
9
            1.87381
                                       -0.94264
            2.09746
10
  Cl
                        -1.36331
                                        0.78711
11
```

Torsion Angle at $140\,^\circ$

• ./CODE/C2H4Cl2_140_degrees.gzmat

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

• ./CODE/C2H4Cl2_140_degrees.xyz

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

Torsion Angle at $160\,^\circ$

• ./CODE/C2H4Cl2_160_degrees.gzmat

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

• ./CODE/C2H4Cl2_160_degrees.xyz

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

Torsion Angle at $180\,^\circ$

• ./CODE/C2H4Cl2_180_degrees.gzmat

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

• ./CODE/C2H4Cl2_180_degrees.xyz

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

Torsion Angle at $200\,^\circ$

• ./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
```

./CODE/C2H4Cl2_200_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 200 degrees.gzmat
   С
             0.00000
                         0.00000
3
                                        0.00000
4
   C
            1.54000
                         0.00000
                                        0.00000
            -0.33381
                         0.00000
5
   H
                                       -0.94264
            -0.33381
                        -0.81635
                                        0.47132
6
7
           -0.55746
                         1.36331
   Cl
                                       0.78711
                        -0.32240
                                       0.88579
8
   H
            1.87381
9
            1.87381
                         0.92832
                                       -0.16369
            2.09746
                        -1.01188
10 Cl
                                       -1.20592
11
```

Torsion Angle at $220\,^\circ$

• ./CODE/C2H4Cl2_220_degrees.gzmat

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

• ./CODE/C2H4Cl2_220_degrees.xyz

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

Torsion Angle at $240\,^\circ$

• ./CODE/C2H4Cl2_240_degrees.gzmat

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

• ./CODE/C2H4Cl2_240_degrees.xyz

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

Torsion Angle at $260\,^\circ$

• ./CODE/C2H4Cl2_260_degrees.gzmat

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

• ./CODE/C2H4Cl2_260_degrees.xyz

```
8
1
  ./CODE/C2H4Cl2_260_degrees.gzmat
2
           0.00000
                        0.00000
                                      0.00000
3
                        0.00000
4
           1.54000
                                      0.00000
5
  H
           -0.33381
                        0.0000
                                    -0.94264
                       -0.81635
6
  H
           -0.33381
                                      0.47132
          -0.55746
7
                        1.36331
                                     0.78711
           1.87381
                       -0.92832
                                     0.16369
8
  H
           1.87381
                        0.60592
                                     0.72211
9
   Cl
           2.09746
                        0.53841
                                     -1.47927
10
11
```

Torsion Angle at $280\,^\circ$

• ./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
```

./CODE/C2H4Cl2_280_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 280 degrees.gzmat
   C
             0.00000
                         0.00000
3
                                        0.00000
4
   C
            1.54000
                         0.00000
                                        0.00000
            -0.33381
                          0.00000
5
   H
                                       -0.94264
            -0.33381
                        -0.81635
                                        0.47132
6
7
           -0.55746
                         1.36331
   Cl
                                       0.78711
                         -0.92832
8
   Η
            1.87381
                                       -0.16369
9
            1.87381
                          0.32240
                                        0.88579
10
  Cl
            2.09746
                         1.01188
                                       -1.20592
11
```

Torsion Angle at $300\,^\circ$

• ./CODE/C2H4Cl2_300_degrees.gzmat

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

• ./CODE/C2H4Cl2_300_degrees.xyz

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

Torsion Angle at $320\,^\circ$

• ./CODE/C2H4Cl2_320_degrees.gzmat

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

• ./CODE/C2H4Cl2_320_degrees.xyz

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

Torsion Angle at $340\,^\circ$

• ./CODE/C2H4Cl2_340_degrees.gzmat

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

• ./CODE/C2H4Cl2_340_degrees.xyz

```
1
   8
   ./CODE/C2H4Cl2_340_degrees.gzmat
2
           0.00000
                        0.00000
                                       0.00000
3
                         0.00000
4
            1.54000
                                       0.00000
5
  H
           -0.33381
                         0.0000
                                      -0.94264
                        -0.81635
6
  H
           -0.33381
                                      0.47132
           -0.55746
7
                         1.36331
                                      0.78711
           1.87381
                        -0.32240
                                      -0.88579
8
   Η
           1.87381
                        -0.60592
                                       0.72211
9
   Cl
           2.09746
                         1.55030
                                       0.27336
10
11
```

Torsion Angle at $360\,^\circ$

• ./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
```

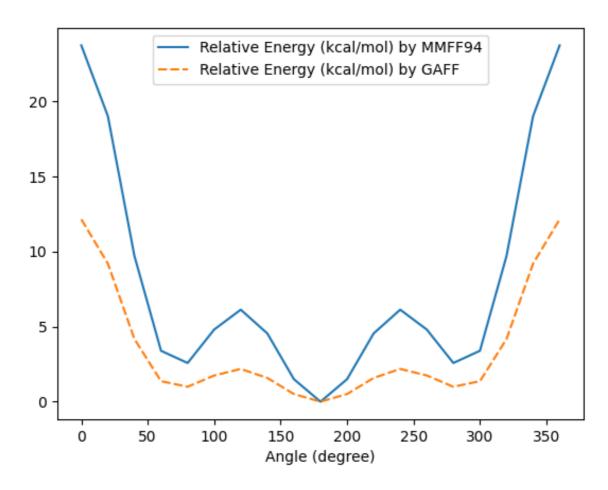
• ./CODE/C2H4Cl2_360_degrees.xyz

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

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

```
15
    C2H4C12
16
17
18
    0 1
19
20
    C 1 1.54
21
    н 1 1.0 2 109.5
    H 1 1.0 2 109.5 3 120.0
2.2
    Cl 1 1.67 2 109.5 4 120.0
23
   H 2 1.0 1 109.5 5 -120.0
24
   н 2 1.0 1 109.5 5 120.0
25
    Cl 2 1.67 1 109.5 5 0.0
26
    0.00
27
28
29
    # Store the code of the 18 modified molecules as a list
    code_list = []
30
31
32
    for n in range(0, 19):
        \# Count the reference number of the atoms to determine which atom to
33
    manipulate
34
        atom_counter = 0
35
        # .xyz code after conversion
36
        code_aft_cnv = ""
37
38
        for line in gzmat_code.split("\n"):
39
            words = line.split()
40
41
            # if the line is empty, do not make modifications
            if len(words) == 0:
42
43
                pass
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")
                code aft cnv = code aft cnv + "-".join(words) + "\n"
49
50
                continue
51
            elif words[0].isalpha() and len(words[0]) in [1, 2]:
52
                atom_counter = atom_counter + 1
53
54
55
                if atom_counter in [6, 7, 8]:
56
                     words[-1] = str(float(words[-1]) + 20 * n)
57
58
                     if float(words[-1]) >= 360:
                         words[-1] = str(float(words[-1]) - 360)
59
60
            code_aft_cnv = code_aft_cnv + " ".join(words) + "\n"
61
        code_list.append(code_aft_cnv)
62
```

```
63
 64
     # Write the code to the .gzmat format
65
     for code, angle in zip(code list, range(0, 380, 20)):
         with open(f"./CODE/C2H4Cl2 {angle} degrees.gzmat", "w") as gzmat file:
 66
 67
             gzmat file.write(code)
 68
     # Set the input format to gzmat and the output format to xyz
 69
     OB converter = openbabel.OBConversion()
 70
     OB_converter.SetInAndOutFormats("gzmat", "xyz")
 71
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
     for angle in range(0, 380, 20):
 77
78
         mol C2H4Cl2 = openbabel.OBMol()
79
80
         # Use MMFF94 and GAFF to calculate the absolute energy
         OB_converter.ReadFile(mol_C2H4Cl2, f"./CODE/C2H4Cl2_{angle}_degrees.gzmat")
81
 82
         MMFF94_forcefield = openbabel.OBForceField.FindForceField("MMFF94")
83
         GAFF forcefield = openbabel.OBForceField.FindForceField("GAFF")
 84
 85
         # Redirect the log output to std::cout
86
 87
         MMFF94 forcefield.SetLogToStdOut()
88
         GAFF forcefield.SetLogToStdOut()
89
 90
         # Set the priority of log to high
         MMFF94 forcefield.SetLogLevel(openbabel.OBFF LOGLVL HIGH)
91
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
         # Energy of C 2H 4Cl 2 with Torsion Angle at `angle` Degrees Starts
98
         # by MMFF94
99
         MMFF94 abs energy in Kcal = MMFF94 forcefield.Energy()
100
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
         OB converter.WriteFile(mol C2H4Cl2, f"./CODE/C2H4Cl2 {angle} degrees.xyz")
107
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)
     ref_GAFF_energy_in_KJ = min(GAFF_abs_energy_in_KJ_list)
111
```

```
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
     GAFF_abs_energy_in_Kcal_vec = GAFF_abs_energy_in_KJ_vec / KCAL2KJ_CONSTANT
117
118
119
     MMFF94_rel_energy_in_Kcal_vec = MMFF94_abs_energy_in_Kcal_vec -
     ref_MMFF94_energy_in_Kcal
     GAFF_rel_energy_in_KJ_vec = GAFF_abs_energy_in_KJ_vec - ref_GAFF_energy_in_KJ
120
121
122
     MMFF94 rel energy in KJ vec = MMFF94 abs energy in KJ vec - KCAL2KJ CONSTANT *
     ref_MMFF94_energy_in_Kcal
     GAFF_rel_energy_in_Kcal_vec = GAFF_abs_energy_in_Kcal_vec - ref_GAFF_energy_in_KJ
123
     / KCAL2KJ CONSTANT
124
125
     data_in_Kcal_dict = {
126
         "Absolute Energy (kcal/mol) by MMFF94" :
     MMFF94 abs energy in Kcal vec.tolist(),
127
         "Absolute Energy (kcal/mol) by GAFF" : GAFF_abs_energy_in_Kcal_vec.tolist(),
128
         "Relative Energy (kcal/mol) by MMFF94" :
     MMFF94 rel energy in Kcal vec.tolist(),
         "Relative Energy (kcal/mol) by GAFF" : GAFF rel energy in Kcal vec.tolist()
129
130
131
     data in KJ dict = {
         "Absolute Energy (kJ/mol) by MMFF94" : MMFF94_abs_energy_in_KJ_vec.tolist(),
132
         "Absolute Energy (kJ/mol) by GAFF" : GAFF abs energy in KJ vec.tolist(),
133
134
         "Relative Energy (kJ/mol) by MMFF94" : MMFF94_rel_energy_in_KJ_vec.tolist(),
         "Relative Energy (kJ/mol) by GAFF" : GAFF_rel_energy_in_KJ_vec.tolist()
135
136
137
138
     data in Kcal df = pd.DataFrame(data in Kcal dict,index=[angle for angle in
     range(0, 380, 20)])
139
     data_in_KJ_df = pd.DataFrame(data_in_KJ_dict,index=[angle for angle in range(0,
     380, 20)1)
140
141
     data_in_Kcal_df.to_csv("./DATA/data_in_Kcal.csv")
     data in KJ df.to csv("./DATA/data in KJ.csv")
142
143
144
     data dict = {
         "Absolute Energy (kcal/mol) by MMFF94":
145
     np.round(MMFF94_abs_energy_in_Kcal_vec.tolist(), 3),
         "Absolute Energy (kcal/mol) by GAFF":
146
     np.round(GAFF abs energy in Kcal vec.tolist(), 3),
         "Relative Energy (kcal/mol) by MMFF94":
147
     np.round(MMFF94 rel energy in Kcal vec.tolist(), 3),
         "Relative Energy (kcal/mol) by GAFF":
148
     np.round(GAFF_rel_energy_in_Kcal_vec.tolist(), 3),
```

```
149
         "Absolute Energy (kJ/mol) by MMFF94":
     np.round(MMFF94 abs energy in KJ vec.tolist(), 3),
150
         "Absolute Energy (kJ/mol) by GAFF":
     np.round(GAFF_abs_energy_in_KJ_vec.tolist(), 3),
151
         "Relative Energy (kJ/mol) by MMFF94":
     np.round(MMFF94_rel_energy_in_KJ_vec.tolist(), 3),
152
         "Relative Energy (kJ/mol) by GAFF":
     np.round(GAFF_rel_energy_in_KJ_vec.tolist(), 3)
153
154
     data df = pd.DataFrame(data dict, index=[angle for angle in range(0, 380, 20)])
155
     data df.index.name = "Angle (degree)"
156
157
     data_df.to_csv("./DATA/data.csv")
158
159
     # Plot the lineplot of relative energy in kcal/mol with respect to angle in
     degrees
     lineplot df = data df.loc[:,["Relative Energy (kcal/mol) by MMFF94","Relative
160
     Energy (kcal/mol) by GAFF"]]
     sns.lineplot(data=lineplot_df)
161
162
163 | plt.savefig("rel_energy.png")
```

code2mkdoc.py

```
1 # This script aims to facilitate the gerneration of the documentation
   # which is not part of the main program.
 2.
   # For the homework solution,
 4
   # pls refer to torsion_angle.py
5
 6
    import sys
7
    # Add heading to the Markdown file
8
9
    def mkdoc heading(heading, level=1):
        heading level = "#" * level + " " + heading + "\n"
10
        print(f"""
11
    {heading_level}""")
12
13
14
    # Wrap the code to make it be recognised by the Markdown parser
15
    def wrap_code(code, lang="python"):
        print(f"""\``{lang}
16
17
    {code}
        *** n n n )
18
19
20
    # Redirect the output to the file writing object.
    with open("XYZ GAMAT SUMMARY.md", "w") as sys.stdout:
21
22
        for angle in range(0, 380, 20):
            mkdoc_heading(f"Torsion Angle at {angle}$\degree$", level= 4)
2.3
24
25
            print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.gzmat\n")
```

II Analysis of the Energy

```
1
2
   АТОМ
           TYPES
3
 4 IDX TYPE RING
5 1 1 NO
6 2 1 NO
 7
   3 5 NO
8 4 5 NO
  5 12 NO
10 6 5 NO
11 7 5 NO
12 8 12 NO
13
14 FORMAL CHARGES
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 PARTIAL CHARGES
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
   8 -0.290000
36
37
38
   SETTING UP CALCULATIONS
39
```

```
40 SETTING UP BOND CALCULATIONS...
   SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
41
42 SETTING UP TORSION CALCULATIONS...
43 SETTING UP OOP CALCULATIONS...
44
   SETTING UP VAN DER WAALS CALCULATIONS...
45
   SETTING UP ELECTROSTATIC CALCULATIONS...
46
47 ATOM TYPES
48
49 IDX TYPE RING
50 1 c3 NO
51 2 c3 NO
52 3 h1 NO
53 4 h1 NO
54 5 cl NO
55 6 h1 NO
56 7 h1 NO
57 8 cl NO
58
59 CHARGES
60
61 IDX CHARGE
62 1 0.036009
63 2 0.036009
64 3 0.044101
65 4 0.044101
66 5 -0.124211
67
   6 0.044101
68 7 0.044101
69 8 -0.124211
70
71 SETTING UP CALCULATIONS
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 ENERGY
81
82
83 BOND STRETCHING
84
85 ATOM TYPES FF BOND
                            IDEAL
                                      FORCE
                                     CONSTANT
86
   I J CLASS LENGTH
                            LENGTH
                                                 DELTA
                                                          ENERGY
87
                                     4.766 -0.093
   5 1 0 1.000 1.093
```

	_								
89			0			1.093			3.578
90			0		540	1.508	4.258	0.032	0.294
91			0			1.093		-0.093	3.578
92			0			1.773		-0.103	2.795
93	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
94	1							-0.103	2.795
95		TOTA	AL BOND	STRETCH	HING ENER	GY = 20.1962	29 kcal/mol		
96									
97	A N	GLI	Е ВЕ	NDII	N G				
98									
99						IDEAL			
100									ENERGY
101						110.549		-1.049	0.015
103								0.606	
104				0		108.162		1.280	
105	1	1	5	0	109.500	110.549			
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		TOTA	AL ANGL	E BENDI	NG ENERGY	= 0.20058	kcal/mol		
115									
116	ST	R E 7	ГСН	BENI	O I N G				
117	7.00	/ MVDI	7.C	DD.	WAT ENGE	DELEN	HODGE	CONCEANE	
118		4 TYPE		FF	VALENCE			CONSTANT	ENEDGY
119 120								J К	
121			 5			-1.049		0.070	
122	5	1		0	109.442	0.606	0.115	0.115	-0.033
123	5	1	12	0		1.280			-0.121
124	1	1	5	0		-1.049			-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		TOTA	AL STRE	TCH BENI	DING ENER	GY = -0.6959	93 kcal/mol		
134									
135	ТО	R S I	ONA	L					
136									

					ANGLE					
										 4 0.59
5	1	1	5	0 -	120.000	0.28	4 –	1.386	0.31	4 -0.65
5	1	1	12	0	120.000	0.678	8 –	0.602	0.39	8 0.11
5	1	1	5	0	120.000	0.28	4 –	1.386	0.31	4 -0.65
5	1	1	5	0	0.000	0.28	4 –	1.386	0.31	4 0.59
5	1	1	12	0 -	120.000	0.678	8 –	0.602	0.39	8 0.13
					120.000					
12	1	1	5	0	120.000	0.678	8 –	0.602	0.39	8 0.11
12	1	1	12	0	-0.000	0.00	0	0.000	0.89	3 0.89
	TOTAL	TORS	IONAL	ENERGY :	1.24400) kcal	/mol			
O U	T - O	F - P	LAN	E B	ENDIN	G				
					OOP					
Ι	J	K	L	CLASS	ANGLE	CONS	TANT	EN	IERGY	
	TOTAL	OUT-	OF-PLA	NE BEND	ING ENERGY	z = 0	.0000	0 kcal	L/mol	
V A	N D	E R	WAA	LS						
ATOM	1 TYPES	;								
I	J		Rij	R*I	J EPSII	LON	ENER	.GY		
					70 0.0					
					70 0.0					
					13 0.0					
5	5		2.746	2.9	70 0.0)22	-0.0	14		
5	5		2.208	2.9	70 0.0)22	0.3	77		
5	12		3.280	3.7	13 0.0)53	0.0	09		
12	5		3.280	3.7	13 0.0)53	0.0	09		
12	5		3.280	3.7	13 0.0)53	0.0	09		
12	12		2.655	4.0	39 0.2	276	20.6	55		
	TOTAL	VAN	DER WA	ALS ENE	RGY = 21.4	1512	kcal/	mol		
ЕL	E C T	R O S	тат	I C	INTER	A C T	ΙO	N S		
ATOM	1 TYPES	;								
I	J		Rij	Qi	(Ωj	E	NERGY		
12	12	2.	705	-0.290	-0.290) .	7.743			
	TOTAL	ELEC	TROSTA	TIC ENE	RGY = 7.7	74347]	kcal/	mol		
TOTA	AL ENER	RGY =	50.103	53 kcal	/mol					
E N	ERG	Y								
11	_ K 0	•								

B O N D	STR	ЕТСЬ	HING						
3.mov. mv		_		T00.07					
				FORCE					
				CONSTA					
				1406.346					
				1406.346					
				1269.019					
				1406.346					
				1168.117					
				1406.346					
				1168.117					
				RGY = 80					
ANGL	Е ВЕ	NDIN	1 G						
ATOM TYI	PES	VALENC	CE II	DEAL	FORCE				
I J	K	ANGLE	E AN	NGLE C	CONSTAN	IT	DELT	A	ENERGY
c3 c3 h	1 109.	500 1	110.070	194.1	100	-0.0	10	0.019	1
n1 c3 h	109.	442 1	109.550	164.0	39	-0.0	02	0.001	
11 c3 c	l 109.	442 1	105.930	183.0	005	0.0	61	0.688	1
c3 c3 h	109.	500 1	110.070	194.1	L00	-0.0	10	0.019	1
23 c3 c	l 109.	500 1	110.330	260.4	119	-0.0	14	0.055	
n1 c3 c	l 109.	442 1	105.930	183.0	05	0.0	61	0.688	}
c3 c3 h	109.	500 1	110.070	194.1	100	-0.0	10	0.019	
h1 c3 h	1 109.	442 1	109.550	164.0)39	-0.0	02	0.001	
h1 c3 c	l 109.	442 1	105.930	183.0	005	0.0	61	0.688	
c3 c3 h	1 109.	500 1	110.070	194.1	100	-0.0	10	0.019	1
c3 c3 c	l 109.	500 1	110.330	260.4	119	-0.0	14	0.055	i
				183.0			61	0.688	ł
TOT	ral angl	E BENDIN	NG ENERGY	Z = 2.9	938 kJ/	/mol			
r o r s	I O N A	L							
				_		SION	-	ENEDGY	
				S					
				0.00					•
				-120.00					
				120.00			0.000		
				120.00			1.303		
				0.00			1.303		
			0				0.000		
				-120.00					
				120.00					
				-0.00			0.000		
				5.210 k					
10.					.,				

```
236 IMPROPER TORSIONAL
237
238 ----ATOM TYPES---- FORCE IMPROPER_TORSION
    I J K L CONSTANT S ANGLE n
239
240
    _____
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
241
242
243 VAN DER WAALS
244
245 ATOM TYPES
246
    I J
            Rij kij ENERGY
247
           2.208
248 h1 h1
                   0.251
249 h1 h1
           2.746 -0.033
           3.280 -0.134
250 h1 cl
251 h1 h1
           2.746
                  -0.033
252 h1 h1
           2.208
                  0.251
253 h1 cl
           3.280 -0.134
           3.280
254 cl h1
                  -0.134
255 cl h1
           3.280
                  -0.134
256 cl cl
                  44.245
            2.655
     TOTAL VAN DER WAALS ENERGY = 44.146 kJ/mol
257
258
259 ELECTROSTATIC INTERACTIONS
260
261 ATOM TYPES
    I J
            Rij 332.17*QiQj ENERGY
262
263
          2.208 1.352
264 h1 h1
                         0.613
265 h1 h1
           2.746
                   1.352
                          0.493
266 h1 cl
           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 cl
           3.280
                  -3.809 -1.161
           3.280 -3.809 -1.161
270 cl h1
271 cl h1
           3.280
                  -3.809 -1.161
                          4.041
272 cl cl
           2.655
                  10.728
     TOTAL ELECTROSTATIC ENERGY = 1.607 kJ/mol
273
274
275 TOTAL ENERGY = 134.023 kJ/mol
276
277 ATOM TYPES
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 FORMAL CHARGES
 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 PARTIAL CHARGES
 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 ATOM TYPES
 314
 315 IDX TYPE RING
 316 1 c3 NO
 317 2 c3 NO
 318 | 3 h1 NO
 319
     4 h1 NO
 320 5 cl NO
     6 h1 NO
 321
     7 h1 NO
 322
 323 8 cl NO
 324
 325 FORMAL CHARGES
 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
    PARTIAL CHARGES
338
    IDX CHARGE
339
340
    1 0.036009
    2 0.036009
341
    3 0.044101
342
    4 0.044101
343
344
    5 -0.124211
345
    6 0.044101
346 7 0.044101
    8 -0.124211
347
348
    ENERGY
349
350
351
    352
353
354
    ATOM TYPES FF BOND
                          IDEAL
                                    FORCE
     I J
                                              DELTA
            CLASS LENGTH
                          LENGTH
                                   CONSTANT
355
                                                       ENERGY
356
357
     5
        1
              0
                   1.000
                            1.093
                                     4.766
                                              -0.093
                                                        3.578
358
     5
        1
              0
                   1.000
                            1.093
                                     4.766
                                              -0.093
                                                        3.578
359
     1
        1
              0
                   1.540
                           1.508
                                     4.258
                                              0.032
                                                        0.294
       5
360
     1
              0
                   1.000
                            1.093
                                     4.766
                                              -0.093
                                                        3.578
361
     1
       12
              0
                    1.670
                            1.773
                                      2.974
                                              -0.103
                                                        2.795
        5
                                      4.766
362
     1
              0
                   1.000
                            1.093
                                              -0.093
                                                       3.578
363
     1 12
              0
                    1.670
                            1.773
                                      2.974
                                              -0.103
                                                        2.795
364
        TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
365
366
    ANGLE BENDING
367
    ATOM TYPES FF VALENCE IDEAL FORCE
368
                                       CONSTANT
369
    I J K
                 CLASS ANGLE
                               ANGLE
                                                  DELTA
                                                           ENERGY
370
    ______
                 0
                     109.500 110.549
        1
            5
371
     1
                                          0.636
                                                  -1.049
                                                            0.015
                                         0.516
372
     5
        1
            5
                  0
                     109.442
                              108.836
                                                  0.606
                                                           0.004
373
     5
        1 12
                 0
                     109.442
                              108.162
                                          0.698
                                                  1.280
                                                           0.025
374
     1
        1 5
                  0
                      109.500
                              110.549
                                          0.636
                                                  -1.049
                                                            0.015
375
            12
                 0
                     109.500
                              108.679
                                          1.056
                                                  0.821
                                                           0.016
     1
        1
     5
        1 12
                     109.442
                                          0.698
                                                  1.280
376
                  0
                              108.162
                                                            0.025
         1
            5
                  0
                      109.500
                             110.549
                                          0.636
                                                  -1.049
                                                           0.015
377
     1
            5
378
     5
        1
                 0
                     109.442
                              108.836
                                          0.516
                                                  0.606
                                                           0.004
379
     5
        1 12
                 0
                     109.442
                              108.162
                                          0.698
                                                  1.280
                                                            0.025
                     109.500
                             110.549
380
     1
         1
            5
                  0
                                          0.636
                                                  -1.049
                                                           0.015
                     109.500
            12
                 0
                              108.679
                                          1.056
                                                  0.821
                                                           0.016
381
     1
        1
382
     5
        1
           12
                  0 109.442 108.162
                                          0.698
                                                  1.280
                                                            0.025
```

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

5	5	2.638	2.970	0.022	0.001		
5	12	3.399	3.713	0.053	-0.028		
5	5	2.831	2.970	0.022	-0.019		
5	5	2.232	2.970	0.022	0.328		
5	12	3.129	3.713	0.053	0.104		
12	5	3.129	3.713	0.053	0.104		
12	5	3.399	3.713	0.053	-0.028		
12	12	2.711	4.089	0.276	16.993		
	TOTAI	L VAN DER WA	AALS ENERG	Y = 17.7815	3 kcal/mol		
ΞL	ЕСТ	ROSTA	ric i	NTERAC	TIONS		
MOTA	TYPES	5					
I	J	Rij	Qi	Qj	ENERGY	7	
						-	
12	12	2.761	-0.290	-0.290	7.587		
	TOTAI	L ELECTROST	ATIC ENERG	Y = 7.5872	1 kcal/mol		
ATO	L ENEF	RGY = 45.389	946 kcal/m	ol			
E N	E R G	Y					
3 0	N D	STRETO	CHING				
3 0	N D	STRET	CHING				
		S T R E T (FORCE			
MOTA	TYPES		IDEAL		T DELTA	A ENERG	Y
ATOM I	TYPES J	BOND LENGTH	IDEAL LENGTH	CONSTAN	T DELTA		Y
ATOM I	TYPES J	S BOND LENGTH	IDEAL LENGTH	CONSTAN			Y
ATOM I n1 c	TYPES J	S BOND LENGTH	IDEAL LENGTH	CONSTAN 		12.163	Y
ATOM I n1 c n1 c	TYPES J 3 3	5 BOND LENGTH 1.000 1.000	IDEAL LENGTH 1.093 1.093	CONSTAN 1406.346 1406.346 1269.019	-0.093 -0.093 0.005	12.163 12.163 0.032	Y
ATOM I h1 c h1 c c3 c	TYPES J 3 3 3	S BOND LENGTH 1.000 1.000 1.540 1.000	IDEAL LENGTH 1.093 1.093 1.535 1.093	CONSTAN 1406.346 1406.346 1269.019 1406.346	-0.093 -0.093 0.005 -0.093	12.163 12.163 0.032	Y
ATOM I h1 c h1 c c3 c c3 h	TYPES J 3 3 3 1	5 BOND LENGTH 1.000 1.000 1.540 1.000 1.670	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718	Y
ATOM I h1 c h1 c c3 c c3 h c3 c	TYPES J 3 3 3 1	5 BOND LENGTH 1.000 1.000 1.540 1.000 1.670	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117	-0.093 -0.093 0.005 -0.093	12.163 12.163 0.032 12.163 15.718	Y
ATOM I n1 c n1 c n3 c c3 h c3 c c3 h	TYPES J 3 3 3 1 1	S BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346	-0.093 -0.093 0.005 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163	Y
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h	TYPES J 3 3 1 1 1	S BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163	Y
ATOM I n1 c n1 c c3 c c3 h c3 c c3 h	TYPES J 3 3 1 1 1	5 BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163	У
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c	TYPES J 3 3 1 1 TOTAL	5 BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163	Y
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c	TYPES J 3 3 1 1 TOTAL	1.000 1.000 1.540 1.000 1.670 1.670 1.670	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163	Y
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h	TYPES J 3 3 1 1 TOTAL	1.000 1.000 1.540 1.000 1.670 1.670 1.670	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 RGY = 80.	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163	Y
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c	TYPES J 3 3 1 1 TOTAL G L E TYPES	E BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000 1.670 E BOND STREE	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163 15.718	
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c	TYPES J 3 3 1 1 TOTAL G L E TYPES J	E BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000 1.670 E BOND STREE B E N D E K ANG	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 RGY = 80.	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116 122 kJ/mol	12.163 12.163 0.032 12.163 15.718 12.163 15.718	ENERGY
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c	TYPES J 3 3 1 1 TOTAL G L E TYPES J	B BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000 1.670 B B N D STREE	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 RGY = 80.	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116 122 kJ/mol	12.163 12.163 0.032 12.163 15.718 12.163 15.718	ENERGY
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c A N ATOM I c3 c	TYPES J TOTAL G L E TYPES J	BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000 1.670 E BOND STREE B E N D E VALI K ANO 109.500	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 RGY = 80. DEAL F NGLE CO	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116 122 kJ/mol	12.163 12.163 0.032 12.163 15.718 12.163 15.718	ENERGY
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c h1 c	TYPES J TOTAL G L E TYPES J TYPES J TYPES	BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000 1.670 E BOND STREE B E N D E VALI K ANO 109.500	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 RGY = 80. DEAL F NGLE CO 194.10 164.03	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116 122 kJ/mol	12.163 12.163 0.032 12.163 15.718 12.163 15.718 DELTA 0.019	ENERGY
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c A N ATOM I c3 c h1 c	TYPES J TOTAL G L E TYPES J TYPES J TYPES J TYPES A 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	B BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.000 1.670 B E N D : B E N D : WALL K ANG 109.500 109.442	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 RGY = 80. DEAL F NGLE CO	-0.093 -0.093 -0.093 -0.093 -0.116 -0.093 -0.116 122 kJ/mol	12.163 12.163 0.032 12.163 15.718 12.163 15.718 DELTA DELTA 0.019 2.0.001 0.688	ENERGY
ATOM I h1 c h1 c c3 c c3 h c3 c c3 h c3 c h1 c h1 c h1 c c3 c	TYPES J 3 3 3 1 1 1 TOTAL G L E TYPES J 3 h1 3 h1 3 c1	B E N D : B E N D : S VALI K ANG 109.500 109.442 109.500	IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786 ICHING ENE	CONSTAN 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 RGY = 80. DEAL F NGLE CO 194.10 164.03 183.00 194.10	-0.093 -0.093 -0.093 -0.093 -0.116 -0.093 -0.116 122 kJ/mol	12.163 12.163 0.032 12.163 15.718 12.163 15.718 DELTA DELTA 0.019 0.088 0.0019	ENERGY

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

```
530 ATOM TYPES
531
               Rij 332.17*QiQj ENERGY
532 -----
533 h1 h1
            2.232
                    1.352
                             0.606
 534 h1 h1
            2.638
                    1.352
                            0.513
            3.399 -3.809 -1.121
535 h1 cl
536 h1 h1
            2.831
                    1.352
                            0.478
 537 h1 h1
            2.232
                    1.352
                            0.606
538 h1 cl
            3.129 -3.809 -1.217
539 cl h1
            3.129 -3.809 -1.217
540 cl h1
             3.399
                    -3.809 -1.121
    cl cl
            2.711 10.728 3.958
541
      TOTAL ELECTROSTATIC ENERGY = 1.484 kJ/mol
542
543
544 TOTAL ENERGY = 121.662 kJ/mol
545
 546 ATOM TYPES
 547
548 IDX TYPE RING
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 FORMAL CHARGES
559
 560 IDX CHARGE
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 PARTIAL CHARGES
 571
 572 IDX CHARGE
 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 SETTING UP CALCULATIONS
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 ATOM TYPES
592
593
    IDX TYPE RING
594 1 c3 NO
    2 c3 NO
595
    3 h1 NO
596
597
    4 h1 NO
598
    5 cl NO
599
    6 h1 NO
600 7 hl NO
601
    8 cl NO
602
603
    CHARGES
604
605 IDX CHARGE
606 1 0.036009
607
    2 0.036009
608 3 0.044101
609
    4 0.044101
610 5 -0.124211
611 6 0.044101
612
    7 0.044101
613 8 -0.124211
614
615
    SETTING UP CALCULATIONS
616
617 SETTING UP BOND CALCULATIONS...
    SETTING UP ANGLE CALCULATIONS...
618
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
    ENERGY
625
626
627 BOND STRETCHING
```

ATOM	TYPES							
I					EAL	ONSTANT	משו שא	ENEDCY
5	1	0	1.0	000 1	.093	4.766	-0.093	3.578
5	1	0	1.0	000 1	.093	4.766	-0.093	3.578
5	1	0	1.0	000 1	.093	4.766	-0.093	3.578
1	1	0	1.5	540 1	.508	4.258	0.032	0.294
1	5	0	1.0	000 1	.093	4.766	-0.093	3.578
1	12	0	1.6	570 1	.773	2.974	-0.103	2.795
1	12	0	1.6	570 1	.773	2.974	-0.103	2.795
	TOTAL	BOND S'	TRETC	HING ENERG	Y = 20.196	29 kcal/mol		
		5 5 11						
A N G) L E	BEN	DII	N G				
MOTA	TYPES		FF	VALENCE	IDEAL	FORCE		
						CONSTANT	DELTA	ENERG
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 1	2	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 1	2	0	109.500	108.679	1.056	0.821	0.016
5	1 1	2	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 1	2	0	109.442	108.162	0.698	1.280	0.025
5	1 1							
1		5	0	109.500	110.549	0.636	-1.049	0.015
1		5				0.636 0.698		
1 5	1 1 1	5	0		108.162	0.698		0.025
1 5 1	1 1 1 1 1	5 12 12	0	109.442 109.500	108.162	0.698 1.056	1.280	0.025
1 5 1	1 1 1 1 1 TOTAL	5 12 2 ANGLE	0 0 BENDII	109.442 109.500 NG ENERGY	108.162 108.679	0.698 1.056	1.280	0.025
1 5 1	1 1 1 1 1 TOTAL	5 12 2 ANGLE	0 0 BENDII	109.442 109.500	108.162 108.679	0.698 1.056	1.280	0.025
1 5 1 S T R	1 1 1 1 1 TOTAL	5 2 2 ANGLE 1	0 0 BENDII E N I	109.442 109.500 NG ENERGY	108.162 108.679 = 0.20058	0.698 1.056	1.280	0.025
1 5 1 S T R	1 1 1 1 TOTAL RETO	5 .2 .2 ANGLE :	0 0 BENDII E N I FF	109.442 109.500 NG ENERGY	108.162 108.679 = 0.20058	0.698 1.056 kcal/mol	1.280 0.821 CONSTANT	0.025
1 5 1 S T R ATOM I	1 1 1 TOTAL RETO TYPES J	5 2 2 ANGLE 1	0 0 BENDII E N I FF CLASS	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE	108.162 108.679 = 0.20058 DELTA ANGLE	0.698 1.056 kcal/mol FORCE I J	1.280 0.821 CONSTANT J K	0.025 0.016 ENERGY
1 5 1 S T R ATOM I	1 1 1 1 TOTAL RETC TYPES J 1	5 2 2 ANGLE 1 2 H B	0 0 BENDIN E N I FF CLASS	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE	108.162 108.679 = 0.20058 DELTA ANGLE 	0.698 1.056 kcal/mol FORCE I J	1.280 0.821 CONSTANT J K	0.025 0.016 ENERGY -0.002
1 5 1 S T R ATOM I 1 5	1 1 1 1 TOTAL R E T C TYPES J 1 1	5 .2 .2 .ANGLE :	0 0 BENDII E N I FF CLASS	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE 109.500 109.442	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606	0.698 1.056 kcal/mol FORCE I J 	1.280 0.821 CONSTANT J K 0.070 0.115	ENERGY -0.002 -0.033
1 5 1 S T R ATOM I 1 5	1 1 1 1 TOTAL RETOTAL TYPES J 1 1 1	5 .2 .2 .2 ANGLE	0 0 BENDIN E N I FF CLASS 0 0	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE 109.500 109.442 109.442	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606 1.280	0.698 1.056 kcal/mol FORCE I J 0.227 0.115 -0.018	1.280 0.821 CONSTANT J K 0.070 0.115 0.380	ENERGY -0.002 -0.033 -0.121
1 5 1 RATOM I 5 5 1	1 1 1 1 TOTAL R E T C TYPES J 1 1 1 1 1 1 1	5 .2 .2 .2 ANGLE	0 0 BENDIN E N I FF CLASS 0 0	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE 109.500 109.442 109.500	108.162 108.679 = 0.20058 DELTA ANGLE 	0.698 1.056 kcal/mol FORCE I J 	1.280 0.821 CONSTANT J K 0.070 0.115 0.380 0.070	ENERGY -0.002 -0.033 -0.121 -0.002
1 5 1 RATOM I 5 5 1 1	1 1 1 1 TOTAL RETOTAL TYPES J 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5 .2 .2 ANGLE	0 0 BENDIN E N I FF CLASS 0 0 0	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606 1.280 -1.049 0.821	0.698 1.056 kcal/mol FORCE I J 0.227 0.115 -0.018 0.227 0.176	1.280 0.821 CONSTANT J K 0.070 0.115 0.380 0.070 0.386	ENERGY -0.002 -0.033 -0.121 -0.002 -0.070
1 5 1 S T R ATOM I 5 5 1 1 5	1 1 1 1 TOTAL R E T C TYPES J 1 1 1 1 1 1 1 1 1	5 .2 .2 .2 ANGLE	0 0 BENDIN E N I FF CLASS 0 0 0 0	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280	0.698 1.056 kcal/mol FORCE I J 	1.280 0.821 CONSTANT J K 0.070 0.115 0.380 0.070 0.386 0.380	ENERGY -0.002 -0.033 -0.121 -0.002 -0.070 -0.121
1 5 1 S T R ATOM I 5 5 1 1 5 5 5	1 1 1 1 TOTAL RETOTAL TYPES J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5 .2 .2	O O O O O O O O O O O O O O O O O O O	109.442 109.500 NG ENERGY D I N G VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.442	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.606	0.698 1.056 kcal/mol FORCE I J 0.227 0.115 -0.018 0.227 0.176 -0.018 0.115	1.280 0.821 CONSTANT J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115	ENERGY -0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033
1 5 1 S T R ATOM I 5 5 1 1 5	1 1 1 1 TOTAL R E T C TYPES J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5 .2 .2 .2 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5	O O O O O O O O O O O O O O O O O O O	109.442 109.500 NG ENERGY O I N G VALENCE ANGLE 	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.606 -1.049	0.698 1.056 kcal/mol FORCE I J 	1.280 0.821 CONSTANT J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115 0.070	ENERGY -0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033 -0.002
1 5 1 RATOM I 5 5 1 1 5 5 1 5 5 1 5	1 1 1 1 TOTAL RETOTAL TYPES J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5 .2 .2	O O O O O O O O O O O O O O O O O O O	109.442 109.500 NG ENERGY O I N G VALENCE ANGLE 109.500 109.442 109.500 109.442 109.442 109.442 109.442 109.442	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.606 -1.049 1.280	0.698 1.056 kcal/mol FORCE I J 	1.280 0.821 CONSTANT J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115 0.070 0.380	ENERGY -0.002 -0.033 -0.121 -0.002 -0.033 -0.121 -0.033 -0.121
1 5 1 S T R ATOM I 5 5 1 1 5	1 1 1 1 TOTAL RETOTAL TYPES J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	5 .2 .2 .2 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5 .5	O O O O O O O O O O O O O O O O O O O	109.442 109.500 NG ENERGY O I N G VALENCE ANGLE 	108.162 108.679 = 0.20058 DELTA ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.606 -1.049 1.280	0.698 1.056 kcal/mol FORCE I J 0.227 0.115 -0.018 0.227 0.176 -0.018 0.115 0.227 -0.018	1.280 0.821 CONSTANT J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115 0.070 0.380 0.070	ENERGY -0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033 -0.002

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

```
726 TOTAL ENERGY = 36.06534 kcal/mol
727
728 E N E R G Y
729
730
731 BOND STRETCHING
732
733 ATOM TYPES BOND
                           FORCE
                   IDEAL
    I J LENGTH
                   LENGTH CONSTANT DELTA ENERGY
734
735
736 hl c3
          1.000
                 1.093
                         1406.346
                                 -0.093
                                         12.163
                        1406.346 -0.093
                 1.093
                                         12.163
   h1 c3
         1.000
737
                         1406.346
738 h1 c3
          1.000
                 1.093
                                  -0.093
                                         12.163
739
   c3 c3
          1.540
                 1.535
                         1269.019
                                  0.005
                                          0.032
                         1406.346 -0.093 12.163
   c3 h1
740
          1.000
                 1.093
                                         15.718
741 c3 c1
          1.670
                 1.786
                         1168.117
                                  -0.116
                         1168.117 -0.116 15.718
742
   c3 cl 1.670
                 1.786
     TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
743
744
745 ANGLE BENDING
746
                       IDEAL
              VALENCE
                               FORCE
747 ATOM TYPES
748
   I J K
               ANGLE
                       ANGLE
                              CONSTANT
                                        DELTA
                                               ENERGY
749
   ______
   c3 c3 h1 109.500
                  110.070
750
                            194.100
                                    -0.010
                                             0.019
751 h1 c3 h1 109.442 109.550
                           164.039
                                    -0.002
                                            0.001
752 h1 c3 cl 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 cl 109.500 110.330
                           260.419
                                    -0.014
                                            0.055
755 h1 c3 cl 109.442 105.930
                           183.005
                                     0.061
                                            0.688
756 h1 c3 h1 109.442
                  109.550
                            164.039
                                    -0.002
                                            0.001
   c3 c3 h1 109.500 110.070
                           194.100
                                    -0.010
757
                                            0.019
758 h1 c3 cl 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 cl 109.442 105.930
                           183.005
                                     0.061
                                            0.688
761 c3 c3 cl 109.500
                  110.330
                           260.419
                                    -0.014
                                            0.055
762
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
763
764 TORSIONAL
765
                                TORSION
    ----ATOM TYPES---- FORCE
766
767
    I J K
              L
                  CONSTANT
                                 ANGLE
                                       n
                                           ENERGY
                           S
   ______
768
   h1 c3 c3 h1 0.651 0
                           40.000 3
769
                                      0.326
                       0
                           -80.000 3
770 h1 c3 c3 h1
              0.651
                                      0.326
771 h1 c3 c3 c1
              0.000
                       0 160.000 3
                                      0.000
772 h1 c3 c3 h1
                       0 160.000 3
                                      0.326
              0.651
                       0
                           40.000 3
              0.651
                                      0.326
773 h1 c3 c3 h1
774 h1 c3 c3 cl 0.000
                                      0.000
                    0 -80.000 3
```

```
775 cl c3 c3 h1 0.000 0 -80.000 3 0.000
776 cl c3 c3 h1
              0.000
                        0 160.000 3
                                        0.000
              0.000 0
777 cl c3 c3 cl
                            40.000 3
                                       0.000
     TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
778
779
780 IMPROPER TORSIONAL
781
782 ----ATOM TYPES---- FORCE IMPROPER_TORSION
    I J K L CONSTANT S ANGLE n ENERGY
783
784
785
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
786
787 VAN DER WAALS
788
   ATOM TYPES
789
790 I J Rij kij ENERGY
791
   _____
792 h1 h1
          2.300
                  0.109
793 h1 h1
           2.518
                  -0.013
794 h1 cl
           3.474
                  -0.129
795 h1 h1
           2.885 -0.031
           2.300
796 h1 h1
                  0.109
797 h1 cl
           2.960
                  0.012
798 cl h1
           2.960
                  0.012
           3.474
799 cl h1
                  -0.129
800 cl cl 2.865 15.169
    TOTAL VAN DER WAALS ENERGY = 15.111 kJ/mol
801
802
803 ELECTROSTATIC INTERACTIONS
804
805 ATOM TYPES
    I J
             Rij 332.17*QiQj ENERGY
806
807
          2.300
808 h1 h1
                  1.352
                         0.588
809 h1 h1
           2.518
                  1.352
                         0.537
810 h1 cl
           3.474 -3.809 -1.097
811 h1 h1
           2.885
                  1.352
                         0.469
           2.300
                  1.352
812 h1 h1
                         0.588
813 h1 cl
           2.960
                  -3.809 -1.287
814 cl h1
           2.960 -3.809 -1.287
           3.474 -3.809 -1.097
815
   cl h1
816 cl cl
           2.865
                  10.728
                         3.745
     TOTAL ELECTROSTATIC ENERGY = 1.160 kJ/mol
817
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
     4 5 NO
827
828 5 12 NO
829 6 5 NO
830 7 5 NO
831 8 12 NO
832
833 FORMAL CHARGES
834
835
     IDX CHARGE
836 1 0.290000
     2 0.290000
837
838
     3 0.000000
839 4 0.000000
840 5 -0.290000
     6 0.000000
841
842 7 0.000000
843 8 -0.290000
844
845 PARTIAL CHARGES
 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
     ATOM TYPES
858
859 IDX TYPE RING
860 1 c3 NO
861
     2 c3 NO
862 3 h1 NO
863
     4 h1 NO
864
     5 cl NO
865
     6 hl NO
866 7 h1 NO
867
     8 cl NO
868
 869
     FORMAL CHARGES
 870
 871 IDX CHARGE
     1 0.036009
 872
```

```
873 2 0.036009
874
    3 0.044101
875
    4 0.044101
876 5 -0.124211
877
    6 0.044101
    7 0.044101
878
879
    8 -0.124211
880
    PARTIAL CHARGES
881
882
883 IDX CHARGE
884
    1 0.036009
885 2 0.036009
886
    3 0.044101
    4 0.044101
887
888 5 -0.124211
889
    6 0.044101
890
    7 0.044101
    8 -0.124211
891
892
893
    ENERGY
894
895
    BOND STRETCHING
896
897
    ATOM TYPES FF BOND IDEAL
898
                                 FORCE
    I J
                                CONSTANT
                                          DELTA
899
           CLASS LENGTH
                        LENGTH
                                                  ENERGY
900
     5 1
            0
                 1.000
                         1.093
901
                                  4.766
                                          -0.093
                                                  3.578
        1
902
     5
            0
                 1.000
                         1.093
                                  4.766
                                          -0.093
                                                  3.578
903
     5
        1
             0
                  1.000
                         1.093
                                  4.766
                                          -0.093
                                                  3.578
                                  4.258
904
    1
        1
            0
                 1.540
                         1.508
                                          0.032
                                                  0.294
905
    1 5
            0
                 1.000
                         1.093
                                  4.766
                                          -0.093
                                                  3.578
                                  2.974
906
    1 12
             0
                  1.670
                         1.773
                                          -0.103
                                                  2.795
                         1.773 2.974 -0.103
907
    1 12
            0
                  1.670
                                                  2.795
908
      TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
909
910 ANGLE BENDING
911
912
    ATOM TYPES
                FF VALENCE
                             IDEAL
                                    FORCE
                             ANGLE CONSTANT DELTA ENERGY
913
     I J K
                CLASS ANGLE
914
    ______
                0 109.500 110.549
915
    1
        1 5
                                       0.636
                                              -1.049
                                                       0.015
        1 5
                0 109.442 108.836
     5
                                      0.516
                                              0.606
                                                      0.004
916
                0 109.442 108.162
                                              1.280
917
    5
        1 12
                                      0.698
                                                      0.025
        1 5
                0 109.500 110.549
918
    1
                                      0.636
                                              -1.049
                                                      0.015
                0 109.500 108.679
                                      1.056
919
    1
        1 12
                                              0.821
                                                      0.016
                0 109.442 108.162
    5
                                              1.280
920
        1 12
                                      0.698
                                                      0.025
921
    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	0.01
	TOTA	AL ANO	GLE BENDI	NG ENERGY	= 0.20058 kg	cal/mol		
сп	חים ח	1 C H	BEN	DINC				
5 1 .	K E 1	. Сп	D E N	DING				
ATOM	TYPE	ES	FF	VALENCE	DELTA	FORCE	CONSTANT	
					ANGLE			
1			0		-1.049			
5	1	5	0	109.442	0.606	0.115	0.115	-0.033
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
5	1	5	0	109.442	0.606	0.115	0.115	-0.033
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
5	1	12	0		1.280			-0.121
1	1	5	0		-1.049			-0.002
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
					0.821 $GY = -0.69593$		0.386	-0.070
то	TOT <i>i</i>	AL STE	RETCH BEN	DING ENER	GY = -0.69593	kcal/mol		-0.070
ТО	TOTA	AL STE	RETCH BEN	DING ENERG		kcal/mol		
T O I	TOTA	L STE	RETCH BEN	FF TO	GY = -0.69593 $ORSION$	kcal/mol FORCE CONST V1 V2	ANT V3 ENER	
T O I	TOT# R S I TYPE J	AL STE	RETCH BEN	FF TO	ORSION 1 ANGLE .000 0.284	kcal/mol FORCE CONST V1 V2 -1.386	ANT V3 ENER	.GY
T O D ATOM I 5	TOTA R S I TYPE J 1	AL STE	RETCH BEN A L L 5	FF TCLASS 1	ORSION 1 ANGLE 000 0.284	kcal/mol FORCE CONST V1 V2 -1.386	ANT V3 ENER 0.314 0.314	GY -0.827
T O 1 ATOM I 5 5	TOTA TYPE J 1	I O N S K 1 1	RETCH BEN L 5 5 12	FF TO CLASS 10 0 60 0 -60	ORSION 1 ANGLE .000 0.284 .000 0.678	FORCE CONST V1 V2 -1.386 -1.386	VANT V3 ENER 0.314 0.314 0.398	GY -0.827 -0.826
T O 1 ATOM I 5 5 5	TOTA TYPE J 1 1	I O N S K 1 1	RETCH BEN A L 5 5 12	FF TCLASS 7 0 60 0 -60 0 -180	ORSION 1 ANGLE000 0.284 .000 0.678 .000 0.284	FORCE CONST V1 V2 -1.386 -1.386 -0.602	VANT V3 ENER 0.314 0.314 0.398	-0.827 -0.826 0.000
T O 1 ATOM I 5 5 5 5 5	TOTA TYPE J 1 1 1 1	I O N SS K 1 1 1 1	L L 5 5 12 5 12	FF TCCLASS 77 0 60 0 -60 0 -180 0 60 0 -60 0 -60 0 -60 0 -60 0 -60 0 -60 0 -60	ORSION 1 ANGLE000 0.284 .000 0.678 .000 0.284 .000 0.678	FORCE CONST V1 V2 -1.386 -1.386 -0.602 -1.386 -0.602	ANT V3 ENER 0.314 0.314 0.398 0.314 0.314 0.398	-0.827 -0.826 0.000 0.000 -0.827 0.057
T O 1 ATOM I 5 5 5 5 12	TOTA TYPE J 1 1 1 1 1	I O N SS K 1 1 1 1 1	L L 5 5 12 5 12 5	FF TO CLASS 7 0 60 0 -60 0 -180 0 60 0 -60 0 -60 0 -60 0 -60 0 -60 0 -60 0 -60	ORSION 1 ANGLE .000 0.284 .000 0.284 .000 0.284 .000 0.284 .000 0.284 .000 0.678 .000 0.678	FORCE CONST V1 V2 -1.386 -1.386 -0.602 -1.386 -0.602 -0.602	VANT V3 ENER 0.314 0.314 0.398 0.314 0.314 0.398 0.318	-0.827 -0.826 0.000 0.000 -0.827 0.057
T O 1 ATOM I 5 5 5 12 12	TOTA R S I TYPE J 1 1 1 1 1 1	I O N SS K 1 1 1 1 1 1	L L 5 5 12 5 12 5 5 5	FF TO CLASS 17 0 60 0 -60 0 -60 0 -60 0 180	ORSION 1 ANGLE	FORCE CONST V1 V2 -1.386 -1.386 -0.602 -1.386 -0.602 -0.602 -0.602	ANT V3 ENER 0.314 0.314 0.398 0.314 0.3198 0.318 0.398 0.398	-0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
T O 1 ATOM I 5 5 5 5	TOTA R S I TYPE J 1 1 1 1 1 1 1	I O N SS K 1 1 1 1 1 1	EETCH BEN L L 5 5 12 5 12 5 12	FF TO CLASS 7 0 60 0 -60 0 -60 0 -60 0 180 0 60 0 60 0 60 0 60 0 60 0 60 0	ORSION 1 ANGLE .000 0.284 .000 0.284 .000 0.284 .000 0.284 .000 0.678 .000 0.678 .000 0.678	FORCE CONST V1 V2 -1.386 -1.386 -0.602 -1.386 -0.602 -0.602 -0.602 -0.602	VANT V3 ENER 0.314 0.314 0.398 0.314 0.314 0.398 0.318	-0.827 -0.826 0.000 0.000 -0.827 0.057
T O 1 ATOM I 5 5 5 12 12	TOTA R S I TYPE J 1 1 1 1 1 1 1	I O N SS K 1 1 1 1 1 1	EETCH BEN L L 5 5 12 5 12 5 12	FF TO CLASS 7 0 60 0 -60 0 -60 0 -60 0 180 0 60 0 60 0 60 0 60 0 60 0 60 0	ORSION 1 ANGLE	FORCE CONST V1 V2 -1.386 -1.386 -0.602 -1.386 -0.602 -0.602 -0.602 -0.602	ANT V3 ENER 0.314 0.314 0.398 0.314 0.3198 0.318 0.398 0.398	-0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
T O 1 ATOM I 5 5 5 12 12 12	TOTA TYPE J 1 1 1 1 1 TOTA	AL STR	RETCH BEN A L L 5 5 12 5 12 5 12 5 12 8SIONAL E	FF TO CLASS 7 0 60 0 -60 0 -60 0 -60 0 180 0 60 0 60 0 60 0 60 0 60 0 60 0	ORSION 1 ANGLE .000 0.284 .000 0.284 .000 0.284 .000 0.284 .000 0.678 .000 0.678 .000 0.678 .000 0.678	FORCE CONST V1 V2 -1.386 -1.386 -0.602 -1.386 -0.602 -0.602 -0.602 -0.602	ANT V3 ENER 0.314 0.314 0.398 0.314 0.3198 0.318 0.398 0.398	-0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
T O 1 ATOM I 5 5 5 12 12 12	TOTA R S I TYPE J 1 1 1 1 TOTA TOTA	I O N SS K 1 1 1 1 1 1 1 1 1 1 1 1	RETCH BEN A L L 5 5 12 5 12 5 12 8 RSIONAL E	FF TO CLASS 7 0 60 0 -60 0 -180 0 60 0 -60 0 180 0 60 0 MERGY = -2	ORSION 1 ANGLE .000 0.284 .000 0.284 .000 0.284 .000 0.284 .000 0.678 .000 0.678 .000 0.678 .000 0.678	FORCE CONST V1 V2 -1.386 -1.386 -0.602 -1.386 -0.602 -0.602 -0.602 0.000	ANT V3 ENER 0.314 0.314 0.398 0.314 0.3198 0.318 0.398 0.398	-0.827 -0.826 0.000 0.000 -0.827 0.057 0.057

```
971 VAN DER WAALS
972
973
   ATOM TYPES
    I J
            Rij R*IJ EPSILON ENERGY
974
975
    _____
    5 5
976
             2.400
                   2.970
                         0.022
                                0.107
977
    5 5
            2.400
                   2.970
                         0.022
                                0.107
    5 12
            3.499
                   3.713
                         0.053 -0.044
978
    5 5
             2.903
                   2.970
                         0.022 -0.021
979
980 5 5
            2.400
                         0.022
                   2.970
                                0.107
981
    5 12
            2.792
                   3.713
                         0.053
                                0.792
    12 5
                         0.053
             2.792
                   3.713
982
                                0.792
983 12 5
            3.499
                   3.713
                         0.053 -0.044
                                3.947
984
    12 12
             3.087
                   4.089
                         0.276
     TOTAL VAN DER WAALS ENERGY = 5.74158 kcal/mol
985
986
987 ELECTROSTATIC INTERACTIONS
988
989 ATOM TYPES
990
            Rij
                 Qi
                       Qj
991
    _____
           3.137
    12 12
                  -0.290
                        -0.290
992
                               6.678
      TOTAL ELECTROSTATIC ENERGY = 6.67788 kcal/mol
993
994
995
    TOTAL ENERGY = 29.75490 kcal/mol
996
997
    ENERGY
998
999
1000 BOND STRETCHING
1001
1002 ATOM TYPES BOND IDEAL FORCE
                                 DELTA ENERGY
1003
    I J
                  LENGTH
                         CONSTANT
          LENGTH
1004
   ______
                1.093 1406.346 -0.093 12.163
1005 h1 c3 1.000
1006 h1 c3
         1.000
                1.093
                       1406.346
                               -0.093
                                      12.163
                                      12.163
1007 h1 c3
         1.000
                1.093
                       1406.346
                               -0.093
                       1269.019
                                0.005
1008 c3 c3
         1.540
                1.535
                                       0.032
1009 c3 h1
         1.000
                               -0.093
                                      12.163
                1.093
                       1406.346
   c3 cl
                       1168.117
1010
         1.670
                1.786
                               -0.116
                                      15.718
    c3 cl 1.670 1.786 1168.117 -0.116 15.718
1011
1012
    TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
1013
1014 ANGLE BENDING
1015
                     IDEAL
1016 ATOM TYPES
              VALENCE
                            FORCE
              ANGLE ANGLE CONSTANT DELTA ENERGY
1017
    I J K
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 cl	109.442	105.930	183.005	5 (0.061	0.688
1022	c3 c3 h1	109.500	110.070	194.100) –(0.010	0.019
1023	c3 c3 cl	109.500	110.330	260.419) –(0.014	0.055
1024	h1 c3 cl	109.442	105.930	183.005	5 (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 cl	109.442	105.930	183.005	5 (0.061	0.688
1028	c3 c3 h1	109.500	110.070	194.100) –(0.010	0.019
1029	h1 c3 cl	109.442	105.930	183.005	5 (0.061	0.688
1030	c3 c3 cl	109.500	110.330	260.419) –(0.014	0.055
1031	TOT	AL ANGLE BEN	DING ENERGY	2.938	kJ/mo	1	
1032							
1033	T O R S	IONAL					
1034							
1035	ATOM	TYPES	FORCE		TORSIO	N	
1036	I J	K L	CONSTANT	S	ANGLE	n	ENERGY
1037							
1038	h1 c3 c3	h1 0.65	1 0	60.000	3	0.000	
1039	h1 c3 c3	h1 0.65	1 0	-60.000	3	0.000	
1040	h1 c3 c3	cl 0.00	0 0	-180.000	3	0.000	
1041	h1 c3 c3	h1 0.65	1 0	-180.000	3	0.000	
1042	h1 c3 c3	h1 0.65	1 0	60.000	3	0.000	
1043	h1 c3 c3	cl 0.00	0 0	-60.000	3	0.000	
1044	cl c3 c3	h1 0.00	0 0	-60.000	3	0.000	
1045	cl c3 c3	h1 0.00	0 0	180.000	3	0.000	
L046	cl c3 c3	cl 0.00	0 0	60.000	3	0.000	
047	TOT	AL TORSIONAL	ENERGY =	0.000 kJ/	'mol		
1048							
L049	IMPR	O P E R T	ORSION	I A L			
1050							
1051	ATOM	TYPES	FORCE	IMPROPER_	TORSIO	N	
052	I J	K L	CONSTANT	S	ANGLE	n	ENERGY
053							
.054	TOT	AL IMPROPER-	TORSIONAL E	ENERGY =	0.000	kJ/mol	
1055							
.056	V A N	DER WA	ALS				
L057							
.058	ATOM TYP						
		Rij	_				
1060							
1061		2.400					
1062		2.400					
1063		3.499					
1064		2.903					
1065		2.400					
1066		2.792					
1067	cl h1	2.792	0.356				
1068	cl h1	3.499	-0.127				

```
1069 cl cl 3.087 4.588
1070
       TOTAL VAN DER WAALS ENERGY = 5.105 kJ/mol
1071
1072 ELECTROSTATIC INTERACTIONS
1073
1074 ATOM TYPES
1075 I J
            Rij 332.17*QiQj ENERGY
1076
    _____
            2.400 1.352 0.563
1077 h1 h1
1078 h1 h1
            2.400
                    1.352
                            0.563
1079 h1 cl
            3.499 -3.809 -1.089
            2.903 1.352
1080 h1 h1
                            0.466
1081 h1 h1
            2.400
                    1.352
                            0.563
1082 h1 cl
            2.792 -3.809 -1.364
            2.792 -3.809 -1.364
1083 cl h1
1084 cl h1
            3.499
                   -3.809 -1.089
            3.087 10.728 3.476
1085 cl cl
     TOTAL ELECTROSTATIC ENERGY = 0.726 kJ/mol
1086
1087
1088 TOTAL ENERGY = 88.891 kJ/mol
1089
1090 ATOM TYPES
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 FORMAL CHARGES
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 PARTIAL CHARGES
1115
1116 IDX CHARGE
1117 | 1 0.290000
```

```
1118 2 0.290000
1119 | 3 0.000000
1120 4 0.000000
1121 5 -0.290000
1122 6 0.000000
1123 7 0.000000
1124 8 -0.290000
1125
1126 A T O M T Y P E S
1127
1128 IDX TYPE RING
1129
     1 c3 NO
1130 2 c3 NO
1131 | 3 h1 NO
1132 | 4 h1 NO
1133 5 cl NO
1134 6 h1 NO
1135 7 h1 NO
1136 8 cl NO
1137
1138 FORMAL CHARGES
1139
1140 IDX CHARGE
1141 1 0.036009
1142 2 0.036009
1143 3 0.044101
1144 4 0.044101
1145 5 -0.124211
1146 6 0.044101
1147 7 0.044101
1148 8 -0.124211
1149
1150 PARTIAL CHARGES
1151
1152 IDX CHARGE
1153 | 1 0.036009
1154 2 0.036009
1155 3 0.044101
1156 4 0.044101
1157 5 -0.124211
     6 0.044101
1158
1159 7 0.044101
1160 8 -0.124211
1161
1162 ENERGY
1163
1164
1165 BOND STRETCHING
1166
```

	ATOM	TYPES	S FF	BONI) I	DEAL	FORCE		
68	I	J	CLASS					DELTA	ENERGY
69									
70	5	1	0	1.0	000	1.093	4.766	-0.093	3.578
71	5	1	0	1.0	000	1.093	4.766	-0.093	3.578
72	5	1	0	1.0	000	1.093	4.766	-0.093	3.578
73	1	1	0	1.5	540	1.508	4.258	0.032	0.294
74	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
75	1	12	0	1.6	570	1.773	2.974	-0.103	2.795
76	1	12	0	1.6	570	1.773	2.974	-0.103	2.795
77		TOTAL	BOND S	TRETCE	HING ENER	GY = 20.19	629 kcal/mol	L	
78									
79	A N (G L E	BEN	DII	N G				
80									
81	ATOM	TYPES	3	FF	VALENCE	IDEAL	FORCE		
82	I	J	K	CLASS	ANGLE	ANGLE	CONSTAN	NT DELTA	ENERGY
83									
84	1	1	5	0	109.500	110.549	0.63	-1.049	0.015
85	5	1	5	0	109.442	108.836	0.51	0.606	0.004
86	5	1	12	0	109.442	108.162	0.69	1.280	0.025
87	1	1	5	0	109.500	110.549	0.63	-1.049	0.015
88	1	1	12	0	109.500	108.679	1.05	0.821	0.016
89	5	1	12	0	109.442	108.162	0.69	1.280	0.025
90	5	1	5	0	109.442	108.836	0.51	0.606	0.004
91	1	1	5	0	109.500	110.549	0.63	-1.049	0.015
92	5	1	12	0	109.442	108.162	0.69	1.280	0.025
93	1	1	5	0	109.500	110.549	0.63	-1.049	0.015
94	5	1	12	0	109.442	108.162	0.69	1.280	0.025
95	1		12			108.679		0.821	0.016
96		TOTAL	ANGLE	BENDI	NG ENERGY	= 0.2005	8 kcal/mol		
98	STI	RET	С Н В	BENI	O I N G				
98									
98 99 00	ATOM	TYPES	3	FF	VALENCE		A FORC		
98 99 00	ATOM	TYPES	3	FF	VALENCE ANGLE	ANGLE	I J	J K	
98 99 00 01 02	ATOM I	TYPES J	S K	FF CLASS	VALENCE ANGLE	ANGLE	I J	J K	
98 99 00 01 02	ATOM I 	TYPES J 1	S K 5	FF CLASS 0	VALENCE ANGLE	ANGLE	I J	J К 	-0.002
98 99 00 01 02 03	ATOM I 1 5	TYPES J 1 1	S K 5 5	FF CLASS 0 0	VALENCE ANGLE 109.500 109.442	ANGLE	0.227 0.115	J K 0.070 0.115	-0.002 -0.033
98 99 00 01 02 03 04	ATOM I 1 5 5	TYPES J 1 1 1	5 5 5 12	FF CLASS 0 0	VALENCE ANGLE 109.500 109.442 109.442	ANGLE1.049 0.606 1.280	0.227 0.115 0.018	J K 0.070 0.115 0.380	-0.002 -0.033 -0.121
98 99 00 01 02 03 04 05	ATOM I	TYPES J 1 1 1 1	5 5 5 12 5	FF CLASS 0 0 0	VALENCE ANGLE 109.500 109.442 109.500	ANGLE1.049 0.606 1.280 -1.049	0.227 0.115 0.018 0.227	J K 0.070 0.115 0.380 0.070	-0.002 -0.033 -0.121 -0.002
98 99 00 01 02 03 04 05 06	ATOM I 1 5 1 1	TYPES J 1 1 1 1 1	5 K 5 5 12 5 12	FF CLASS 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500	ANGLE1.049 0.606 1.280 -1.049 0.821	0.227 0.115 -0.018 0.227 0.176	J K 0.070 0.115 0.380 0.070 0.386	-0.002 -0.033 -0.121 -0.002 -0.070
997 998 999 000 001 002 003 004 005 006 007	ATOM I	TYPES J 1 1 1 1 1 1	5 5 5 12 5 12	FF CLASS 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018	J K 0.070 0.115 0.380 0.070 0.386 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121
98 99 000 01 002 003 004 005 006 007	ATOM I 1 5 1 1 5 5 1 1 5 5	TYPES J 1 1 1 1 1 1 1	5 K 5 5 12 5 12 12 5 5	FF CLASS 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500 109.442 109.442	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 0.606	0.227 0.115 -0.018 0.227 0.176 -0.018 0.115	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033
98 999 000 01 002 03 004 005 006 007 008	ATOM I 1 5 5 1 1 5 1	TYPES J 1 1 1 1 1 1 1 1	5 K 5 5 12 5 12 12 5 5 5	FF CLASS 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442	-1.049 0.606 1.280 -1.049 0.821 1.280 0.606 -1.049	0.227 0.115 -0.018 0.227 0.176 -0.018 0.115 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115 0.070	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033 -0.002
98 999 000 01 002 003 004 005 006 007 008 009 110	ATOM I 1 5 5 1 1 5 5 1 5 5 1	TYPES J 1 1 1 1 1 1 1 1 1	5 K 5 5 12 5 12 5 5 12 12 12 12 12 12	FF CLASS 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.442	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 0.606 -1.049 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018 0.115 0.227 -0.018	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115 0.070 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033 -0.002 -0.121
98 99 99 99 99 99 99 99	ATOM I 1 5 5 1 1 5 1 1 5 1	TYPES J 1 1 1 1 1 1 1 1 1 1 1 1	5 K 5 5 12 5 12 5 5 12 5 5 5 12 5 5 5 12 5 5 5 12 5 5 5 12 5 5 5 12 5 5 5 5	FF CLASS 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500 109.442 109.500 109.442 109.500	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 0.606 -1.049 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018 0.115 0.227 -0.018 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115 0.070 0.380 0.070	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033 -0.002 -0.121 -0.002
98 999 000 01 002 003 004 005 006 007 008 009 110	ATOM I 1 5 5 1 1 5 5 1 5 5 1	TYPES J 1 1 1 1 1 1 1 1 1 1 1 1	5 K 5 5 12 5 12 5 5 12 12 12 12 12 12	FF CLASS 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.442 109.500 109.442	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 0.606 -1.049 1.280 -1.049	0.227 0.115 -0.018 0.227 0.176 -0.018 0.115 0.227 -0.018	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.115 0.070 0.380 0.070 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.033 -0.002 -0.121 -0.002 -0.121

```
1216
1217
   TORSIONAL
1218
                   FF TORSION FORCE CONSTANT
1219 ATOM TYPES
                                  V1 V2 V3
1220
    I J K L CLASS ANGLE
                                             ENERGY
1221
    ______
1222
    5
       1 1 5
                   0
                       80.000
                              0.284 - 1.386
                                          0.314
                                                  -1.099
                                                  -0.243
1223
    5
       1
           1
              5
                   0 \quad -40.000 \quad 0.284 \quad -1.386
                                          0.314
          1 12
       1
                   0 -160.000 0.678 -0.602 0.398
    5
                                                  0.050
1224
           1 5
                   0 -160.000 0.284 -1.386
1225 5
       1
                                          0.314
                                                  -0.075
    5
                       80.000 0.284 -1.386
1226
       1
           1
              5
                   0
                                          0.314
                                                  -1.099
                   0 -40.000 0.678 -0.602
    5
           1 12
                                          0.398
1227
       1
                                                  0.449
1228 12
       1
           1 5
                   0 -40.000 0.678 -0.602
                                          0.398
                                                  0.449
           1
1229
    12
              5
                   0 -160.000 \quad 0.678 \quad -0.602 \quad 0.398
                                                  0.050
       1
                       80.000 0.000 0.000 0.893 0.223
1230
       1
           1 12
    12
                   0
      TOTAL TORSIONAL ENERGY = -1.29534 kcal/mol
1231
1232
1233 OUT-OF-PLANE BENDING
1234
    ATOM TYPES
1235
                   FF
                         OOP FORCE
                  CLASS ANGLE CONSTANT
1236
    I J K
              L
                                       ENERGY
1237
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
1238
1239
    VAN DER WAALS
1240
1241
    ATOM TYPES
1242
    I J Rij
                    R*IJ EPSILON ENERGY
1243
1244
1245
    5 5
             2.518
                    2.970
                           0.022
                                  0.036
1246
    5 5
             2.300
                    2.970
                           0.022
                                  0.215
    5 12
             3.474
                    3.713
                           0.053 -0.041
1247
1248 5 5
             2.885
                    2.970
                           0.022 -0.021
1249
    5 5
             2.518
                    2.970
                           0.022
                                  0.036
             2.647
                    3.713
                                  1.520
1250
    5 12
                           0.053
1251 12 5
                    3.713
                           0.053
             2.647
                                  1.520
1252 12 5
             3.474
                    3.713
                           0.053 -0.041
                                  1.129
                    4.089
                           0.276
    12 12
             3.338
1253
      TOTAL VAN DER WAALS ENERGY = 4.35500 kcal/mol
1254
1255
    ELECTROSTATIC INTERACTIONS
1256
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
   ENERGY
1266
1267
1268
    BOND STRETCHING
1269
1270
1271 ATOM TYPES BOND
                    IDEAL
                           FORCE
                                      DELTA
                                              ENERGY
12.72
            LENGTH
                    LENGTH
                            CONSTANT
    I J
1273
1274 h1 c3
           1.000
                   1.093
                          1406.346
                                    -0.093
                                            12.163
           1.000
1275 h1 c3
                   1.093
                          1406.346
                                   -0.093
                                           12.163
                          1406.346 -0.093
                   1.093
1276
   h1 c3
          1.000
                                           12.163
1277 c3 c3
           1.540
                   1.535
                          1269.019
                                    0.005
                                            0.032
1278 c3 h1
           1.000
                   1.093
                          1406.346
                                   -0.093
                                           12.163
1279 c3 cl
                   1.786
                          1168.117
           1.670
                                   -0.116
                                           15.718
1280 c3 cl
                  1.786
                          1168.117
           1.670
                                   -0.116
                                           15.718
      TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
1281
1282
1283 ANGLE BENDING
1284
1285 ATOM TYPES VALENCE IDEAL FORCE
    I J K
                ANGLE
                        ANGLE
                                CONSTANT
                                          DELTA ENERGY
1286
1287
1288 c3 c3 h1 109.500 110.070
                             194.100
                                      -0.010
                                              0.019
1289 h1 c3 h1 109.442
                    109.550
                             164.039
                                      -0.002
                                               0.001
                             183.005
                                      0.061
1290 h1 c3 cl 109.442 105.930
                                              0.688
                             194.100 -0.010
1291 c3 c3 h1 109.500 110.070
                                              0.019
1292
    c3 c3 cl
           109.500
                    110.330
                             260.419
                                      -0.014
                                               0.055
1293 h1 c3 cl 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 cl 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 cl 109.442
                    105.930
                             183.005
                                      0.061
                                               0.688
    c3 c3 c1 109.500 110.330 260.419 -0.014 0.055
1299
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
1300
1301
1302 TORSIONAL
1303
1304
    ----ATOM TYPES----
                    FORCE
                                  TORSION
               L CONSTANT
1305
                                  ANGLE n ENERGY
                             S
1306
    ______
1307 h1 c3 c3 h1
               0.651
                        0
                             80.000 3
                                        0.326
                        0 -40.000 3
    h1 c3 c3 h1
               0.651
1308
                                         0.326
                        0 -160.000 3
1309 h1 c3 c3 cl
               0.000
                                        0.000
1310 h1 c3 c3 h1
               0.651
                        0 -160.000 3
                                        0.326
               0.651
                             80.000 3
                                        0.326
1311 h1 c3 c3 h1
                         0
                        0
               0.000
                            -40.000 3
                                        0.000
1312 h1 c3 c3 cl
1313 cl c3 c3 h1
                                        0.000
               0.000
                      0 -40.000 3
```

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

```
1363 2 1 NO
1364 | 3 5 NO
1365 4 5 NO
1366 5 12 NO
1367
     6 5 NO
1368 7 5 NO
1369 8 12 NO
1370
1371 FORMAL CHARGES
1372
1373 IDX CHARGE
1374
     1 0.000000
1375 2 0.000000
1376 3 0.000000
1377
     4 0.000000
1378 5 0.000000
1379
     6 0.000000
1380 7 0.000000
1381 8 0.000000
1382
1383 PARTIAL CHARGES
1384
1385 IDX CHARGE
1386 1 0.290000
1387 2 0.290000
1388 3 0.000000
1389 4 0.000000
1390 5 -0.290000
1391 6 0.000000
1392 7 0.000000
1393
     8 -0.290000
1394
1395 SETTING UP CALCULATIONS
1396
1397 SETTING UP BOND CALCULATIONS...
1398 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
1399
     SETTING UP TORSION CALCULATIONS...
1400
     SETTING UP OOP CALCULATIONS...
1401
     SETTING UP VAN DER WAALS CALCULATIONS...
1402
     SETTING UP ELECTROSTATIC CALCULATIONS...
1403
1404 ATOM TYPES
1405
1406
     IDX TYPE RING
1407 1 c3 NO
1408 2 c3 NO
1409
     3 h1 NO
1410 4 h1 NO
1411 | 5 cl NO
```

```
1412 6 h1 NO
1413 7 h1 NO
1414 8 cl NO
1415
1416 C H A R G E S
1417
1418 IDX CHARGE
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
    8 -0.124211
1426
1427
1428 SETTING UP CALCULATIONS
1429
1430 | SETTING UP BOND CALCULATIONS...
1431
    SETTING UP ANGLE CALCULATIONS...
1432
    SETTING UP TORSION CALCULATIONS...
1433 SETTING UP IMPROPER TORSION CALCULATIONS...
    SETTING UP VAN DER WAALS CALCULATIONS...
1434
1435 SETTING UP ELECTROSTATIC CALCULATIONS...
1436
1437 ENERGY
1438
1439
1440 BOND STRETCHING
1441
1442 ATOM TYPES FF BOND IDEAL
                                  FORCE
    I J CLASS LENGTH
                         LENGTH
                                 CONSTANT
1443
                                           DELTA ENERGY
1444
           0
                          1.093
1445
     5
        1
                  1.000
                                   4.766
                                           -0.093
                                                    3.578
1446 5 1
            0
                  1.000
                          1.093
                                   4.766 -0.093
                                                   3.578
1447
    1
        1
            0
                  1.540
                          1.508
                                   4.258
                                           0.032
                                                   0.294
1448
    1 5
            0
                  1.000
                          1.093
                                   4.766
                                           -0.093
                                                   3.578
    1 12
                  1.670
            0
                          1.773
                                   2.974
                                           -0.103
                                                   2.795
1449
1450 1 5
            0
                  1.000
                          1.093
                                   4.766
                                           -0.093
                                                   3.578
                                   2.974
                                                   2.795
1451
    1 12
             0
                  1.670
                          1.773
                                           -0.103
1452
      TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
1453
1454 ANGLE BENDING
1455
1456 ATOM TYPES
                FF VALENCE
                             IDEAL
                                     FORCE
    I J K
1457
               CLASS ANGLE
                              ANGLE
                                    CONSTANT
                                               DELTA
1458
    ______
    1 1 5
                0 109.500 110.549
                                       0.636
                                              -1.049
1459
                                                       0.015
    5 1 5 0 109.442 108.836 0.516 0.606
1460
                                                       0.004
```

1461	5	1	12	0	109.442	108.162	0.698	1.280	0.02
1462	1	1	5	0	109.500	110.549	0.636	-1.049	0.0
463	1	1	12	0	109.500	108.679	1.056	0.821	0.0
464	5	1	12	0	109.442	108.162	0.698	1.280	0.02
465	1	1	5	0	109.500	110.549	0.636	-1.049	0.0
466	5	1	5	0	109.442	108.836	0.516	0.606	0.0
467	5	1	12	0	109.442	108.162	0.698	1.280	0.0
468	1	1	5	0	109.500	110.549	0.636	-1.049	0.0
469	1	1	12	0	109.500	108.679	1.056	0.821	0.0
470	5	1	12	0	109.442	108.162	0.698	1.280	0.0
471		TOT	AL ANG	LE BENDI	NG ENERGY	= 0.20058	kcal/mol		
472									
473	ST	RE'	ГСН	BENI	DING				
474									
475	ATOM	I TYP	ES	FF	VALENCE	DELTA	FORCE	CONSTANT	
476	I	J	K	CLASS	ANGLE	ANGLE	ΙJ	JК	ENERG
477									
478	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
479	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
480	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
481	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
482	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
483	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
484	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
485	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
486	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
487	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
488	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
489	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
490		TOT	AL STR	ETCH BEN		SY = -0.6959			
491									
492	ТО	R S	I O N	A L					
493									
	ATOM	1 TYP	ES		FF TO	ORSION	FORCE CONST	ANT	
494	ATOM I	I TYPI			FF TO			'ANT V3 ENER	GY
493 494 495 496									GY
494 495	I 				CLASS A	ANGLE		V3 ENER	GGY 0.349

1494	ATOM	TYPES			FF	TORSION	F	ORCE CONS	TANT	
1495	I	J	K	L	CLASS	ANGLE		V1 V2	V3 I	ENERGY
1496										
1497	5	1	1	5	0	-20.000	0.284	-1.386	0.314	0.349
1498	5	1	1	5	0	100.000	0.284	-1.386	0.314	-0.991
1499	5	1	1	12	0	-140.000	0.678	-0.602	0.398	0.129
1500	5	1	1	5	0	100.000	0.284	-1.386	0.314	-0.991
1501	5	1	1	5	0	-140.000	0.284	-1.386	0.314	-0.304
1502	5	1	1	12	0	-20.000	0.678	-0.602	0.398	0.886
1503	12	1	1	5	0	-140.000	0.678	-0.602	0.398	0.129
1504	12	1	1	5	0	-20.000	0.678	-0.602	0.398	0.886
1505	12	1	1	12	0	100.000	0.000	0.000	0.893	0.670
1506		TOTAL	TOR	SIONAL	ENERGY	r = 0.76131	kcal/m	ol		
1 - 0 -										

1508 OUT-OF-PLANE BENDING

TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol V A N D E R W A A L S ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.638 2.970 0.022 0.001 5 5 2.232 2.970 0.022 0.028 5 5 2.831 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.019 5 5 12 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 2.298 12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY HI 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 c3 1.000 1.093 1406.346 -0.093 12.163 c3 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 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	I	TYPES		FF			FNFDCV
ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.638 2.970 0.022 0.001 5 5 2.232 2.970 0.022 0.328 5 12 3.399 3.713 0.053 -0.028 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 0.001 5 12 2.547 3.713 0.053 2.298 12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 2.298 12 5 3.399 3.713 0.053 2.298 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY I J LENGTH LENGTH CONSTANT DELTA ENERGY I J LENGTH LENGTH CONSTANT DELTA ENERGY ATOM TYPES BOND 1.093 1406.346 -0.093 12.163 and 1 c3 1.000 1.093 1406.346 -0.093 12.163 and 1 c3 c1 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol							
ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.638 2.970 0.022 0.001 5 5 2.232 2.970 0.022 0.328 5 12 3.399 3.713 0.053 -0.028 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 12 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 2.298 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY TOTAL ENERGY = 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 c4 1.670 1.786 1168.117 -0.116 15.718 c3 c1 1.670 1.786 1168.117 -0.116 15.718 c3 c1 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol		TOTAL	OUT-OF-PL	ANE BENDING	G ENERGY =	0.00000	kcal/mol
ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.638 2.970 0.022 0.001 5 5 2.232 2.970 0.022 0.328 5 12 3.399 3.713 0.053 -0.028 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 -0.019 5 12 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 2.298 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY TOTAL ENERGY = 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 c4 1.670 1.786 1168.117 -0.116 15.718 c3 c1 1.670 1.786 1168.117 -0.116 15.718 c3 c1 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol							
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I J Rij R*IJ EPSILON ENERGY 5 5 2.638 2.970 0.022 0.001 5 5 5 2.232 2.970 0.022 0.328 5 12 3.399 3.713 0.053 -0.028 5 5 2.831 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.019 5 12 2.547 3.713 0.053 2.298 12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY 1 C J LENGTH LENGTH CONSTANT DELTA ENERGY 1 ATOM TYPES BOND 1.093 1406.346 -0.093 12.163 2							
5 5 2.638 2.970 0.022 0.001 5 5 5 2.232 2.970 0.022 0.328 5 12 3.399 3.713 0.053 -0.028 5 5 2.831 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 0.001 5 12 2.547 3.713 0.053 2.298 12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 2.298 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH CONSTANT DELTA ENERGY I J LENGTH CONSTANT DELTA ENERGY ATOM TYPES BOND IDEAL FORCE I J LENGTH CONSTANT DELTA ENERGY ATOM TYPES BOND 1.093 1406.346 -0.093 12.163 hl c3 1.000 1.093 1406.346 -0.093 12.163 c3 c3 1.540 1.535 1269.019 0.005 0.032 c3 hl 1.000 1.093 1406.346 -0.093 12.163 c3 c1 1.670 1.786 1168.117 -0.116 15.718 c3 hl 1.000 1.093 1406.346 -0.093 12.163 c3 c1 1.670 1.786 1168.117 -0.116 15.718				D≠TT	EDCTION	EMEDCV	
5 5 2.638 2.970 0.022 0.001 5 5 5 2.232 2.970 0.022 0.328 5 12 3.399 3.713 0.053 -0.028 5 5 2.831 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 -0.001 5 12 2.547 3.713 0.053 2.298 12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY I J LENGTH LENGTH CONSTANT DELTA ENERGY ATOM TYPES BOND 1.093 1406.346 -0.093 12.163 hl c3 1.000 1.093 1406.346 -0.093 12.163 hl c3 1.000 1.093 1406.346 -0.093 12.163 c3 c3 1.540 1.535 1269.019 0.005 0.032 c3 hl 1.000 1.093 1406.346 -0.093 12.163 c3 c1 1.670 1.786 1168.117 -0.116 15.718 c3 hl 1.000 1.093 1406.346 -0.093 12.163 c3 c1 1.670 1.786 1168.117 -0.116 15.718 c3 hl 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							
5 12 3.399 3.713 0.053 -0.028 5 5 2.831 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 0.001 5 12 2.547 3.713 0.053 2.298 12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY h1 c3 1.000 1.093 1406.346 -0.093 12.163 h1 c3 1.000 1.093 1406.346 -0.093 12.163 c3 c3 1.540 1.535 1269.019 0.005 0.032 c3 h1 1.000 1.093 1406.346 -0.093 12.163 c3 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							
5 5 2.831 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 0.001 5 12 2.547 3.713 0.053 2.298 12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY	5	5	2.232	2.970	0.022	0.328	
5 5 2.638 2.970 0.022 0.001 5 12 2.547 3.713 0.053 2.298 12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY h1 c3 1.000 1.093 1406.346 -0.093 12.163 h1 c3 1.000 1.093 1406.346 -0.093 12.163 c3 c3 1.540 1.535 1269.019 0.005 0.032 c3 h1 1.000 1.093 1406.346 -0.093 12.163 c3 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 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	5	12	3.399	3.713	0.053	-0.028	
12						-0.019	
12 5 2.547 3.713 0.053 2.298 12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY 11 J LENGTH LENGTH CONSTANT DELTA ENERGY 12 12 12 12 12 12 12 12 12 12 12 12 12 1							
12 5 3.399 3.713 0.053 -0.028 12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY 11 1 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 11 1.000 1.093 1406.346 -0.093 12.163 12 1.670 1.786 1168.117 -0.116 15.718 15 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol							
12 12 3.587 4.089 0.276 0.100 TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY 10 DELTA ENERGY = 1.000 1.093 1406.346 -0.093 12.163 h1 c3 1.000 1.093 1406.346 -0.093 12.163 h1 c3 1.540 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 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 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 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 STRETCHING ENERGY = 80.122 kJ/mol							
TOTAL VAN DER WAALS ENERGY = 4.94916 kcal/mol E L E C T R O S T A T I C I N T E R A C T I O N S ATOM TYPES I J Rij Qi Qj ENERGY TOTAL ELECTROSTATIC ENERGY = 5.7592 kcal/mol TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY							
ELECTROSTATIC INTERACTIONS ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol ENERGY BOND STRETCHING ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY							1
ATOM TYPES I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY							
I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY	ELF	ЕСТ	ROSTA	TIC II	NTERA	CTION	5
I J Rij Qi Qj ENERGY 12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY							
12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY							
12 12 3.637 -0.290 -0.290 5.759 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY							RGY
TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol TOTAL ENERGY = 31.17064 kcal/mol E N E R G Y B O N D S T R E T C H I N G ATOM TYPES BOND IDEAL FORCE I J LENGTH LENGTH CONSTANT DELTA ENERGY							
ENERGY BOND STRETCHING 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 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 c3 c1 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol							1
ENERGY BOND STRETCHING 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 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 c3 c1 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol							
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	TOTAI	LENER	GY = 31.17	064 kcal/mo	ol		
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							
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 1.535 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 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	E N E	ERG	Y				
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 1.535 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 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							
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 1.535 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 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	B O F	1 D :	STRET	CHING			
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		, ,		0 11 1 1, 0			
h1 c3							
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 c3 c1 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol	ATOM	TYPES	BOND	IDEAL	FORCE		
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							LTA ENERGY
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	I 	J	LENGTH	LENGTH	CONSTAI	NT DE	
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	I h1 c3	J 	LENGTH 	LENGTH	CONSTAN	NT DE:	12.163
C3 Cl 1.670 1.786 1168.117 -0.116 15.718 C3 hl 1.000 1.093 1406.346 -0.093 12.163 C3 Cl 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol	I h1 c3 h1 c3	J 3 3	LENGTH	LENGTH	CONSTANT 1406.346 1406.346	-0.093	12.163 12.163
c3 h1 1.000 1.093 1406.346 -0.093 12.163 c3 cl 1.670 1.786 1168.117 -0.116 15.718 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol	I h1 c3 h1 c3 c3 c3	J 3 3	LENGTH 1.000 1.000 1.540	LENGTH 1.093 1.093 1.535	CONSTAI 1406.346 1406.346 1269.019	-0.093 -0.093 0.005	12.163 12.163 0.032
TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol	I h1 c3 h1 c3 c3 c3	J 3 3 3	LENGTH 1.000 1.000 1.540 1.000	LENGTH 1.093 1.093 1.535 1.093	CONSTANT 1406.346 1406.346 1269.019 1406.346	-0.093 -0.093 0.005 -0.093	12.163 12.163 0.032 12.163
	I h1 c3 h1 c3 c3 c3 c3 h1 c3 c1	J 3 3 3 1 L	LENGTH 1.000 1.000 1.540 1.000 1.670	LENGTH 1.093 1.093 1.535 1.093 1.786	CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718
	I h1 c3 h1 c3 c3 c3 h1 c3 c1 c3 h1	J 33 33 34 44 44 44 44 44 44 44 44 44 44	LENGTH 1.000 1.000 1.540 1.000 1.670 1.000	1.093 1.093 1.535 1.093 1.786 1.093	CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346	-0.093 -0.093 0.005 -0.093 -0.116 -0.093	12.163 12.163 0.032 12.163 15.718 12.163
	I h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1 c3 c1	J 3 3 4 1 L L	LENGTH 1.000 1.000 1.540 1.000 1.670 1.000 1.670	LENGTH 1.093 1.093 1.535 1.093 1.786 1.093 1.786	CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718 12.163 15.718

59									
0		S VAL							
1		K AN						TA I	ENERGY
		100 500						0.010	
1	h1 c3 h1	109.500					0.010		
5	h1 c3 cl	109.442 109.442					0.061		
6	c3 c3 h1	109.442			194.100		0.010		
7	c3 c3 c1	109.500			260.419		0.014		
8	h1 c3 cl	109.442					0.061		
9	c3 c3 h1	109.500	110.070		194.100		0.010		
0	h1 c3 h1	109.442			164.039		0.002		
	h1 c3 cl	109.442	105.930				0.061		
72	c3 c3 h1	109.500			194.100		0.010		
3	c3 c3 cl	109.500	110.330		260.419		0.014	0.055	
74	h1 c3 cl	109.442	105.930		183.005	(0.061	0.688	
5	TOTAL	ANGLE BEN	DING ENER	.GY =	2.938	kJ/mo]	L		
	T O R S I	ONAL							
3									
9	ATOM T	TYPES	FORCE		1	TORSION	N		
0	I J	K L	CONSTAN	T	S	ANGLE	n	ENERGY	
2		1 0.65							
3	h1 c3 c3 h	1 0.65			.00.000	3	0.977		
1	h1 c3 c3 c				40.000		0.000		
	h1 c3 c3 h								
	h1 c3 c3 h				40.000				
	h1 c3 c3 c						0.000		
	cl c3 c3 h								
	cl c3 c3 h								
	cl c3 c3 c						0.000		
	TOTAL	J TORSIONAL	ENERGY =	3.	908 KJ/1	mol			
2	T M D D O		0 D G T 0	. NT 70 T					
3 4	IMPRU	PER T	ORSIO	NAI	1				
5	лπ∩м п	TYPES	FORCE	TI	(DDADED '	TODCTON	vī.		
	I J				_			FNEDCV	
	TOTAL								
	10111		1010101111	LIVETC	, -		10 / 1110 1		
	V A N D	ER WA	ALS						
	-	_							
	ATOM TYPES	3							
	I J		kij		ENERGY				
4									
5	h1 h1	2.638	-0.029						
6	h1 h1	2.232	0.205						
	h1 cl								

```
1608 h1 h1 2.831 -0.032
1609 h1 h1
            2.638
                   -0.029
1610 h1 cl
            2.547
                    2.064
1611 cl h1
            2.547
                    2.064
1612 cl h1
            3.399
                   -0.133
1613 cl cl 3.587 -0.326
     TOTAL VAN DER WAALS ENERGY = 3.650 kJ/mol
1614
1615
1616 ELECTROSTATIC INTERACTIONS
1617
1618 ATOM TYPES
     I J
            Rij 332.17*QiQj ENERGY
1619
1620 -----
1621 h1 h1
           2.638
                    1.352
                           0.513
            2.232
                    1.352
                           0.606
1622 h1 h1
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
            2.547
1626 h1 cl
                   -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
      TOTAL ELECTROSTATIC ENERGY = -0.132 kJ/mol
1630
1631
1632 TOTAL ENERGY = 90.486 kJ/mol
1633
1634 ATOM TYPES
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 FORMAL CHARGES
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
```

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1657
1658
     PARTIAL CHARGES
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
     2 c3 NO
1674
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 FORMAL CHARGES
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 PARTIAL CHARGES
1695
1696 IDX CHARGE
     1 0.036009
1697
1698 2 0.036009
1699 3 0.044101
1700
     4 0.044101
1701 5 -0.124211
1702
     6 0.044101
     7 0.044101
1703
     8 -0.124211
1704
1705
```

1706 ENERGY 1707 1708 1709 BOND STRETCHING 1710 ATOM TYPES FF BOND IDEAL FORCE 1711 1712 I J LENGTH CONSTANT DELTA CLASS LENGTH ENERGY 1713 ______ 1 0 1.093 1.000 1714 5 4.766 -0.093 3.578 1715 5 1 0 1.000 1.093 4.766 -0.093 3.578 1716 0 1.540 1.508 4.258 0.032 0.294 1 1 5 1717 1 0 1.000 1.093 4.766 -0.093 3.578 1718 1 12 0 1.670 1.773 2.974 -0.103 2.795 1719 1 5 1.000 1.093 4.766 -0.093 0 3.578 1.773 2.974 -0.103 1720 1 12 0 1.670 2.795 1721 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol 1722 ANGLE BENDING 1723 1724 1725 FF VALENCE IDEAL FORCE ATOM TYPES ANGLE 1726 CLASS ANGLE CONSTANT DELTA ENERGY I J K 1727 1728 1 1 5 0 109.500 110.549 0.636 -1.049 0.015 1729 5 1 5 0 109.442 108.836 0.516 0.606 0.004 109.442 1730 5 1 12 0 108.162 0.698 1.280 0.025 0.636 1731 1 1 5 0 109.500 110.549 -1.0490.015 1732 1 1 12 0 109.500 108.679 1.056 0.821 0.016 1733 5 1 12 0 109.442 108.162 0.698 1.280 0.025 1 5 109.500 110.549 1734 1 0 0.636 -1.049 0.015 1735 5 1 5 0 109.442 108.836 0.516 0.606 0.004 1736 5 1 12 0 109.442 108.162 0.698 1.280 0.025 1 5 0 109.500 110.549 1737 1 0.636 -1.0490.015 1738 1 1 12 0 109.500 108.679 1.056 0.821 0.016 108.162 1739 5 1 12 0 109.442 0.698 1.280 0.025 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol 1740 1741 1742 1743 ATOM TYPES FF VALENCE FORCE CONSTANT 1744 DELTA IJ JK 1745 I J K CLASS ANGLE ANGLE ENERGY 1746 1747 1 1 5 0 109.500 -1.049 0.227 0.070 -0.0025 0.606 0.115 1748 1 5 0 109.442 0.115 -0.033 109.442 1 12 0 1.280 0.380 1749 5 -0.018 -0.1215 1750 1 0 109.500 -1.0490.227 0.070 1 -0.0021751 1 1 12 0 109.500 0.821 0.176 0.386 -0.070109.442 1 12 1.280 -0.018 1752 5 0 0.380 -0.1211 5 0 109.500 0.227 1753 -1.0490.070 1 -0.002 1754 5 1 5 0 109.442 0.606 0.115 0.115 -0.033

5 1	1	12	0			0 010	0 000	0 101
1			0	109.442	1.280	-0.018	0.380	-0.121
	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
	TOTA	AL STE	RETCH BEN	DING ENERGY	Y = -0.6959	3 kcal/mol		
ТО	R S I	ON	A L					
ATOM	I TYPE	ES		FF TOF	RSION	FORCE CONS	TANT	
I	J	K	L	CLASS AN	NGLE	V1 V2	V3 ENE	ERGY
5	1	1	5	0 0.0	000 0.28	4 -1.386	0.314	0.598
5	1	1	5	0 120.0	000 0.28	4 -1.386	0.314	-0.654
5	1		12		000 0.67		0.398	0.116
5	1	1	5		000 0.28			-0.655
5	1		5					
5	1	1						1.076
12	1			0 -120.0				
12	1					8 -0.602		
12						0 0.000		
. 2				0 = 120.0 $NERGY = 1.$			0.033	0.093
	1018	ıl IOF	OTOMAL E	., 1.	JIIJU KUAI	, mor		
UU	Т – С) F -	PLAN	E BENI	DING			
MOTA	I TYPE	ES		FF C	OOP FOR	CE		
						CE TANT EN	ERGY	
I 	J	К	L	CLASS AN	NGLE CONS	TANT EN		
I 	J	К	L	CLASS AN	NGLE CONS			
I 	J	К	L	CLASS AN	NGLE CONS	TANT EN		
I 	J TOTA	K AL OUT	L	CLASS AN	NGLE CONS	TANT EN		
I 	J TOTA	K AL OUT	L '-OF-PLAN	CLASS AN	NGLE CONS	TANT EN		
I 	J TOTA N D TYPE	K AL OUT D E R	L C-OF-PLAN W A A	CLASS AN	NGLE CONS	TANT EN		
I V A ATOM	J TOTA N D TYPE	K AL OUT D E R	L C-OF-PLAN W A A	CLASS AN	NGLE CONS	TANT EN		
I / A ATOM I	J TOTA N D TYPE J	K AL OUT DER	L C-OF-PLAN W A A	CLASS AN	NGLE CONS	TANT EN 00000 kcal ENERGY		
I V A ATOM I 5	J TOTA N E TYPE J 5	K AL OUT DER	L C-OF-PLAN W A A Rij 	CLASS AN E BENDING F L S R*IJ 2.970	NGLE CONS ENERGY = 0 EPSILON 0.022	TANT EN00000 kcal ENERGY0.014		
I V A ATOM I 5	J TOTA N E TYPE J 5	K AL OUT DER	L C-OF-PLAN W A A Rij 	CLASS AN	NGLE CONS ENERGY = 0 EPSILON 0.022	TANT EN00000 kcal ENERGY0.014		
I V A ATOM I 5 5	J TOTA I TYPE J 5 5	K AL OUT DER	L C-OF-PLAN W A A Rij 	CLASS AN E BENDING F L S R*IJ 2.970	EPSILON 0.022 0.022	ENERGY0.014 0.377		
I V A AATOM I 5 5 5 5	J TOTA N C TYPE J 5 5 12	K AL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280	CLASS AN E BENDING F L S R*IJ 2.970 2.970	EPSILON 0.022 0.022 0.053	ENERGY -0.014 0.377 0.009		
I V A ATOM I 5 5 5 5 5	J TOTA N C TYPE J 5 5 12	K AL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713	EPSILON 0.022 0.022 0.053 0.022	ENERGY -0.014 0.377 0.009		
I	J TOTA I TYPE J 5 5 12 5 5	K AL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713 2.970	EPSILON 0.022 0.022 0.053 0.022 0.022	ENERGY0.014 0.377 0.009 -0.014 -0.014		
I V A ATOM I 5 5 5 5 5 5 5 5	J TOTA I TYPE J 5 5 12 5 5	K AL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746 2.512	CLASS AN E BENDING E L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713	EPSILON 0.022 0.022 0.053 0.022 0.053	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649		
I	J TOTA N C TYPE J 5 5 12 5 12 5 12 5	K AL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746 2.512 2.512	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 3.713 3.713	EPSILON 0.022 0.022 0.053 0.022 0.053 0.053	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649		
I V A ATOM I 5 5 5 5 5 12 12	J TOTA N C TYPE J 5 5 12 5 12 5 5 5	KAL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.512 2.512 3.280	CLASS AN E BENDING E L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 3.713 3.713 3.713	EPSILON 0.022 0.022 0.053 0.022 0.053 0.053 0.053	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649 0.009		
I V A ATOM I 5 5 5 5 5 12 12	J TOTA N C TYPE J 5 5 12 5 12 5 12	K AL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746 2.512 2.512 3.280 3.806	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 4.089	EPSILON 0.022 0.022 0.053 0.022 0.053 0.053 0.053 0.053 0.276	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649 0.009 -0.201		
I	J TOTA N C TYPE J 5 5 12 5 12 5 12	K AL OUT DER	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746 2.512 2.512 3.280 3.806	CLASS AN E BENDING E L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 3.713 3.713 3.713	EPSILON 0.022 0.022 0.053 0.022 0.053 0.053 0.053 0.053 0.276	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649 0.009 -0.201		
I	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12 7 TOTA	K AL OUT AL VAN	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746 2.512 2.512 3.280 3.806 H DER WAA	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 4.089 LS ENERGY =	EPSILON 0.022 0.022 0.053 0.022 0.053 0.053 0.053 0.053 0.276 = 5.44875	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649 0.009 -0.201 kcal/mol		
I	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12 7 TOTA	K AL OUT AL VAN	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746 2.512 2.512 3.280 3.806 H DER WAA	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 4.089	EPSILON 0.022 0.022 0.053 0.022 0.053 0.053 0.053 0.053 0.276 = 5.44875	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649 0.009 -0.201 kcal/mol		
I V A ATOM I 5 5 5 5 12 12 12 12	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12 TOTA	K AL OUT O E R ES T R O	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.746 2.512 2.512 3.280 3.806 H DER WAA	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 4.089 LS ENERGY =	EPSILON 0.022 0.022 0.053 0.022 0.053 0.053 0.053 0.053 0.276 = 5.44875	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649 0.009 -0.201 kcal/mol		
I V A ATOM I 5 5 5 5 12 12 12 12	J TOTA N C TYPE J 5 5 12 5 12 5 12 5 12 TOTA	K AL OUT AL VAN	L C-OF-PLAN W A A Rij 2.746 2.208 3.280 2.746 2.512 2.512 3.280 3.806 W DER WAA	CLASS AN E BENDING F L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 4.089 LS ENERGY =	EPSILON O.022 O.022 O.022 O.053 O.022 O.053 O.053 O.053 O.276 = 5.44875 FERACT	ENERGY0.014 0.377 0.009 -0.014 -0.014 2.649 2.649 0.009 -0.201 kcal/mol		

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

```
1853 h1 c3 c3 cl 0.000 0 -120.000 3 0.000
1854 h1 c3 c3 h1
              0.651
                        0
                           120.000 3
                                       1.303
1855 h1 c3 c3 h1
              0.651
                       0 -120.000 3
                                       1.303
                            0.000 3
1856 h1 c3 c3 cl
              0.000
                        0
                                       0.000
                       0 -120.000 3
1857 cl c3 c3 h1
              0.000
                                       0.000
1858 cl c3 c3 h1
              0.000
                        0
                            -0.000 3
                                       0.000
              0.000 0 120.000 3
1859 cl c3 c3 cl
                                       0.000
      TOTAL TORSIONAL ENERGY = 5.210 kJ/mol
1860
1861
1862 IMPROPER TORSIONAL
1863
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
1864
1865 I J K L CONSTANT S ANGLE N ENERGY
1866
    ______
     TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
1867
1868
1869 VAN DER WAALS
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
           2.746
1877 h1 h1
                  -0.033
1878 h1 h1
           2.746 -0.033
1879 h1 cl
           2.512
                  2.571
           2.512
                  2.571
1880 cl h1
1881 cl h1
           3.280 -0.134
                  -0.542
1882 cl cl
           3.806
1883
     TOTAL VAN DER WAALS ENERGY = 4.485 kJ/mol
1884
1885 ELECTROSTATIC INTERACTIONS
1886
1887 ATOM TYPES
    I J
                Rij 332.17*QiQj ENERGY
1888
1889
    _____
           2.746 1.352 0.493
1890 h1 h1
1891 h1 h1
           2.208
                  1.352
                         0.613
1892 h1 cl
           3.280 -3.809 -1.161
    h1 h1
           2.746
                  1.352
1893
                         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 \text{ kJ/mol}
1900
1901 TOTAL ENERGY = 92.310 \text{ kJ/mol}
```

```
1902
1903 ATOM TYPES
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 FORMAL CHARGES
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 PARTIAL CHARGES
1928
1929 IDX CHARGE
1930 1 0.290000
1931 2 0.290000
1932 | 3 0.000000
1933 4 0.000000
1934 5 -0.290000
     6 0.000000
1935
1936 7 0.000000
1937 8 -0.290000
1938
1939 SETTING UP CALCULATIONS
1940
1941 SETTING UP BOND CALCULATIONS...
1942
     SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
1943 SETTING UP TORSION CALCULATIONS...
     SETTING UP OOP CALCULATIONS...
1944
1945
     SETTING UP VAN DER WAALS CALCULATIONS...
1946 SETTING UP ELECTROSTATIC CALCULATIONS...
1947
1948 A T O M T Y P E S
1949
1950 IDX TYPE RING
```

```
1951 1 c3 NO
1952 2 c3 NO
1953 3 h1 NO
1954 4 h1 NO
1955 | 5 cl NO
    6 h1 NO
1956
1957
    7 h1 NO
1958
    8 cl 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
    SETTING UP CALCULATIONS
1972
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...
    SETTING UP ELECTROSTATIC CALCULATIONS...
1979
1980
1981
    ENERGY
1982
1983
1984 BOND STRETCHING
1985
1986 ATOM TYPES FF BOND IDEAL FORCE
     I J CLASS LENGTH
1987
                            LENGTH
                                     CONSTANT
                                                DELTA
                                                         ENERGY
1988
    5 1
              0
                    1.000
                                       4.766
                                                -0.093
1989
                             1.093
                                                         3.578
1990
    5
                    1.000
                             1.093
                                       4.766
                                                -0.093
                                                         3.578
         1
              0
     1
         1
              0
                    1.540
                             1.508
                                       4.258
1991
                                                0.032
                                                         0.294
1992
    1 5
              0
                    1.000
                             1.093
                                       4.766
                                                -0.093
                                                         3.578
1993
    1 12
                    1.670
                             1.773
                                       2.974
                                                -0.103
                                                         2.795
              0
1994
     1 12
              0
                    1.670
                             1.773
                                       2.974
                                                -0.103
                                                          2.795
    1 5
                                       4.766
                                               -0.093
1995
              0
                    1.000
                             1.093
                                                         3.578
1996
        TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
1997
1998 ANGLE BENDING
1999
```

2000	ATOM	TYPI	ES	FF	VALENCE	E ID	EAL	FORCE		
2001	I	J	K	CLASS	ANGLE	AN	GLE	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		1		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					109.500		679		0.821	
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		TOTA	AL ANG	LE BENDI	NG ENERGY	Z = 0.2	0058 k	cal/mol		
2016										
2017	ST	RE:	ГСН	BENI	DING					
2018										
2019								FORCE		
2020									JК	
2021									0.070	
2022									0.070	
								0.115		-0.033
2024					109.442					
2025				0				0.227		
2026		1		0				0.176		
2027				0				-0.018		
								0.227		-0.002
2029							280 606	0.115	0.380 0.115	-0.121
2030	5	1	5	0	109.442					-0.033
2031	1		12 5	0	109.500		821 049	0.176 0.227	0.386 0.070	-0.070
2032	5	1	12	0						-0.121
2033	J				109.442			kcal/mol	0.300	-0.121
2034		1012	лг оти	EICH BEN	DING ENER	(61 – -0	.09393	KCa1/IIIO1		
2036	ΤО	RS -	I O N	A T.						
2037			,							
2038	ATOM	TYPI	ES		FF I	CORSION]	FORCE CONS	TANT	
2039	I		K	L (ANGLE		V1 V2	V3 ENE	RGY
2040										
2041	5	1	1	5	0 20	0.000	0.284	-1.386	0.314	0.349
2042	5	1	1	12	0 -100	0.000	0.678	-0.602	0.398	-0.005
2043	5	1	1	5	0 140	0.000	0.284	-1.386	0.314	-0.304
2044	5	1	1	5	0 140	0.000	0.284	-1.386	0.314	-0.304
2045	5	1	1	12	0 20	0.000	0.678	-0.602	0.398	0.886
2046	5	1	1	5	0 -100	0.000	0.284	-1.386	0.314	-0.991
2047	12	1	1	5	0 -100	0.000	0.678	-0.602	0.398	-0.005
2048	12	1	1	12	0 140	0.000	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 OUT-OF-PLANE BENDING
2053
    ATOM TYPES
                   FF OOP FORCE
2054
    I J K
2055
                  CLASS ANGLE CONSTANT
              L
2056
    ______
2057
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
2058
2059 VAN DER WAALS
2060
2061 ATOM TYPES
2062
             Rij R*IJ EPSILON ENERGY
    I J
2063
    5 5
              2.831
                     2.970
2.064
                            0.022
                                   -0.019
   5 5
                     2.970
2065
             2.232
                            0.022
                                   0.328
                           0.053
                                   0.104
2066 5 12
             3.129
                    3.713
   5 5
2067
             2.638
                     2.970
                            0.022
                                   0.001
2068 5 5
             2.831
                     2.970
                           0.022 -0.019
             2.547
2069
    5 12
                     3.713
                           0.053
                                   2.298
2070 12 5
             2.547
                     3.713
                            0.053
                                   2.298
    12 5
              3.129
                     3.713
                           0.053
2071
                                   0.104
                           0.276 -0.269
2.072
    12 12
              3.975
                     4.089
      TOTAL VAN DER WAALS ENERGY = 4.82482 kcal/mol
2073
2074
   ELECTROSTATIC INTERACTIONS
2075
2076
2077 ATOM TYPES
             Rij Qi Qj ENERGY
2078
    I J
2079
    12 12 4.025 -0.290 -0.290 5.204
2080
    TOTAL ELECTROSTATIC ENERGY = 5.20367 kcal/mol
2081
2082
2083 | TOTAL ENERGY = 30.90959 kcal/mol
2084
2085 ENERGY
2086
2087
2088 BOND STRETCHING
2089
2090 ATOM TYPES BOND
                   IDEAL
                           FORCE
    I J
                           CONSTANT
2.091
           LENGTH
                   LENGTH
                                     DELTA
                                            ENERGY
2092
2093 h1 c3
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12,163
2094 h1 c3
          1.000
                         1406.346
                  1.093
                                  -0.093
                                          12.163
                  1.535
                         1269.019
2095 c3 c3
          1.540
                                   0.005
                                          0.032
                  1.093
                         1406.346
          1.000
                                         12.163
2096 c3 h1
                                  -0.093
2097 c3 cl
          1.670 1.786 1168.117 -0.116 15.718
```

```
2098 c3 cl 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 ANGLE BENDING
2103
2104 ATOM TYPES
               VALENCE IDEAL FORCE
2105
    I J K
                ANGLE
                        ANGLE
                               CONSTANT
                                         DELTA ENERGY
    _____
2106
                   110.070
2107 c3 c3 h1 109.500
                             194.100
                                      -0.010
                                              0.019
2108 h1 c3 h1 109.442 109.550
                             164.039
                                     -0.002
                                              0.001
2109 h1 c3 cl 109.442 105.930
                            183.005
                                      0.061
                                              0.688
                                              0.019
2110 c3 c3 h1 109.500 110.070
                             194.100
                                     -0.010
2111 c3 c3 c1 109.500 110.330
                            260.419
                                     -0.014
                                              0.055
2112 h1 c3 cl 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 cl 109.442 105.930
                             183.005
                                      0.061
                                              0.688
                            164.039 -0.002
2115 h1 c3 h1 109.442 109.550
                                              0.001
2116 c3 c3 cl 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 cl 109.442 105.930 183.005
                                      0.061
                                              0.688
     TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
2119
2120
2121 T O R S I O N A L
2122
2123 ----ATOM TYPES---- FORCE
                                 TORSION
    I J K L CONSTANT
2124
                                  ANGLE n ENERGY
                            S
2125
2126 h1 c3 c3 h1 0.651 0
                            20.000 3
                                        0.977
2127 h1 c3 c3 cl
               0.000
                        0 -100.000 3
                                        0.000
                        0
2128 h1 c3 c3 h1
               0.651
                            140.000 3
                                        0.977
2129 h1 c3 c3 h1 0.651
                        0
                            140.000 3
                                        0.977
2130 h1 c3 c3 cl
               0.000
                        0
                            20.000 3
                                        0.000
2131 h1 c3 c3 h1
               0.651
                        0 -100.000 3
                                        0.977
              0.000
                        0 -100.000 3
2132 cl c3 c3 h1
                                        0.000
2133 cl c3 c3 cl
                        0
                            140.000 3
               0.000
                                        0.000
2134
    cl c3 c3 h1
               0.000
                        0
                            20.000 3
                                        0.000
     TOTAL TORSIONAL ENERGY = 3.908 kJ/mol
2135
2136
2137 IMPROPER TORSIONAL
2138
2139 ----ATOM TYPES---- FORCE IMPROPER_TORSION
    I J K L CONSTANT
                            s ANGLE n ENERGY
2140
2141
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2142
2143
2144 VAN DER WAALS
2145
2146 ATOM TYPES
```

```
2147 I J Rij kij ENERGY
2148
2149 h1 h1
            2.831 -0.032
2150 h1 h1
            2.232
                   0.205
2151 h1 cl
            3.129
                   -0.106
2152 h1 h1
            2.638 -0.029
2153 h1 h1
            2.831
                   -0.032
2154 h1 cl
            2.547
                   2.064
                   2.064
2155 cl h1
            2.547
2156 cl h1
            3.129
                   -0.106
            3.975 -0.548
2157 cl cl
     TOTAL VAN DER WAALS ENERGY = 3.480 kJ/mol
2158
2159
2160 ELECTROSTATIC INTERACTIONS
2161
2162 ATOM TYPES
    I J
2163
                Rij 332.17*QiQj ENERGY
2164
    _____
            2.831
2165 h1 h1
                   1.352
                           0.478
2166 h1 h1
            2.232
                   1.352
                           0.606
            3.129 -3.809 -1.217
2167 h1 cl
            2.638
                   1.352
2168 h1 h1
                           0.513
2169 h1 h1
            2.831
                   1.352
                           0.478
2170 h1 cl
            2.547 -3.809 -1.495
            2.547
2171 cl h1
                   -3.809
                           -1.495
2172 cl h1
            3.129 -3.809 -1.217
            3.975 10.728
2173 cl cl
                           2.699
      TOTAL ELECTROSTATIC ENERGY = -0.652 kJ/mol
2174
2175
2176 TOTAL ENERGY = 89.796 kJ/mol
2177
2178 ATOM TYPES
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 FORMAL CHARGES
2191
2192 IDX CHARGE
2193 | 1 0.000000
2194 2 0.000000
2195 | 3 0.000000
```

```
2196 4 0.000000
2197 5 0.000000
2198 6 0.000000
2199 7 0.000000
2200 8 0.000000
2201
2202 PARTIAL CHARGES
2203
2204 IDX CHARGE
2205 | 1 0.290000
2206 2 0.290000
     3 0.000000
2207
2208 4 0.000000
2209 5 -0.290000
2210
     6 0.000000
2211 7 0.000000
2212 8 -0.290000
2213
2214 SETTING UP CALCULATIONS
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 ATOM TYPES
2224
2225 IDX TYPE RING
2226 1 c3 NO
2227 2 c3 NO
2228 | 3 h1 NO
2229
     4 h1 NO
2230 5 cl NO
2231 6 h1 NO
2232 7 h1 NO
2233 8 cl 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 SETTING UP CALCULATIONS
2248
2249
    SETTING UP BOND CALCULATIONS...
2250
    SETTING UP ANGLE CALCULATIONS...
2251
    SETTING UP TORSION CALCULATIONS...
    SETTING UP IMPROPER TORSION CALCULATIONS...
2252
    SETTING UP VAN DER WAALS CALCULATIONS...
2253
    SETTING UP ELECTROSTATIC CALCULATIONS...
2254
2255
2256
    ENERGY
2257
2258
    BOND STRETCHING
2259
2260
2261 ATOM TYPES FF BOND
                         IDEAL
                                  FORCE
                         LENGTH
                                  CONSTANT
                                            DELTA
2262
    I J CLASS LENGTH
                                                    ENERGY
2263
2264
    5 1
            0
                  1.000
                          1.093
                                    4.766
                                           -0.093
                                                    3.578
2265
     5
        1
             0
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                    3.578
                  1.670
        1
                          1.773
                                    2.974
2266 12
             0
                                            -0.103
                                                    2.795
2267
    1
        1
             0
                  1.540
                          1.508
                                    4.258
                                            0.032
                                                    0.294
                                    4.766
                                            -0.093
2268
    1 5
             0
                  1.000
                          1.093
                                                    3.578
2269
    1 12
             0
                  1.670
                          1.773
                                    2.974
                                            -0.103
                                                    2.795
                          1.093 4.766 -0.093
2270
    1 5
            0
                  1.000
                                                    3.578
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
2271
2272
2273 ANGLE BENDING
2274
2275
    ATOM TYPES
                FF VALENCE
                              IDEAL
                                      FORCE
               CLASS ANGLE
2276
    I J K
                              ANGLE CONSTANT
                                               DELTA ENERGY
2277
                            110.549
2278
     1
        1
            5
                 0
                    109.500
                                        0.636
                                                -1.049
                                                         0.015
        1 5
                 0 109.442 108.836
2279
    5
                                       0.516
                                               0.606
                                                        0.004
                 0 109.442
                                       0.698
                                                1.280
2280
    5
        1 12
                            108.162
                                                        0.025
2281
        1
           5
                 0
                    109.500
                            110.549
                                        0.636
                                               -1.049
                                                        0.015
    1
                 0 109.500 108.679
    1
        1 12
                                        1.056
                                                0.821
2282
                                                        0.016
2283
    5
        1 12
                 0
                    109.442
                            108.162
                                       0.698
                                                1.280
                                                        0.025
2284
    5
        1 12
                    109.442 108.162
                                        0.698
                                                1.280
                                                         0.025
                 0
        1 5
                   109.500 110.549
2285
     1
                 0
                                        0.636
                                                -1.049
                                                         0.015
    5
        1
            5
                 0 109.442
                            108.836
                                       0.516
                                                0.606
                                                        0.004
2286
                 0 109.500 108.679
                                        1.056
2287
    1
        1 12
                                               0.821
                                                        0.016
                    109.442 108.162
        1 12
2288
     5
                 0
                                        0.698
                                                1.280
                                                        0.025
    1
        1
            5
                    109.500
                            110.549
                                               -1.049
2289
                 0
                                       0.636
                                                        0.015
2290
       TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
2291
2292 STRETCH BENDING
2293
```

294	ATOM	TYPE	ES	FF	VALE	NCE D	ELTA	FOR	CE CONSTAN	1T
295	I	J	K	CLASS	ang Ang	LE A	NGLE	ΙJ	J	K ENERGY
296										
297	1	1	5	0	109.5	00 -1	.049	0.227	0.07	70 -0.002
298	5	1	5	0	109.4	42 0	.606	0.115	0.11	-0.033
299	5	1	12	0	109.4	42 1	.280	-0.018	0.38	-0.121
300	1	1	5	0	109.5	00 -1	.049	0.227	0.07	70 -0.002
301	1	1	12	0	109.5	00	.821	0.176	0.38	-0.070
302	5	1	12	0	109.4	42 1	.280	-0.018	0.38	-0.121
303	5	1	12	0	109.4	42 1	.280	-0.018	0.38	-0.121
304	1	1	5	0	109.5	00 -1	.049	0.227	0.07	70 -0.002
305	5	1	5	0	109.4	42 0	.606	0.115	0.11	L5 -0.033
306	1	1	12	0	109.5	00 0	.821	0.176	0.38	-0.070
307	5	1	12	0	109.4	42 1	.280	-0.018	0.38	-0.121
808	1	1	5	0	109.5	00 -1	.049	0.227	0.07	70 -0.002
09		TOTA	AL STE	RETCH BEI	DING E	NERGY = -	0.69593	kcal/mo	1	
10										
11	т о :	R S I	ON	A L						
12										
13	ATOM	TYPE	ES		FF	TORSION	[]	FORCE CO	NSTANT	
14	I	J	K	L	CLASS	ANGLE		V1 V2	V3	ENERGY
15										
16	5	1	1	5	0	40.000	0.284	-1.38	6 0.314	-0.243
17	5	1	1	12	0	-80.000	0.678	-0.60	2 0.398	-0.086
18	5	1	1	5	0	160.000	0.284	-1.38	6 0.314	-0.075
19	5	1	1	5	0	160.000	0.284	-1.38	6 0.314	-0.075
20	5	1	1	12	0	40.000	0.678	-0.60	2 0.398	0.449
21	5	1	1	5	0	-80.000	0.284	-1.38	6 0.314	-1.099
322	12	1	1	5	0	-80.000	0.678	-0.60	2 0.398	-0.086
323	12	1	1	12	0	160.000	0.000	0.00	0 0.893	0.223
24	12	1	1	5	0	40.000	0.678	-0.60	2 0.398	0.449
25		TOTA	L TOI	RSIONAL E	NERGY	= -0.5433	6 kcal/ı	mol		
26										
27	O U	т – С) F -	P L A N	Е В	ENDIN	I G			
328										
329	ATOM	TYPE	ES		FF	OOP	FORC	E		
	I	J	K	L	CLASS	ANGLE	CONST	ANT	ENERGY	
30										
					IF BENIC	ING ENERG	SY = 0.	00000 kc	al/mol	
31			Tr On.	r-of-plan	IL DENL	THO DIVINO				
31			AL OU'.	r-or-plan	IE DENE	THO BREK				
331 332 333		TOTA		r-of-plan W A A		THO BINDING				
331 332 333 334		TOTA				ING ENERG				
331 332 333 334 335		TOT <i>P</i>) E R			ING ENERG				
331 332 333 334 335	V A	TOT <i>E</i> N [DER ES	W A A	L S	J EPSI	LON 1	ENERGY		
331 332 333 334 335 336	V A :	TOTA N I TYPE J	DER ES	W A A	L S					
330 331 332 333 334 335 336 337 338	V A I	TOTA TYPE J	DER ES	W A A	L S R*I	J EPSI				
331 332 333 334 335 336 337 338	V A : ATOM I 5	TOTA N I TYPE J 5	DER	W A A Rij2.885	L S R*I 2.9	J EPSI	022	-0.021		
331 332 333 334 335 336 337 338 339	V A : ATOM I 5 5	TOTA TYPE J 5 5	DER	W A A Rij 2.885 2.300	R*I	J EPSI 70 0.	022	 -0.021 0.215		

5 5	2.8	2.970	0.022	-0.021		
5 12	2.6	47 3.713	0.053	1.520		
12 5	2.6	47 3.713	0.053	1.520		
12 5	2.9	60 3.713	0.053	0.331		
12 12	4.0	4.089	0.276	-0.276		
TC	TAL VAN DER	WAALS ENERG	3.6366	3 kcal/mol		
ELEC	TROST	ATIC I	NTERAC	TIONS		
ATOM TY						
	Rij					
					-	
	4.132					
TC	TAL ELECTRO	STATIC ENERG	3Y = 5.0691	5 kcal/mol		
		0.6005 1 7/				
rotal E	ENERGY = 27.8	86335 KCal/m	IOT			
) C V					
ENEF	GI					
	STRE!	r C H T N C				
5 O N L) SIKE	ICHING				
атом тү	PES BOND	TDEAL.	FORCE			
	LENGTH			T DELT	A ENER	GY
	1.000					
	1.000					
cl c3	1.670	1.786	1168.117	-0.116	15.718	
c3 c3	1.540	1.535	1269.019	0.005	0.032	
c3 h1	1.000	1.093	1406.346	-0.093	12.163	
c3 cl	1.670	1.786	1168.117	-0.116	15.718	
c3 h1	1.000	1.093	1406.346	-0.093	12.163	
TC	TAL BOND ST	RETCHING ENE	ERGY = 80.	122 kJ/mol		
ANGI	E BENI	DING				
	PES V					
I J	K Z	ANGLE A	NGLE CO	NSTANT	DELTA	ENERGY
	109.500					
h1 c3 h		109.550		9 -0.00		
h1 c3 c		105.930		5 0.06		
c3 c3 h						
c3 c3 c		110.330				
h1 c3 c				5 0.06		
h1 c3 c				5 0.06		
c3 c3 h						
h1 c3 h		109.550				
c3 c3 c	109.500	110.330	260.41	9 -0.01	4 0.05	5

```
2392 h1 c3 cl 109.442 105.930 183.005 0.061 0.688
2393 c3 c3 h1 109.500 110.070
                           194.100 -0.010
                                            0.019
2394
     TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
2395
2396 TORSIONAL
2397
                                TORSION
2398 ----ATOM TYPES---- FORCE
2399
    I J K
              L
                  CONSTANT
                                ANGLE n ENERGY
                           s
2400 | -----
2401 h1 c3 c3 h1
                            40.000 3
              0.651
                       0
                                       0.326
2402 h1 c3 c3 cl
              0.000
                       0 -80.000 3
                                      0.000
                       0 160.000 3
2403 h1 c3 c3 h1 0.651
                                      0.326
                       0 160.000 3
2404 h1 c3 c3 h1
              0.651
                                      0.326
                       0
2405 h1 c3 c3 c1
                           40.000 3
              0.000
                                      0.000
2406 h1 c3 c3 h1 0.651
                       0 -80.000 3
                                      0.326
2407 cl c3 c3 h1
              0.000
                       0 -80.000 3
                                      0.000
2408 cl c3 c3 cl
                       0
                           160.000 3
              0.000
                                      0.000
              0.000 0
2409 cl c3 c3 h1
                           40.000 3
                                      0.000
     TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
2410
2411
2412 IMPROPER TORSIONAL
2413
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
2414
    I J K L CONSTANT S ANGLE N ENERGY
2415
2416
2417
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2418
2419 VAN DER WAALS
2.42.0
2421 ATOM TYPES
    I J Rij kij ENERGY
2422
2423
2424 h1 h1 2.885 -0.031
2425 h1 h1
           2.300
                  0.109
                 0.012
2426 h1 cl
           2.960
2427 h1 h1
           2.518
                 -0.013
2428 h1 h1
           2.885
                 -0.031
           2.647
                 1.083
2429 h1 cl
2430 cl h1
           2.647
                  1.083
2431 cl h1
           2.960
                  0.012
    cl cl
           4.082 -0.522
2432
2433
    TOTAL VAN DER WAALS ENERGY = 1.704 kJ/mol
2434
2435 ELECTROSTATIC INTERACTIONS
2436
2437 ATOM TYPES
    I J
2438
           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 cl
             2.960
                     -3.809 -1.287
                              0.537
2443 h1 h1
             2.518
                      1.352
2444 h1 h1
             2.885
                      1.352
                              0.469
2445 h1 cl
             2.647
                     -3.809
                             -1.439
2446 cl h1
             2.647 -3.809 -1.439
2447 cl h1
             2.960
                     -3.809
                             -1.287
2448
     cl cl
              4.082
                     10.728
                              2.628
      TOTAL ELECTROSTATIC ENERGY = -0.761 kJ/mol
2449
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 FORMAL CHARGES
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 PARTIAL CHARGES
2478
2479 IDX CHARGE
2480 1 0.290000
    2 0.290000
2481
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 SETTING UP CALCULATIONS
```

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

2539	5	1	0	1.0	000 1	1.093	4.766	-0.093	3.578
2540	12	1	0	1.6	570 1	1.773	2.974	-0.103	2.795
2541	5	1	0	1.0	000 1	1.093	4.766	-0.093	3.578
2542	1	1	0	1.5	540 1	1.508	4.258	0.032	0.294
2543	1	5	0	1.0	000 1	1.093	4.766	-0.093	3.578
2544	1		0			1.773	2.974	-0.103	2.795
2545	1		0					-0.093	3.578
2546		TOTA	L BOND	STRETCH	HING ENERG	GY = 20.1962	29 kcal/mol		
2547									
2548	A N	GLE	ВЕ	NDII	1 G				
2549			_						
2550						IDEAL			
2551		J						DELTA	ENERGY
2552									0.015
2553		1						-1.049	
2554 2555	5					108.836		0.606 1.280	
	5	1	12 5	0	109.442				
2556 2557	1	1	12	0	109.500		0.636	-1.049 0.821	
2558	5	1	12	0	109.500	108.162	0.698		
2559	5	1	12	0	109.442	108.162	0.698		
2560	1	1	12	0	109.500			0.821	
2561	5		12	0	109.442			1.280	
2562	1		5	0	109.500		0.636		
2563	5	1		0	109.442			0.606	
2564		1		0			0.636		
2565		TOTA	L ANGI	E BENDI	NG ENERGY	= 0.20058	kcal/mol		
2566									
2567	ST	RET	СН	BENI	O I N G				
2568									
2569	ATOM	TYPE	S	FF	VALENCE	DELTA	FORCE	CONSTANT	
2570	I	J	K	CLASS	ANGLE	ANGLE	ΙJ	JК	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					0.227		
2576		1	12				0.176		
2577		1	12		109.442		-0.018		
	5						-0.018		
2579		1	12				0.176		
2580			12				-0.018		
2581							0.227		
2582							0.115		
2583								0.070	-0.002
2584 2585		TOTA	r Sikt	TOU BENI	YTMG ENER(GY = -0.6959	22 VCGT/WOT		
2586	ΤО	RST	O N A	Т.					
2587	1 0	I O I	O IN P.	. 11					
2307									

ATOM	TYPES	1		F'F'	TORSION	I	ORCE	CONS	TANT	
I	J	K	L	CLASS	ANGLE		V1	V2	V3	ENERGY
										0.05
										-0.82
										0.00
										0.05
					-180.000					0.00
					-60.000					
										0.00
										0.05
								602	0.39	0.05
	TOTAL	TOE	RSIONAL	ENERGY	= -1.42500) kcal/m	nol			
O U	T - O	F -	PLAN	I E B	ENDIN	G				
							_			
					OOP					
					ANGLE				ERGY	
	TOTAL	UO	Γ-OF-PL <i>I</i>	ANE BENI	DING ENERGY	z = 0.0	00000	kcal	/mol	
V A	N D	E R	WAA	ALS						
ATOM	I TYPES	;								
			Rij	R*1	IJ EPSII	ON E	ENERGY	7.		
I 	J							-		
I 5	J 5		2.903	2.9	970 0.0)22 -	-0.021	-		
I 5 5	J 5 5		2.903	2.9	970 0.0 970 0.0)22 -)22	0.107	- - 7		
I 5 5	J 5 5		2.903	2.9	970 0.0)22 -)22	0.107	- - 7		
I 5 5	J 5 5		2.903	2.9 2.9 3.7	970 0.0 970 0.0 713 0.0)22 -)22	0.107	- - !		
5 5 5 5	J 5 5 12 5		2.903 2.400 2.792	2.9 2.9 3.7 2.9	970 0.0 970 0.0 713 0.0 970 0.0)22 -)22 -)23)53	0.107	- - - - - - - - - - - - - - - - - - -		
5 5 5 5 5	J 5 5 12 5		2.903 2.400 2.792 2.400	2.9 2.9 3.7 2.9	970 0.0 970 0.0 713 0.0 970 0.0)22 -)22 -)23)53	0.107 0.792 0.107 0.021	- 7 2 2 7		
I 5 5 5 5	J 5 5 12 5		2.903 2.400 2.792 2.400 2.903 2.792	2.9 2.9 3.7 2.9	970 0.0 970 0.0 713 0.0 970 0.0 970 0.0	022 - 022 053 022	0.107 0.792 0.107 0.021 0.792	2		
1 5 5 5 5 5 5 5	J 5 5 12 5 12		2.903 2.400 2.792 2.400 2.903 2.792	2.9 2.9 3.7 2.9 2.9 3.7	970 0.0 970 0.0 713 0.0 970 0.0 970 0.0 713 0.0		0.107 0.792 0.107 0.021 0.792 0.792	2.		
5 5 5 5 5 5 12	J 5 5 12 5 12 5 5 5		2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792	2.9 2.9 3.7 2.9 2.9 3.7	970 0.0 970 0.0 970 0.0 970 0.0 970 0.0 970 0.0 9713 0.0 9713 0.0	022 - 022 053 022 022 - 053	0.107 0.792 0.107 0.107 0.107 0.792 0.792 0.792	2.		
5 5 5 5 5 5 12	J 5 5 12 5 12 5 12 5 12 5 12		2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792 4.118	2.9 2.9 3.7 2.9 3.7 3.7 3.7	970 0.0 970 0.0 970 0.0 970 0.0 970 0.0 970 0.0 9713 0.0 9713 0.0	022 - 022 - 022 - 022 - 022 - 023 - 023 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 -	0.107 0.792 0.107 0.107 0.107 0.792 0.792 0.792	- 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7		
1 5 5 5 5 5 5 5 12	J 5 5 12 5 12 5 12 5 12 5 12		2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792 4.118	2.9 2.9 3.7 2.9 3.7 3.7 3.7	970 0.0 970 0.0 713 0.0 970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0	022 - 022 - 022 - 022 - 023 - 023 - 025 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 - 053 -	0.107 0.792 0.107 0.107 0.107 0.792 0.792 0.792	- 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7		
I 5 5 5 5 5 5 12 12 12 12	J 5 5 12 5 12 5 12 5 12 5 TOTAL	· VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 3.7 4.0	970 0.0 970 0.0 713 0.0 970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0	022 - 022 - 022 - 022 - 023 - 023 - 053 - 053 - 053 - 06216 kg	0.107 0.792 0.107 0.107 0.021 0.792 0.792 0.792	- - - - - - - - - - - - - - - - - - -		
I 5 5 5 5 5 12 12 12	J 5 5 12 5 12 5 12 5 12 5 TOTAL	· VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 3.7 4.0	970 0.0 970 0.0 713 0.0 970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0	022 - 022 - 022 - 022 - 023 - 023 - 053 - 053 - 053 - 06216 kg	0.107 0.792 0.107 0.107 0.021 0.792 0.792 0.792	- - - - - - - - - - - - - - - - - - -		
I 5 5 5 5 5 12 12 12 E L	J 5 5 12 5 12 5 12 5 12 5 TOTAL	VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 3.7 4.0	970 0.0 970 0.0 713 0.0 970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0	022 - 022 - 022 - 022 - 023 - 023 - 053 - 053 - 053 - 06216 kg	0.107 0.792 0.107 0.107 0.021 0.792 0.792 0.792	- - - - - - - - - - - - - - - - - - -		
I 5 5 5 5 5 5 12 12 12 12 E L	J 5 5 12 5 12 5 12 5 12 TOTAL	VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	970 0.0 970 0.0 713 0.0 970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0 713 0.0		0.107 0.792 0.107 0.792 0.792 0.792 0.792 -0.275 cal/mo	2. 2. 2. 2. 3. 5. 5. 5. 5. 5. 5. S.		
I 5 5 5 5 5 5 12 12 12 12 E L	J 5 5 12 5 12 5 12 5 12 TOTAL E C T	VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	970 0.0 970 0.0 970 0.0 970 0.0 970 0.0 9713 0.0 9713 0.0 9713 0.0 9713 0.0 9713 0.0 9713 0.0 9713 0.0 9713 0.0 9713 0.0		0.107 0.792 0.107 0.792 0.792 0.792 0.792 -0.275 cal/mo	2. 2. 2. 2. 3. 5. 5. 5. 5. 5. 5. S.		
I 5 5 5 5 5 5 12 12 12 12 E L ATOM	J 5 5 12 5 12 5 12 5 12 TOTAL E C T TYPES J	VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	970 0.0 970 0.0 970 0.0 970 0.0 970 0.0 9713 0.0	022 - 022 - 022 - 023 - 023 - 025 - 027 - 053 - 053 - 053 - 06216 kc	0.107 0.792 0.107 0.107 0.792 0.792 0.792 0.792	2. 2. 2. 2. 3. 5. 5. 5. 5. 5. 5. S.		
I 5 5 5 5 5 5 12 12 12 12 E L ATOM	J 5 5 12 5 12 5 12 5 12 TOTAL E C T TYPES J	VAI	2.903 2.400 2.792 2.400 2.903 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	970 0.0 970 0.0 9713 0.0 970 0.0 9713 0.0		0.107 0.792 0.107 0.792 0.792 0.792 0.792 0.792	e e e e e e e e e e e e e e e e e e e		
I 5 5 5 5 5 5 12 12 12 12 E L ATOM	J 5 5 12 5 12 5 12 5 12 TOTAL E C T TYPES J	VAI	2.903 2.400 2.792 2.400 2.903 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	770 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 773 0.0 774 0.0 775 0.0 776 0.0 777 0.		0.107 0.792 0.107 0.792 0.792 0.792 0.792 0.792	e e e e e e e e e e e e e e e e e e e		
I 5 5 5 5 5 5 12 12 12 12 12 12 12	J 5 5 12 5 12 5 12 5 12 7 12 TOTAL 1 TYPES J 12 TOTAL	VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	770 0.0 773 0.0 774 0.0 775 0.		0.107 0.792 0.107 0.792 0.792 0.792 0.792 0.792	e e e e e e e e e e e e e e e e e e e		
I 5 5 5 5 5 5 12 12 12 12 12 12 12	J 5 5 12 5 12 5 12 5 12 7 12 TOTAL 1 TYPES J 12 TOTAL	VAN	2.903 2.400 2.792 2.400 2.903 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	770 0.0 773 0.0 774 0.0 775 0.		0.107 0.792 0.107 0.792 0.792 0.792 0.792 0.792	e e e e e e e e e e e e e e e e e e e		
I 5 5 5 5 5 5 12 12 12 12 12 TOTA	J 5 5 12 5 12 5 12 5 12 7 12 TOTAL 1 TYPES J 12 TOTAL	R O	2.903 2.400 2.792 2.400 2.903 2.792 2.792 4.118 N DER WA	2.9 2.9 3.7 2.9 3.7 3.7 4.0 AALS ENE	770 0.0 773 0.0 774 0.0 775 0.		0.107 0.792 0.107 0.792 0.792 0.792 0.792 0.792	e e e e e e e e e e e e e e e e e e e		

BOND	STRET	CHING					
ATOM TYP	ES BOND	IDEAL	FORCE				
I J	LENGTH	LENGTH	CONSTANT	DE	LTA	ENERGY	
h1 c3	1.000	1.093	1406.346	-0.093	12.	163	
cl c3	1.670	1.786	1168.117	-0.116	15.	718	
h1 c3	1.000	1.093	1406.346	-0.093	12.	163	
c3 c3	1.540	1.535	1269.019	0.005	0.	032	
c3 h1	1.000	1.093	1406.346	-0.093	12.	.163	
c3 cl	1.670	1.786	1168.117	-0.116	15.	718	
c3 h1	1.000	1.093	1406.346	-0.093	12.	163	
TOTA	AL BOND STRE	TCHING ENER	RGY = 80.1	.22 kJ/mo	1		
ANGLI	E BEND	I N G					
	ES VAL						
	K AN						
	100 500						
	109.500						
	109.442			0.			
h1 c3 cl c3 c3 h1		105.930 110.070			010		
c3 c3 c1		110.070		-0.			
h1 c3 c1			183.005				
h1 c3 c1		105.930		0.			
c3 c3 cl			260.419				
h1 c3 cl		105.930		0.			
	109.442						
	109.442			-0.			
	109.500						
	AL ANGLE BEN						
				,			
rors:	IONAL						
ATOM	TYPES	FORCE		TORSION			
I J	K L	CONSTANT	S	ANGLE	n E	ENERGY	
h1 c3 c3	cl 0.00	0 0	-60.000	3	0.000		
h1 c3 c3	h1 0.65	1 0	60.000	3	0.000		
h1 c3 c3	h1 0.65	1 0	-180.000	3	0.000		
h1 c3 c3	cl 0.00	0 0	60.000	3	0.000		
h1 c3 c3		1 0		3	0.000		
h1 c3 c3			-60.000	3	0.000		
	cl 0.00			3	0.000		
	h1 0.00				0.000		
	h1 0.00				0.000		
TOTA	AL TORSIONAL	ENERGY =	0.000 kJ/	mol			

```
2686
2687 IMPROPER TORSIONAL
2688
2689 ----ATOM TYPES---- FORCE IMPROPER_TORSION
                           s ANGLE n ENERGY
2690
    I J K L CONSTANT
2691
    ______
2692
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2693
2694 VAN DER WAALS
2695
2696 ATOM TYPES
           Rij kij ENERGY
    I J
2697
2698 -----
2699 h1 h1
          2.903 -0.031
           2.400
                  0.030
2700
   h1 h1
2701 h1 cl
           2.792
                  0.356
2702 h1 h1
           2.400
                  0.030
           2.903 -0.031
   h1 h1
2703
           2.792
                  0.356
2704 h1 cl
2705
   cl h1
           2.792
                  0.356
2706 cl h1
           2.792
                  0.356
2707 cl cl
           4.118
                 -0.510
     TOTAL VAN DER WAALS ENERGY = 0.910 kJ/mol
2708
2709
2710 ELECTROSTATIC INTERACTIONS
2711
2712 ATOM TYPES
    I J
2713
           Rij 332.17*QiQj ENERGY
2.714
    _____
2715 h1 h1 2.903 1.352
                        0.466
                         0.563
           2.400
2716 h1 h1
                  1.352
2717 h1 cl
           2.792 -3.809 -1.364
2718 h1 h1
           2.400
                  1.352
                         0.563
2719 hl hl
           2.903
                  1.352
                         0.466
           2.792 -3.809 -1.364
2720 h1 cl
2721 cl h1
           2.792 -3.809 -1.364
2722 cl h1
           2.792
                 -3.809
                        -1.364
    cl cl 4.118 10.728 2.605
2723
    TOTAL ELECTROSTATIC ENERGY = -0.794 kJ/mol
2724
2725
    TOTAL ENERGY = 83.176 kJ/mol
2726
2727
2728 ATOM TYPES
2729
2730 IDX TYPE RING
2731 | 1 1 NO
2732 | 2 1 NO
2733 3 5 NO
2734 4 5 NO
```

```
2735 5 12 NO
2736 6 5 NO
2737 7 5 NO
2738 8 12 NO
2739
2740 FORMAL CHARGES
2741
2742 IDX CHARGE
2743 1 0.000000
2744 2 0.000000
2745 3 0.000000
     4 0.000000
2746
2747 5 0.000000
2748 6 0.000000
2749
     7 0.000000
2750 8 0.000000
2751
2752 PARTIAL CHARGES
2753
2754 IDX CHARGE
     1 0.290000
2755
2756 2 0.290000
2757
     3 0.000000
2758 4 0.000000
2759 5 -0.290000
     6 0.000000
2760
2761 7 0.000000
     8 -0.290000
2762
2763
2764 SETTING UP CALCULATIONS
2765
2766 SETTING UP BOND CALCULATIONS...
2767
     SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
2768
     SETTING UP TORSION CALCULATIONS...
2769
     SETTING UP OOP CALCULATIONS...
2770
     SETTING UP VAN DER WAALS CALCULATIONS...
2771
     SETTING UP ELECTROSTATIC CALCULATIONS...
2772
2773 ATOM TYPES
2774
2775
     IDX TYPE RING
2776 | 1 c3 NO
2777
     2 c3 NO
2778
     3 h1 NO
     4 h1 NO
2779
2780 5 cl NO
     6 h1 NO
2781
2782 7 hl NO
2783
     8 cl NO
```

```
2784
2785 C H A R G E S
2786
2787 IDX CHARGE
2788 1 0.036009
    2 0.036009
2789
2790 3 0.044101
    4 0.044101
2.791
2792 5 -0.124211
2793 6 0.044101
2794 7 0.044101
2795
    8 -0.124211
2796
2797 SETTING UP CALCULATIONS
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 ENERGY
2807
2808
2809 BOND STRETCHING
2810
    ATOM TYPES FF BOND IDEAL
2811
                                  FORCE
    I J CLASS LENGTH
                         LENGTH
                                 CONSTANT
                                           DELTA
                                                   ENERGY
2812
2813
    _____
             0
2814
    12
                  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
    1 5
2818
             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
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
2821
2822
2823 ANGLE BENDING
2824
2825 ATOM TYPES
                FF VALENCE
                             IDEAL
                                     FORCE
    I J K CLASS ANGLE
2826
                             ANGLE
                                    CONSTANT
                                               DELTA
                                                       ENERGY
2827
    1
        1 5
                0 109.500
                            110.549
2828
                                       0.636
                                              -1.049
                                                        0.015
    5
                0 109.442 108.836
                                       0.516
2829
       1 5
                                               0.606
                                                       0.004
                0 109.442 108.162
    5
                                               1.280
2830
        1 12
                                       0.698
                                                       0.025
                0 109.500 110.549
    1 1 5
                                       0.636
2831
                                              -1.049
                                                       0.015
               0 109.500 108.679
2832
    1 1 12
                                     1.056
                                               0.821
                                                        0.016
```

_									
5	1	12	0	109.44	2 108	.162	0.698	1.280	0.025
5			0		2 108			1.280	
1		12			0 108			0.821	
5		12	0	109.44		.162		1.280	
1		5			0 110				
			0					0.606	
			0					-1.049	0.01
	TOTA	AL ANO	GLE BEND	ING ENER	dGY = 0.3	20058 kc	al/mol		
ST	RET	Г С Н	BEN	DING					
		7.0						GOVERNVE	
							FORCE		ENEDGY
								JК	
								0.070	
			0				0.227		-0.002 -0.033
		12 5					-0.018 0.227		
1		12	0				0.227		
5		12	0	109.44			-0.018		
		12					-0.018		
1		12	0				0.176		
5			0				-0.018		
1		5	0	109.50			0.227		
			0				0.115		
			0					0.070	
	TOTF	AL STE	RETCH BE		ERGY = -				
т о	R S J	I O N	A L						
ATOM	I TYPE	ES		FF	TORSION	F	ORCE CONS	TANT	
	J			CLASS	ANGLE		V1 V2	V3 ENE	RGY
I 		K	L						
I 5	1	K 1	L 12	0 –	40.000	0.678	-0.602	0.398	0.449
I 5 5	1 1	к 1 1	L 12 5	0 – 0	40.000	0.678 0.284	-0.602 -1.386	0.398 0.314	0.449 -1.099
I 5 5 5	1 1 1	1 1 1	L 12 5 5	0 - 0 0 0 -1	40.000 80.000 60.000	0.678 0.284 0.284	-0.602 -1.386 -1.386	0.398 0.314 0.314	0.449 -1.099 -0.075
5 5 5 5	1 1 1 1	K 1 1 1 1	12 5 5 12	0 - 0 0 0 -1	40.000 80.000 60.000 80.000	0.678 0.284 0.284 0.678	-0.602 -1.386 -1.386 -0.602	0.398 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086
5 5 5 5 5	1 1 1 1 1	K 1 1 1 1 1	L 12 5 5 12 5	0 - 0 0 - 1 0 0 - 1	40.000 80.000 60.000 80.000 60.000	0.678 0.284 0.284 0.678 0.284	-0.602 -1.386 -1.386 -0.602 -1.386	0.398 0.314 0.314 0.398 0.314	0.449 -1.099 -0.075 -0.086 -0.075
5 5 5 5 5 5	1 1 1 1 1 1	K 1 1 1 1 1 1 1 1	12 5 5 12 5	0 -1 0 -1 0 -1	40.000 80.000 60.000 80.000 60.000 40.000	0.678 0.284 0.284 0.678 0.284 0.284	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386	0.398 0.314 0.314 0.398 0.314	0.449 -1.099 -0.075 -0.086 -0.075 -0.243
I 5 5 5 5 5 5 12	1 1 1 1 1 1 1	K 1 1 1 1 1 1 1	L 12 5 5 12 5 12 5 12	0 -1 0 -1 0 -1 0 -1	40.000 80.000 60.000 80.000 60.000 40.000	0.678 0.284 0.284 0.678 0.284 0.284 0.000	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386	0.398 0.314 0.314 0.398 0.314 0.314 0.893	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223
I 5 5 5 5 5 5 5 12 12	1 1 1 1 1 1 1 1	K 1 1 1 1 1 1 1 1 1	L 12 5 5 12 5 12 5 12 5 5	0 -1 0 -1 0 -1 0 -1 0 -1	40.000 80.000 60.000 80.000 40.000 40.000 40.000	0.678 0.284 0.284 0.678 0.284 0.284 0.000 0.678	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386 0.000 -0.602	0.398 0.314 0.314 0.398 0.314 0.314 0.893 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
I 5 5 5 5 5 5 12 12	1 1 1 1 1 1 1 1	K 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	L 12 5 5 12 5 12 5 12 5 5 5 12 5 5	0 -1 0 -1 0 -1 0 -1 0 -1 0 -1	40.000 80.000 60.000 80.000 60.000 40.000 40.000 80.000	0.678 0.284 0.284 0.678 0.284 0.000 0.678	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386 0.000 -0.602 -0.602	0.398 0.314 0.314 0.398 0.314 0.314 0.893	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
I 5 5 5 5 5 5 12 12	1 1 1 1 1 1 1 1	K 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	L 12 5 5 12 5 12 5 12 5 5 5 12 5 5	0 -1 0 -1 0 -1 0 -1 0 -1 0 -1	40.000 80.000 60.000 80.000 40.000 40.000 40.000	0.678 0.284 0.284 0.678 0.284 0.000 0.678	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386 0.000 -0.602 -0.602	0.398 0.314 0.314 0.398 0.314 0.314 0.893 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
I 5 5 5 5 5 5 12 12 12	1 1 1 1 1 1 1 TOTA	1 1 1 1 1 1 1 1 1 1	L 12 5 12 5 12 5 5 12 5 5 12 5 RSIONAL	0 - 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	40.000 80.000 60.000 80.000 40.000 40.000 40.000 80.000 -0.54330	0.678 0.284 0.284 0.678 0.284 0.284 0.000 0.678 0.678	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386 0.000 -0.602 -0.602	0.398 0.314 0.314 0.398 0.314 0.314 0.893 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
I 5 5 5 5 5 12 12 12	1 1 1 1 1 1 1 TOTA	1 1 1 1 1 1 1 1 1 1	L 12 5 12 5 12 5 5 12 5 5 12 5 RSIONAL	0 - 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	40.000 80.000 60.000 80.000 60.000 40.000 40.000 80.000	0.678 0.284 0.284 0.678 0.284 0.284 0.000 0.678 0.678	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386 0.000 -0.602 -0.602	0.398 0.314 0.314 0.398 0.314 0.314 0.893 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
I 5 5 5 5 5 12 12 12 O U	1 1 1 1 1 1 TOTF	1 1 1 1 1 1 1 1 1 1 0 F -	L 12 5 5 12 5 12 5 5 12 7 PLAN	0 -1 0 -1 0 -1 0 -1 0 -2 ENERGY =	40.000 80.000 60.000 80.000 40.000 40.000 40.000 80.000 -0.54330	0.678 0.284 0.284 0.284 0.284 0.284 0.000 0.678 0.678 6 kcal/m		0.398 0.314 0.314 0.398 0.314 0.314 0.893 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
I 5 5 5 5 5 5 12 12 12 12 O U	1 1 1 1 1 1 TOTA T - C	K 1 1 1 1 1 1 1 1 CAL TOP	L 12 5 5 12 5 12 5 5 RSIONAL P L A N	0 - 0 0 0 - 1 0 0 0 - 1 0 0 0 0 0 0 0 0	40.000 80.000 60.000 80.000 40.000 40.000 80.000 -0.54330	0.678 0.284 0.284 0.678 0.284 0.284 0.000 0.678 0.678 6 kcal/m		0.398 0.314 0.314 0.398 0.314 0.314 0.893 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449

```
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
2883
2884 VAN DER WAALS
2885
2886 ATOM TYPES
    I J
           Rij R*IJ EPSILON ENERGY
2887
2888
              2.885
                     2.970
2889
    5 5
                            0.022
                                   -0.021
    5 5
              2.518
                     2.970
                            0.022
                                   0.036
2890
2891 5 12
                            0.053
              2.647
                     3.713
                                    1.520
    5 5
              2.300
                     2.970
2892
                            0.022
                                    0.215
    5 5
                            0.022
              2.885
                     2.970
2893
                                   -0.021
2894
    5 12
              2.960
                     3.713
                            0.053
                                    0.331
2895 12 5
              2.960
                     3.713
                            0.053
                                    0.331
              2.647
2896 12 5
                     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 ELECTROSTATIC INTERACTIONS
2901
2902 ATOM TYPES
    I J
             Rij Qi Qj ENERGY
2903
2904
2905
    12 12
           4.132 -0.290 -0.290
                                  5.069
     TOTAL ELECTROSTATIC ENERGY = 5.06915 kcal/mol
2906
2907
2908 TOTAL ENERGY = 27.86335 kcal/mol
2909
2910 ENERGY
2911
2912
2913 BOND STRETCHING
2914
2915 ATOM TYPES BOND
                   IDEAL
                            FORCE
    I J
           LENGTH
                    LENGTH
                           CONSTANT DELTA ENERGY
2916
2917
2918 cl c3
          1.670
                  1.786
                          1168.117
                                  -0.116
                                           15.718
                         1406.346
                                          12.163
2919 h1 c3
          1.000
                  1.093
                                  -0.093
2920 h1 c3
          1.000
                  1.093
                                   -0.093
                          1406.346
                                           12.163
2921 c3 c3
          1.540
                  1.535
                          1269.019
                                    0.005
                                           0.032
                                   -0.093 12.163
    c3 h1
          1.000
                  1.093
                          1406.346
2922
2923 c3 cl
          1.670
                  1.786
                          1168.117
                                   -0.116
                                           15.718
2924 c3 h1
          1.000
                                   -0.093
                  1.093
                          1406.346
                                           12.163
    TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
2925
2926
2927 ANGLE BENDING
2928
2929 ATOM TYPES
               VALENCE
                        IDEAL
                                FORCE
    I J K ANGLE ANGLE CONSTANT DELTA ENERGY
2930
```

31								
32	c3 c3 h1	109.500	110.070	194.100	-0.	010	0.019	
33	h1 c3 h1	109.442	109.550		-0.			
34	h1 c3 cl	109.442	105.930					
35	c3 c3 h1	109.500	110.070	194.100	-0.	010	0.019	
36	c3 c3 cl	109.500	110.330		-0.			
37	h1 c3 cl	109.442			0.	061	0.688	
38	h1 c3 cl	109.442	105.930		0.			
39	c3 c3 cl	109.500	110.330		-0.			
40	h1 c3 cl	109.442	105.930	183.005	0.	061	0.688	
41	c3 c3 h1		110.070			010		
42	h1 c3 h1		109.550					
13			110.070				0.019	
4	TOTAI	L ANGLE BEI	NDING ENERGY	= 2.938	kJ/mol			
5								
6	TORSI	ONAL						
7								
8			FORCE					
9			CONSTANT					
0								
1			0 0					
2			51 0					
3			51 0					
4			0 0					
5			51 0			0.326		
6	h1 c3 c3 h		51 0			0.326		
7			00 0					
8			00 0					
9			00 0			0.000		
	TOTAL	_ TORSIONAL	L ENERGY =	1.303 KJ/	MOT			
1	T W D D O			2 7				
2	IMPRO	PER T	ORSION	А Ь				
3	л пом п	TVDEC	FORCE	TMDDODED	ПОВСТОМ			
4 5			CONSTANT				ENEDCV	
6	1 3	к п	CONSTANT	5	ANGLE	11	ENERGI	
7	ποπа τ	TMDDODFD.	-TORSIONAL E	VEDCV =	0 000 ka	[/mo]		
8	IOIAI	J IMPROPER-	-IONDIONAL EL	VERGI —	0.000 K	/ IIIOI		
9	W A N D	ER WA	A T. S					
0	VAND	LK WA	A L U					
1	ATOM TYPES	3						
			kij	ENERGY				
3		_						
4		2.885						
75		2.885						
6	h1 cl							
U		2.300						
77		4.300	0.109					
77			0 021					
7 8 9	h1 h1 h1 cl	2.885						

```
2980 cl h1 2.960 0.012
2981 cl h1
            2.647
                    1.083
2982 cl cl 4.082 -0.522
    TOTAL VAN DER WAALS ENERGY = 1.704 kJ/mol
2983
2984
2985 ELECTROSTATIC INTERACTIONS
2986
2987 ATOM TYPES
    I J
            Rij 332.17*QiQj ENERGY
2988
2989
    _____
                   1.352
2990 h1 h1 2.885
                           0.469
    h1 h1
           2.518
                   1.352
                           0.537
2991
            2.647 -3.809 -1.439
2992 h1 cl
2993 h1 h1
            2.300
                    1.352
                           0.588
            2.885
                   1.352
                           0.469
2994 h1 h1
2995 h1 cl
            2.960
                   -3.809 -1.287
2996 cl h1
            2.960 -3.809 -1.287
            2.647 -3.809 -1.439
2997 cl h1
                            2.628
2998 cl cl
            4.082 10.728
      TOTAL ELECTROSTATIC ENERGY = -0.761 kJ/mol
2999
3000
3001 TOTAL ENERGY = 85.306 \text{ 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 FORMAL CHARGES
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 PARTIAL CHARGES
3028
```

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

```
3078 SETTING UP VAN DER WAALS CALCULATIONS...
    SETTING UP ELECTROSTATIC CALCULATIONS...
3079
3080
3081
    ENERGY
3082
3083
3084
    BOND STRETCHING
3085
                                  FORCE
    ATOM TYPES FF BOND IDEAL
3086
    I J
                                            DELTA
3087
            CLASS LENGTH
                          LENGTH
                                  CONSTANT
                                                    ENERGY
3088
3089
              0
                  1.670
                          1.773
                                     2.974
                                                     2.795
                                            -0.103
3090
    5
        1
             0
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                     3.578
                                            0.032
3091
             0
                  1.540
                          1.508
                                    4.258
                                                     0.294
    1
        1
        5
             0
                  1.000
                          1.093
                                    4.766
                                            -0.093
3092
     1
                                                     3.578
                  1.000
3093
    1
       5
             0
                          1.093
                                    4.766
                                            -0.093
                                                     3.578
    1 5
3094
              0
                  1.000
                           1.093
                                    4.766
                                            -0.093
                                                     3.578
                                     2.974 -0.103
     1 12
3095
             0
                   1.670
                           1.773
                                                     2.795
3096
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
3097
3098
    ANGLE BENDING
3099
                FF VALENCE
                              IDEAL
                                      FORCE
3100
    ATOM TYPES
                              ANGLE
3101
                                     CONSTANT
    I J K
                CLASS ANGLE
                                                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
                    109.442
3105
     5
        1
           12
                 0
                             108.162
                                        0.698
                                                1.280
                                                         0.025
        1 5
                 0 109.500 110.549
3106
    1
                                        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
                 0 109.500 108.679
    1
        1 12
                                        1.056
                                                0.821
                                                         0.016
3109
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
                    109.500 110.549
    1
        1 5
                 0
                                         0.636
3112
                                                -1.049
                                                         0.015
            5
3113
    1
        1
                 0 109.500
                             110.549
                                        0.636
                                               -1.049
                                                         0.015
3114
     5
            5
                 0
                    109.442
                             108.836
                                        0.516
                                                0.606
                                                         0.004
        1
        TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
3115
3116
    STRETCH BENDING
3117
3118
3119
    ATOM TYPES
                FF VALENCE
                                        FORCE CONSTANT
                              DELTA
                                             JК
    I J K CLASS ANGLE
3120
                              ANGLE
                                        ΙJ
                                                       ENERGY
3121
           5
                 0
                                              0.070
    1
        1
                    109.500
                              -1.049
                                       0.227
                                                       -0.002
3122
3123
    5
        1 5
                 0 109.442
                              0.606
                                      0.115
                                              0.115
                                                       -0.033
                                     -0.018
                                              0.380
3124
    5
        1 12
                 0 109.442
                              1.280
                                                       -0.121
        1 5
                 0 109.500
                                      0.227
    1
                              -1.049
                                              0.070
3125
                                                       -0.002
                 0 109.500
                              0.821
        1 12
                                      0.176 0.386
                                                       -0.070
3126
```

1 1 12 0 109.500 0.821 0.176 0.38 5 1 12 0 109.442 1.280 -0.018 0.38 5 1 12 0 109.442 1.280 -0.018 0.38 1 1 5 0 109.500 -1.049 0.227 0.03 1 1 5 0 109.500 -1.049 0.227 0.03 5 1 5 0 109.442 0.606 0.115 0.11	$ \begin{array}{rcl} & -0.12 \\ & 0.12 \\ & 0.12 \\ & 0.00 \end{array} $
5 1 12 0 109.442 1.280 -0.018 0.38 5 1 12 0 109.442 1.280 -0.018 0.38 1 1 5 0 109.500 -1.049 0.227 0.07 1 1 5 0 109.500 -1.049 0.227 0.07 5 1 5 0 109.442 0.606 0.115 0.11	30 -0.12 30 -0.12 70 -0.00 70 -0.00
5 1 12 0 109.442 1.280 -0.018 0.38 1 1 5 0 109.500 -1.049 0.227 0.07 1 1 5 0 109.500 -1.049 0.227 0.07 5 1 5 0 109.442 0.606 0.115 0.11	$ \begin{array}{rcl} & -0.12 \\ & -0.00 \\ & -0.00 \end{array} $
1 1 5 0 109.500 -1.049 0.227 0.07 1 1 5 0 109.500 -1.049 0.227 0.07 5 1 5 0 109.442 0.606 0.115 0.11	$ \begin{array}{rrr} 70 & -0.00 \\ 70 & -0.00 \end{array} $
1 1 5 0 109.500 -1.049 0.227 0.07 5 1 5 0 109.442 0.606 0.115 0.11	70 -0.00
5 1 5 0 109.442 0.606 0.115 0.11	
	15 -0.03
TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol	
TORSIONAL	
ATOM TYPES FF TORSION FORCE CONSTANT	
I J K L CLASS ANGLE V1 V2 V3	ENERGY
12 1 1 5 0 -20.000 0.678 -0.602 0.398	0.886
12 1 1 5 0 100.000 0.678 -0.602 0.398	-0.005
12 1 1 12 0 -140.000 0.000 0.000 0.893	0.670
5 1 1 5 0 100.000 0.284 -1.386 0.314	-0.991
5 1 1 5 0 -140.000 0.284 -1.386 0.314	-0.304
5 1 1 12 0 -20.000 0.678 -0.602 0.398	0.886
5 1 1 5 0 -140.000 0.284 -1.386 0.314	4 -0.304
5 1 1 5 0 -20.000 0.284 -1.386 0.314	0.349
5 1 1 12 0 100.000 0.678 -0.602 0.398	-0.005
TOTAL TORSIONAL ENERGY = 1.18015 kcal/mol	
OUT-OF-PLANE BENDING	
ATOM TYPES FF OOP FORCE	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol	
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 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	
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	
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	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol V A N D E R W A A L S ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.831 2.970 0.022 -0.019	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol V A N D E R W A A L S ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.831 2.970 0.022 -0.019 5 5 5 2.638 2.970 0.022 0.001	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol V A N D E R W A A L S ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.831 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 0.001 5 12 2.547 3.713 0.053 2.298	
ATOM TYPES	
ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol V A N D E R W A A L S ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.831 2.970 0.022 -0.019 5 5 2.638 2.970 0.022 0.001 5 12 2.547 3.713 0.053 2.298 5 5 2.232 2.970 0.022 0.328 5 5 2.831 2.970 0.022 0.328 5 5 2.831 2.970 0.022 -0.019 5 12 3.129 3.713 0.053 0.104 12 5 3.129 3.713 0.053 0.104 12 5 3.129 3.713 0.053 2.298	

```
3176
3177 ATOM TYPES
    I J Rij Qi Qj ENERGY
3178
3179
3180
    12 12 4.025 -0.290 -0.290
                                   5.204
     TOTAL ELECTROSTATIC ENERGY = 5.20367 kcal/mol
3181
3182
3183 TOTAL ENERGY = 30.90959 kcal/mol
3184
3185 ENERGY
3186
3187
3188 BOND STRETCHING
3189
3190 ATOM TYPES BOND IDEAL FORCE
                                      DELTA ENERGY
3191 I J LENGTH
                    LENGTH
                            CONSTANT
3192
    ______
          1.670
                          1168.117
                                   -0.116
                                           15.718
3193 cl c3
                  1.786
3194 h1 c3
           1.000
                   1.093
                          1406.346
                                           12.163
                                   -0.093
3195 c3 c3
          1.540
                   1.535
                          1269.019
                                    0.005
                                            0.032
                          1406.346 -0.093 12.163
3196 c3 h1
          1.000
                  1.093
                   1.093
                          1406.346
                                           12.163
3197 c3 h1
           1.000
                                    -0.093
3198 c3 h1
          1.000
                   1.093
                          1406.346
                                    -0.093
                                           12.163
                          1168.117
3199 c3 cl
          1.670
                   1.786
                                    -0.116
                                           15.718
     TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
3200
3201
3202 ANGLE BENDING
3203
3204 ATOM TYPES VALENCE IDEAL FORCE
                                CONSTANT DELTA ENERGY
3205
    I J K
                ANGLE
                        ANGLE
3206
    c3 c3 h1 109.500 110.070
3207
                             194.100
                                      -0.010
                                              0.019
3208 h1 c3 h1 109.442
                   109.550
                             164.039
                                      -0.002
                                               0.001
                             183.005
3209 h1 c3 cl 109.442 105.930
                                      0.061
                                               0.688
3210 c3 c3 h1 109.500 110.070
                             194.100
                                      -0.010
                                              0.019
3211 c3 c3 cl 109.500 110.330
                             260.419
                                      -0.014
                                              0.055
3212 h1 c3 cl 109.442
                   105.930
                             183.005
                                      0.061
                                              0.688
3213 c3 c3 cl 109.500 110.330
                             260.419
                                      -0.014
                                              0.055
3214 h1 c3 cl 109.442
                   105.930
                             183.005
                                      0.061
                                              0.688
                             183.005
3215 h1 c3 cl 109.442 105.930
                                      0.061
                                              0.688
    c3 c3 h1 109.500 110.070
                             194.100
3216
                                     -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
                                      -0.002
                             164.039
                                              0.001
     TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
3219
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 -----
                           -20.000 3
3226 cl c3 c3 h1
              0.000
                       0
                                       0.000
3227 cl c3 c3 h1
              0.000
                       0 100.000 3
                                       0.000
3228 cl c3 c3 cl
              0.000
                       0 -140.000 3
                                       0.000
3229 h1 c3 c3 h1
              0.651
                       0
                           100.000 3
                                       0.977
3230 h1 c3 c3 h1 0.651
                       0 -140.000 3
                                       0.977
3231 h1 c3 c3 cl
              0.000
                       0 -20.000 3
                                       0.000
3232 h1 c3 c3 h1
                       0 -140.000 3
              0.651
                                       0.977
3233 h1 c3 c3 h1
              0.651
                        0
                           -20.000 3
                                       0.977
3234 h1 c3 c3 c1
                       0
                           100.000 3
              0.000
                                       0.000
      TOTAL TORSIONAL ENERGY = 3.908 kJ/mol
3235
3236
3237 IMPROPER TORSIONAL
3238
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
3239
    I J K L CONSTANT S ANGLE n ENERGY
3240
3241
3242
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
3243
3244 VAN DER WAALS
3245
3246 ATOM TYPES
           Rij kij ENERGY
3247
    I J
3248
    _____
           2.831
3249 h1 h1
                 -0.032
3250 h1 h1
           2.638 -0.029
           2.547
3251 h1 cl
                  2.064
           2.232
                  0.205
3252 h1 h1
3253 h1 h1
           2.831
                 -0.032
3254 h1 cl
           3.129
                 -0.106
3255 cl h1
           3.129
                  -0.106
           2.547
                  2.064
3256 cl h1
3257 cl cl
           3.975
                 -0.548
3258
      TOTAL VAN DER WAALS ENERGY = 3.480 kJ/mol
3259
3260 ELECTROSTATIC INTERACTIONS
3261
3262 ATOM TYPES
               Rij 332.17*QiQj ENERGY
3263
3264
    ______
    h1 h1
           2.831 1.352 0.478
3265
3266 h1 h1
           2.638
                  1.352
                         0.513
3267 h1 cl
           2.547 -3.809 -1.495
    h1 h1
           2.232
                  1.352
3268
                         0.606
3269 h1 h1
           2.831
                  1.352
                         0.478
3270 h1 cl
           3.129
                 -3.809 -1.217
3271 cl h1
           3.129 -3.809 -1.217
           2.547
                 -3.809 -1.495
3272 cl h1
3273 cl cl
          3.975 10.728 2.699
```

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

```
3323 7 hl NO
3324 8 cl NO
3325
3326 FORMAL CHARGES
3327
3328 IDX CHARGE
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 PARTIAL CHARGES
3339
3340 IDX CHARGE
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 BOND STRETCHING
3354
3355 ATOM TYPES FF BOND IDEAL FORCE
    I J CLASS LENGTH
3356
                          LENGTH
                                   CONSTANT
                                             DELTA
                                                      ENERGY
3357
3358 12 1
             0
                   1.670
                           1.773
                                     2.974
                                             -0.103
                                                      2.795
3359
    5
        1
             0
                   1.000
                           1.093
                                     4.766
                                             -0.093
                                                      3.578
                   1.540
    1
        1
             0
                           1.508
                                     4.258
                                             0.032
                                                      0.294
3360
3361
    1 5
             0
                   1.000
                           1.093
                                     4.766
                                             -0.093
                                                      3.578
                   1.000
3362
    1 5
             0
                           1.093
                                     4.766
                                             -0.093
                                                      3.578
                                     4.766
3363
    1
        5
              0
                   1.000
                           1.093
                                             -0.093
                                                      3.578
3364
    1 12
             0
                   1.670
                           1.773
                                     2.974
                                             -0.103
                                                      2.795
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
3365
3366
3367 ANGLE BENDING
3368
3369 ATOM TYPES FF VALENCE IDEAL FORCE
    I J K
                CLASS ANGLE
                               ANGLE
                                      CONSTANT
                                                 DELTA
3370
                                                         ENERGY
3371
```

.11							8 _0 602		
10	12	1	1	5	0 0.0	0.678	3 -0.602	0.398	1.076
08					спчээ Аг		VI VZ \		
) /							FORCE CONSTA		!v
7	ΣπΩм	пvр	70		FF TO	STON	FORCE CONCE	MΠ	
) 5	Τ 0	K S .	ON	А Ь					
) 4	шо	D C 3	. O N	7. T					
03		TOTA	AL STR	ETCH BEN	DING ENERGY	r = -0.69593	3 kcal/mol		
)2	5						0.115	0.115	-0.033
01							0.227		
00							0.227		
99	5	1		0	109.442	1.280	-0.018	0.380	-0.12
8 (1		0		1.280		0.380	-0.12
97	1	1	12	0		0.821		0.386	-0.07
96	5	1	12	0		1.280	-0.018	0.380	-0.12
95	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
94	1	1	5	0	109.500	-1.049	0.227	0.070	-0.00
93	5	1	12	0	109.442	1.280	-0.018	0.380	-0.12
2	5	1	5	0	109.442	0.606	0.115	0.115	-0.03
1	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
0 (
39	I	J	K	CLASS	ANGLE	ANGLE	ΙJ	JК	ENER
88	ATOM	TYPE	ES	FF	VALENCE	DELTA	FORCE C	CONSTANT	
37									
36	ST	RET	гс н	B E N	DING				
85									
34						0.20058			
33				0			0.516		
32				0		110.549		-1.049	
31		1		0	109.500	110.549	0.636	-1.049	
30	5		12	0	109.442	108.162		1.280	
79		1	12	0	109.442	108.079	0.698	1.280	0.
78		1	12	0	109.442	108.679		0.821	
77	5	1	12	0	109.300	108.162	0.698	1.280	0.
76	1	1	12	0	109.500	10.549		0.821	
74 75		1	12 5	0	109.442	108.162 110.549	0.698 0.636	1.280 -1.049	0.
73	5	1	5	0	109.442	108.836	0.516	0.606	0.0
	_	1	_	0	109.500	110.549			

3411 12 1 1 5 0 120.000 0.678 -0.602 0.398 0.116 12 0 -120.000 0.000 0.000 0.893 0.893 3412 12 1 1 3413 5 1 1 5 0 120.000 0.284 -1.386 0.314 -0.654 5 1 5 0 -120.000 -0.655 3414 1 0.284 -1.386 0.314 3415 5 1 1 12 0 -0.000 0.678 -0.602 0.398 1.076 3416 5 1 5 0 -120.000 0.284 -1.386 0.314 -0.655 1 5 0.598 3417 5 1 1 0.000 0.284 -1.386 0.314 3418 5 1 1 12 0 120.000 0.678 -0.602 0.398 0.116 TOTAL TORSIONAL ENERGY = 1.91150 kcal/mol 3419

3420

```
3421 OUT-OF-PLANE BENDING
3422
3423 ATOM TYPES
                   FF
                          OOP FORCE
3424 I J K
                  CLASS ANGLE CONSTANT
               L
3425
    _____
3426
       TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
3427
3428 VAN DER WAALS
3429
3430 ATOM TYPES
3431
             Rij R*IJ EPSILON ENERGY
    I J
3432
3433
    5 5
              2.746
                     2.970
                             0.022
                                   -0.014
3434
    5 5
             2.746
                     2.970
                            0.022 -0.014
                     3.713
    5 12
             2.512
                            0.053
                                   2.649
3435
3436 5 5
             2.208
                     2.970
                            0.022
                                   0.377
    5 5
              2.746
                     2.970
                            0.022
3437
                                   -0.014
              3.280
                            0.053
                                   0.009
3438
    5 12
                     3.713
3439 12 5
              3.280
                     3.713
                            0.053
                                   0.009
3440 12 5
              2.512
                     3.713
                            0.053
                                   2.649
                     4.089 0.276
3441 12 12
              3.806
                                   -0.201
      TOTAL VAN DER WAALS ENERGY = 5.44875 kcal/mol
3442
3443
3444 ELECTROSTATIC INTERACTIONS
3445
3446 ATOM TYPES
             Rij Qi Qj ENERGY
    I J
3447
3448
    12 12 3.856 -0.290 -0.290 5.432
3449
     TOTAL ELECTROSTATIC ENERGY = 5.43239 kcal/mol
3450
3451
3452 | TOTAL ENERGY = 32.49359 kcal/mol
3453
3454 ENERGY
3455
3456
3457 BOND STRETCHING
3458
3459 ATOM TYPES BOND
                   IDEAL FORCE
           LENGTH
                   LENGTH
3460
    I J
                           CONSTANT
                                     DELTA
                                             ENERGY
3461
3462 cl c3
          1.670
                  1.786
                         1168.117
                                  -0.116
                                          15.718
3463 h1 c3
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
                  1.535
                         1269.019
3464 c3 c3
          1.540
                                   0.005
                                           0.032
3465 c3 h1
          1.000
                  1.093
                         1406.346
                                          12.163
                                   -0.093
3466 c3 h1
          1.000
                  1.093
                         1406.346
                                   -0.093
                                          12.163
3467 c3 h1
          1.000
                  1.093
                         1406.346
                                   -0.093
                                          12.163
3468 c3 cl
                  1.786
                         1168.117
                                          15.718
          1.670
                                  -0.116
     TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
```

ушОм шальа	777 77	NCE IDEA	T 50	DCF			
		LE ANGL			DEL	תים	FNFDCV
		ANGL					
		110.070					
h1 c3 h1	109.442	109.550	164.039	-0.	002	0.001	
h1 c3 cl	109.442	105.930	183.005	0.	061	0.688	
c3 c3 h1	109.500	110.070	194.100	-0.	010	0.019	
c3 c3 cl	109.500	110.330	260.419	-0.	014	0.055	
h1 c3 cl	109.442	105.930	183.005	0.	061	0.688	
c3 c3 cl		110.330					
h1 c3 cl		105.930					
h1 c3 cl		105.930					
		110.070				0.019	
		110.070					
		109.550 ING ENERGY =				0.001	
IOIAL	ANGLE DEND	ING ENERGI -	2.930	KU/IIIOI			
TORSI	ONAT.						
	0 11 11 11						
ATOM T	YPES	FORCE		TORSION			
		CONSTANT				ENERGY	
cl c3 c3 h	1 0.000	0	0.000	3	0.000		
cl c3 c3 h	1 0.000	0	120.000	3	0.000		
cl c3 c3 c	0.000	0	-120.000	3	0.000		
h1 c3 c3 h	1 0.651	0	120.000	3	1.303		
		0			1.303		
		0					
		0					
		0					
		0			0.000		
TOTAL	TORSTONAL	ENERGY =	J.210 KJ/	шОТ			
TMPPO	рер по	RSIONA	т.				
		RUIUNA	. 1				
ATOM T	YPES	FORCE	IMPROPER	TORSION			
		CONSTANT				ENERGY	
TOTAL	IMPROPER-T	ORSIONAL ENE	RGY =	0.000 kJ	/mol		
V A N D	ER WAA	L S					
ATOM TYPES							
I J	Rij	kij	ENERGY				

```
3519 h1 h1 2.746 -0.033
3520 h1 cl
             2.512
                     2.571
3521 h1 h1
             2.208
                     0.251
3522 h1 h1
             2.746 -0.033
3523 h1 cl
             3.280
                    -0.134
3524 cl h1
             3.280 -0.134
3525 cl h1
             2.512
                     2.571
             3.806
                    -0.542
3526 cl cl
      TOTAL VAN DER WAALS ENERGY = 4.485 kJ/mol
3527
3528
3529 ELECTROSTATIC INTERACTIONS
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
             2.512 -3.809 -1.516
3536 h1 cl
             2.208
                     1.352
3537 h1 h1
                             0.613
3538 h1 h1
             2.746
                     1.352
                             0.493
3539 h1 cl
             3.280 -3.809 -1.161
             3.280
3540 cl h1
                    -3.809
                            -1.161
3541 cl h1
             2.512
                    -3.809 -1.516
3542 cl cl
             3.806
                    10.728
                             2.819
      TOTAL ELECTROSTATIC ENERGY = -0.446 kJ/mol
3543
3544
3545 TOTAL ENERGY = 92.310 \text{ kJ/mol}
3546
3547 ATOM TYPES
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 FORMAL CHARGES
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 PARTIAL CHARGES
3572
3573 IDX CHARGE
3574 1 0.290000
3575 2 0.290000
3576 3 0.000000
3577 4 0.000000
3578 5 -0.290000
3579 6 0.000000
3580 7 0.000000
3581 8 -0.290000
3582
3583 A T O M T Y P E S
3584
3585 IDX TYPE RING
3586 1 c3 NO
3587 2 c3 NO
3588 3 h1 NO
3589 4 h1 NO
3590 5 cl NO
3591 6 hl NO
3592 7 h1 NO
3593 8 cl NO
3594
3595 FORMAL CHARGES
3596
3597 IDX CHARGE
3598 1 0.036009
3599 2 0.036009
3600 3 0.044101
3601 4 0.044101
3602 5 -0.124211
3603 6 0.044101
3604 7 0.044101
3605 8 -0.124211
3606
3607 PARTIAL CHARGES
3608
3609 IDX CHARGE
3610 1 0.036009
3611 2 0.036009
3612 3 0.044101
3613 4 0.044101
3614 5 -0.124211
3615 6 0.044101
3616 7 0.044101
```

3617 8 -0.124211 3618 3619 ENERGY 3620 3621 3622 BOND STRETCHING 3623 3624 ATOM TYPES FF BOND IDEAL FORCE I J CLASS LENGTH LENGTH CONSTANT DELTA ENERGY 3625 3626 12 0 1.670 2.974 2.795 3627 1 1.773 -0.103 4.766 3628 5 1 0 1.000 1.093 -0.093 3.578 3629 1 1 0 1.540 1.508 4.258 0.032 0.294 -0.093 3630 1 5 0 1.000 1.093 4.766 3.578 5 0 1.000 3631 1 1.093 4.766 -0.093 3.578 1 5 0 1.000 1.093 3632 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 ANGLE BENDING 3637 IDEAL FF VALENCE FORCE ATOM TYPES 3638 3639 I J K CLASS ANGLE ANGLE CONSTANT DELTA ENERGY 3640 ______ 3641 5 0 109.500 110.549 0.636 -1.0490.015 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 1 5 3644 1 0 109.500 110.549 0.636 -1.0490.015 1 12 0 109.500 108.679 3645 1 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 0 109.442 108.162 3648 5 1 12 0.698 1.280 0.025 3649 5 1 12 0 109.442 108.162 0.698 1.280 0.025 110.549 3650 1 1 5 0 109.500 0.636 -1.0490.015 109.500 110.549 1 1 5 0 0.636 -1.0493651 0.015 3652 5 0 109.442 108.836 0.516 0.606 0.004 3653 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol 3654 STRETCH BENDING 3655 3656 ATOM TYPES FF VALENCE DELTA 3657 FORCE CONSTANT I J K CLASS ANGLE 3658 ΙJ JК ANGLE ENERGY 3659 ______ 0 109.500 -1.049 0.227 0.070 3660 1 1 5 -0.002 5 1 5 0 109.442 0.606 -0.033 3661 0.115 0.115 3662 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121109.500 -1.049 0.227 -0.002 3663 1 1 5 0 0.070 0 109.500 0.821 0.176 1 1 12 0.386 3664 -0.070 3665 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121

3666				0		0.821				
3667				0	109.442		-0.0			
3668				0		1.280				
						-1.049				
3670						-1.049				
3671	5								0.115	-0.033
3672		TOTA	L STF	RETCH BEN	IDING ENERG	SY = -0.695	93 kcal/	mol		
3673		D 0 T								
3674	TO	RSI	ON	АЬ						
3675 3676	л пом	ם מעטם	C		EE MC	RSION	FORCE	CONC	m 7. N/m	
3677									V3 ENE	PCV
3678										
3679									0.398	0.886
3680									0.398	
3681									0.893	
3682						000 0.2			0.314	
3683						000 0.2		386	0.314	-0.991
3684	5	1	1	12	0 20.	000 0.6	78 -0.	602	0.398	0.886
3685	5	1	1	5	0 -100.	000 0.2	84 -1.	386	0.314	-0.991
3686	5	1	1	5	0 20.	000 0.2	84 -1.	386	0.314	0.349
3687	5	1	1	12	0 140.	000 0.6	78 -0.	602	0.398	0.129
3688		TOTA	L TOF	RSIONAL E	ENERGY = 0	.76131 kca	1/mol			
3689										
3690	O U	Т - О	F -	P L A N	E B E N	DING				
3691										
3692	ATOM	TYPE	S		FF	OOP FO	RCE			
3693	I	J	K	L	CLASS A	NGLE CON	STANT	EN	ERGY	
3694										
3695		TOTA	T OO1	'-OF'-PLAN	NE BENDING	ENERGY =	0.00000	kcal	/mol	
3696 3697	77 A	M D	ת קו	WAA	T. C					
3698	VA	IN D	EK	WAA	υр					
3699	ΔͲΩΝ	I TYPE	.s							
3700				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	3		
3705	5	5		2.232	2.970	0.022	0.328	3		
3706	5	5		2.638	2.970	0.022	0.001			
3707	5	12		3.399	3.713	0.053	-0.028	3		
3708	12	5		3.399	3.713	0.053	-0.028	3		
3709	12	5		2.547	3.713	0.053	2.298	3		
3710	12	12		3.587	4.089	0.276	0.100)		
3711		TOTA	L VAN	DER WAR	ALS ENERGY	= 4.94916	kcal/mc	1		
3712										
3712 3713 3714	ΕL	ЕСТ	'RO	STAT	I C I N	TERAC	TION	S		

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

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

```
3813
3814
     TOTAL ENERGY = 90.486 \text{ kJ/mol}
3815
3816 ATOM TYPES
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 FORMAL CHARGES
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 PARTIAL CHARGES
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 SETTING UP CALCULATIONS
3853
3854 SETTING UP BOND CALCULATIONS...
     SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
3855
3856
     SETTING UP TORSION CALCULATIONS...
3857 SETTING UP OOP CALCULATIONS...
     SETTING UP VAN DER WAALS CALCULATIONS...
3858
     SETTING UP ELECTROSTATIC CALCULATIONS...
3859
3860
3861 ATOM TYPES
```

```
3862
3863 IDX TYPE RING
3864 1 c3 NO
3865 2 c3 NO
3866 3 h1 NO
    4 h1 NO
3867
3868
    5 cl NO
    6 hl NO
3869
    7 h1 NO
3870
3871
    8 cl NO
3872
3873
    CHARGES
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
    SETTING UP CALCULATIONS
3885
3886
3887
    SETTING UP BOND CALCULATIONS...
3888
    SETTING UP ANGLE CALCULATIONS...
3889
    SETTING UP TORSION CALCULATIONS...
    SETTING UP IMPROPER TORSION CALCULATIONS...
3890
3891 SETTING UP VAN DER WAALS CALCULATIONS...
3892
    SETTING UP ELECTROSTATIC CALCULATIONS...
3893
3894 ENERGY
3895
3896
3897 BOND STRETCHING
3898
    ATOM TYPES FF BOND IDEAL FORCE
3899
    I J
                           LENGTH
3900
            CLASS LENGTH
                                    CONSTANT
                                               DELTA
                                                        ENERGY
3901
    ______
              0
3902
    12
        1
                   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
                   1.000
                            1.093
                                      4.766
                                               -0.093
                                                        3.578
             0
3905
        1
              0
                   1.540
                            1.508
                                      4.258
                                               0.032
                                                        0.294
     1
        5
             0
3906
    1
                   1.000
                            1.093
                                      4.766
                                               -0.093
                                                        3.578
3907
    1 12
               0
                   1.670
                            1.773
                                      2.974
                                               -0.103
                                                        2.795
                            1.093 4.766
    1 5
                                             -0.093
3908
              0
                    1.000
                                                         3.578
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
3909
3910
```

ANO	G L E	Е В	ENDI	N G				
АТОМ	TYPE	ES	FF	VALENCE	IDEAL	FORCE		
						CONSTANT	DELTA	ENERGY
						0.636		
						0.516		
				109.442			1.280	
				109.500		0.636		
1			0	109.500			0.821	
			0			0.698		
5			0	109.442				
1			0	109.500		1.056		
				109.442		0.698		
						0.636		
						0.516		
						0.636		
					= 0.20058		20019	00020
	1011	11110		NO DIVIDICOT	0.20030	noul, mol		
S T 1	вЕт	гс н	BENI	DING				
		. 0 11	2 2 1, .	3 1 1 0				
АТОМ	ТҮРБ	S	नन	VALENCE	DELTA	FORCE	CONSTANT	
						I J		ENERGY
						0.227		
						0.115		
						-0.018		
						0.227		
						0.176		
		12		109.442			0.380	-0.121
5	1	12	0	109.442	1.280		0.380	-0.121
1	1	12	0			0.176		-0.070
5	1	12	0		1.280			-0.121
1	1	5	0			0.227		-0.002
5	1		0			0.115		-0.033
1	1		0			0.227		
-						93 kcal/mol	0.070	0.002
	1011		dion but	JING LIVLING	1 00000	oo noar, mor		
т О 1	RSI	ON	A Tı					
_ 0 1		J 11						
АТОМ	ТАБЕ	ES		FF TO	RSION	FORCE CONS	TANT	
I					NGLE		V3 ENER	GY
5						78 -0.602		0.449
5	1	1	5	0 -80.	000 0.28	34 -1.386	0.314	-1.099
5	1	1	5	0 160.	000 0.28	34 -1.386	0.314	-0.075
		1	12	0 160.	000 0.67	78 -0.602	0.398	0.050
5	1							
5 5	1		5	0 40.			0.314	-0.243

```
3960 12 1 1 12 0 -80.000 0.000 0.000 0.893 0.223
3961
             5
                  0 160.000 0.678 -0.602
                                        0.398
   12
                                                0.050
                  0 40.000 0.678 -0.602 0.398 0.449
3962 12 1 1
             5
3963
      TOTAL TORSIONAL ENERGY = -1.29534 kcal/mol
3964
3965 OUT-OF-PLANE BENDING
3966
   ATOM TYPES
                  FF
3967
                        OOP
                             FORCE
    I J K L CLASS ANGLE CONSTANT ENERGY
3968
3969
3970
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
3971
3972 VAN DER WAALS
3973
3974
   ATOM TYPES
   I J
            Rij R*IJ EPSILON ENERGY
3975
3976
    ______
            2.518
3977
   5 5
                   2.970
                         0.022
                                0.036
   5 5
                   2.970
                          0.022 -0.021
             2.885
3978
3979
   5 12
            2.647
                   3.713
                          0.053
   5 5
3980
            2.300
                   2.970
                         0.022
                                0.215
   5 5
            2.518
                   2.970
                          0.022
                                0.036
3981
                   3.713
   5 12
                          0.053 -0.041
3982
             3.474
3983 12 5
             3.474
                         0.053 -0.041
                   3.713
3984 12 5
                          0.053
             2.647
                   3.713
                                1.520
            3.338
                   4.089 0.276
3985
   12 12
                                1.129
    TOTAL VAN DER WAALS ENERGY = 4.35500 kcal/mol
3986
3987
3988 ELECTROSTATIC INTERACTIONS
3989
3990
   ATOM TYPES
            Rij
3991
    I J
                 Qi
                        Qj
                               ENERGY
3992
    ______
3993
   12 12 3.388
                  -0.290
                        -0.290
                               6.182
3994
      TOTAL ELECTROSTATIC ENERGY = 6.18170 kcal/mol
3995
3996
   TOTAL ENERGY = 28.94230 kcal/mol
3997
   ENERGY
3998
3999
4000
4001 BOND STRETCHING
4002
   ATOM TYPES BOND IDEAL FORCE
4003
   I J
          LENGTH
                  LENGTH
                         CONSTANT
                                  DELTA ENERGY
4004
4005
   ______
                                       15.718
4006
   cl c3 1.670 1.786
                       1168.117 -0.116
                1.093
                       1406.346
4007 h1 c3
         1.000
                               -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 cl
          1.670
                  1.786
                         1168.117
                                  -0.116
                                          15.718
4012 c3 h1
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
      TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
4013
4014
4015 ANGLE BENDING
4016
    ATOM TYPES VALENCE IDEAL FORCE
4017
    I J K
                ANGLE
                        ANGLE
                               CONSTANT
                                         DELTA ENERGY
4018
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 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
                            194.100 -0.010
    c3 c3 h1 109.500 110.070
4023
                                             0.019
4024 c3 c3 cl 109.500
                   110.330
                            260.419
                                     -0.014
                                             0.055
                            183.005
4025 h1 c3 cl 109.442 105.930
                                     0.061
                                             0.688
4026 h1 c3 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
4027 c3 c3 cl 109.500
                   110.330
                            260.419
                                     -0.014
                                             0.055
4028 h1 c3 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
                            194.100 -0.010
4029
    c3 c3 h1 109.500 110.070
                                             0.019
                   109.550
                            164.039
4030 h1 c3 h1 109.442
                                             0.001
                                     -0.002
    c3 c3 h1 109.500 110.070 194.100
                                    -0.010
4031
                                             0.019
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
4032
4033
4034 TORSIONAL
4035
4036
    ----ATOM TYPES----
                   FORCE
                                 TORSION
    I J K L
                  CONSTANT
                                 ANGLE n ENERGY
4037
                            S
4038
    ______
4039
    h1 c3 c3 cl
               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 -80.000 3
              0.651
                                       0.326
4045
    cl c3 c3 cl
               0.000
                        0
                            -80.000 3
                                       0.000
4046 cl c3 c3 h1
               0.000
                        0
                           160.000 3
                                       0.000
                            40.000 3
4047
    cl c3 c3 h1
               0.000
                        0
                                       0.000
4048
       TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
4049
4050 IMPROPER TORSIONAL
4051
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
4052
    I J K
                  CONSTANT
                            s ANGLE n ENERGY
4053
              T.
4054
4055
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
4056
4057 VAN DER WAALS
```

```
4058
4059 ATOM TYPES
    I J Rij kij ENERGY
4060
4061
4062 h1 h1
           2.518
                   -0.013
4063 h1 h1
            2.885 -0.031
4064 h1 cl
            2.647
                    1.083
4065 h1 h1
            2.300
                    0.109
4066 h1 h1
            2.518 -0.013
4067 h1 cl
            3.474
                   -0.129
4068 cl h1
            3.474
                   -0.129
                    1.083
4069 cl h1
            2.647
4070 cl cl
            3.338
                    0.738
      TOTAL VAN DER WAALS ENERGY = 2.701 kJ/mol
4071
4072
4073 ELECTROSTATIC INTERACTIONS
4074
4075 ATOM TYPES
    I J
            Rij 332.17*QiQj ENERGY
4076
4077
4078 hl hl
           2.518 1.352 0.537
4079 h1 h1
            2.885
                    1.352
                           0.469
4080 h1 cl
            2.647 -3.809 -1.439
                    1.352
                           0.588
4081 h1 h1
            2.300
4082 h1 h1
            2.518
                    1.352
                           0.537
4083 h1 cl
            3.474 -3.809 -1.097
4084 cl h1
            3.474 -3.809 -1.097
            2.647
4085 cl h1
                   -3.809
                           -1.439
4086 cl cl 3.338 10.728 3.214
     TOTAL ELECTROSTATIC ENERGY = 0.273 kJ/mol
4087
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 FORMAL CHARGES
4104
4105 IDX CHARGE
4106 | 1 0.000000
```

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

```
4156 6 0.044101
    7 0.044101
4157
4158 8 -0.124211
4159
4160 SETTING UP CALCULATIONS
4161
4162 | SETTING UP BOND CALCULATIONS...
    SETTING UP ANGLE CALCULATIONS...
4163
    SETTING UP TORSION CALCULATIONS...
4164
    SETTING UP IMPROPER TORSION CALCULATIONS...
4165
4166
    SETTING UP VAN DER WAALS CALCULATIONS...
4167
    SETTING UP ELECTROSTATIC CALCULATIONS...
4168
4169 ENERGY
4170
4171
4172 BOND STRETCHING
4173
4174 ATOM TYPES FF BOND
                         IDEAL
                                 FORCE
    I J
           CLASS LENGTH
                         LENGTH
4175
                                 CONSTANT
                                           DELTA
    _____
4176
             0
        1
4177
    5
                  1.000
                          1.093
                                    4.766
                                           -0.093
                                                    3.578
4178 12
        1
            0
                  1.670
                          1.773
                                   2.974
                                           -0.103
                                                   2.795
    5
4179
        1
            0
                  1.000
                          1.093
                                   4.766
                                           -0.093
                                                   3.578
                  1.540
                                           0.032
4180
    1
        1
            0
                          1.508
                                   4.258
                                                   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
    1 5
4183
             0
                  1.000
                          1.093
                                   4.766
                                           -0.093
                                                   3.578
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
4184
4185
    ANGLE BENDING
4186
4187
4188 ATOM TYPES
                FF VALENCE IDEAL
                                     FORCE
4189
    I J K CLASS ANGLE
                             ANGLE
                                    CONSTANT
                                               DELTA
                                                       ENERGY
4190
        1 5
                0 109.500
                            110.549
                                              -1.049
4191
    1
                                       0.636
                                                       0.015
4192
    5
        1
           5
                0
                    109.442
                            108.836
                                       0.516
                                               0.606
                                                       0.004
                0 109.442 108.162
    5
        1 12
                                       0.698
                                               1.280
4193
                                                       0.025
        1 5
4194
    1
                0 109.500 110.549
                                       0.636
                                              -1.049
                                                       0.015
4195
        1 12
                0 109.500 108.679
                                       1.056
                                               0.821
                                                       0.016
    1
                0 109.442 108.162
4196
    5
        1 12
                                       0.698
                                               1.280
                                                       0.025
4197
    5
        1 12
                0 109.442
                            108.162
                                       0.698
                                               1.280
                                                       0.025
                0 109.500 108.679
                                       1.056
4198
    1
        1 12
                                               0.821
                                                       0.016
                   109.442 108.162
        1 12
                0
                                       0.698
4199
     5
                                               1.280
                                                       0.025
        1 5
                0 109.500 110.549
4200
    1
                                       0.636
                                              -1.049
                                                       0.015
    5
           5
4201
        1
                0 109.442 108.836
                                       0.516
                                               0.606
                                                       0.004
                0 109.500 110.549
                                       0.636 -1.049
4202
    1
       1
           5
                                                        0.015
      TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
4203
4204
```

ST	RET	СН	BEN	DING						
ATOM	TYPE	S	FF	VALENCE	E DE	ELTA	FO	RCE CON	STANT	
										ENERGY
				109.500						
				109.442						
				109.442						
				109.500						
			0							
5			0	109.442				8 (
			0							
				109.500				6 (
			0					8 (
				109.500						
				109.442						
				109.500					0.070	-0.002
	TOTA	L STR	RETCH BEN	IDING ENER	RGY = -(.69593	kcal/m	ol		
T O	RSI	ON	AL							
				FF I						
Ι	J	K	L	CLASS	ANGLE		V1 V	2 V3	EN	NERGY
										0.057
								86 0	.314	-0.826
				0 -180						0.000
										0.000
5	1	1	5	0 60	.000	0.284	-1.3	86 0	.314	-0.827
									.314	-0.826
				0 -60					.893	
				0 180						
12	1	1	5	0 60	0.000	0.678	-0.6	02 0	.398	0.057
	TOTA	L TOR	SIONAL E	ENERGY = -	-2.36550	kcal/r	nol			
O U	T - C) F -	P L A N	E BEN	DIN	G				
		S		FF	OOP	FORCE	Ξ			
ATOM	TYPE		L	CLASS	ANGLE	CONST	ANT	ENERGY		
		K								
		K 								
I 	J 			E BENDING	ENERGY	z = 0.0	00000 k	cal/mol		
I 	J 			E BENDING	G ENERGY	<i>y</i> = 0.0	00000 k	cal/mol		
I 	J TOTA	L OUT			G ENERGY	Z = 0.0	00000 k	cal/mol		
I 	J TOTA	L OUT	 '-OF-PLAN		G ENERGY	z = 0.0	00000 k	cal/mol		
I V A	J TOTA	AL OUT	 '-OF-PLAN		G ENERGY	z = 0.0	00000 k	cal/mol		
I V A	J TOTA N D TYPE	L OUT	'-OF-PLAN					cal/mol		
I V A : ATOM	J TOTA TYPE J	AL OUT	P-OF-PLAN WAA	L S	EPSII	LON I	ENERGY	cal/mol		
I V A ATOM I	J TOTA TOTA TYPE J	L OUT	C-OF-PLAN WAA	L S R*IJ	EPSII	JON I	ENERGY	cal/mol		

5	1	.2	2.792	3.713	3 0	.053	0.792		
				2.970		.022	0.107		
5		5	2.400	2.970			0.107		
		.2		3.713		.053	-0.044		
12		5	3.499	3.713	3 0	.053	-0.044		
12		5	2.792	3.713	3 0	.053	0.792		
12	1	2	3.087	4.089	9 0	.276	3.947		
	Ţ	COTAL	VAN DER V	VAALS ENERG	GY = 5	.74158	kcal/mol		
E L	Е	СТІ	ROSTA	T I C I	NTEI	RAC	r I O N S		
		YPES							
Ι		J	Rij	Qi		Qj	ENERG	Y	
								-	
L2	1	.2	3.137	-0.290	-0.29	90	6.678		
	I	COTAL	ELECTROS	TATIC ENERG	GY = 6	.67788	kcal/mol		
rot <i>i</i>	ΑL	ENER	GY = 29.75	5490 kcal/r	mol				
E N	Е	R G	Y						
3 0	N	D S	STRET	CHING					
				IDEAL					
Ι		J	LENGTH	LENGTH	COI	NSTANT	DELTA	A ENER	RGY
				1.093					
				1.786					
				1.093					
				1.535					
				1.093					
				1.786					
				1.093				12.163	
	T	COTAL	BOND STRE	ETCHING EN	ERGY =	80.12	22 kJ/mol		
A N	G	L E	B E N D	I N G					
				LENCE					
								DELTA	
								0.01	.9
h1 c	23	h1	109.442	109.550)1
h1 c	23			105.930			0.06	0.68	88
c3 c	23	h1	109.500	110.070	19	94.100	-0.01	0.01	.9
c3 c			109.500	110.330		60.419		4 0.05	55
h1 c	23	cl	109.442	105.930			0.06		88
h1 c	23	cl	109.442	105.930	18	83.005	0.06	0.68	88
c3 c	23	cl	109.500	110.330	20	60.419	-0.01	4 0.05	55

```
4303 h1 c3 cl 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
                   FORCE
                                TORSION
4311
    ----ATOM TYPES----
    I J K L CONSTANT
                                 ANGLE n ENERGY
4312
                           S
4313
    _____
                      0
                          60.000 3 0.000
4314 h1 c3 c3 cl 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 cl 0.000
                       0 -180.000 3
                                      0.000
                           60.000 3
4318 h1 c3 c3 h1
              0.651
                       0
                                      0.000
4319 h1 c3 c3 h1
                       0
              0.651
                           -60.000 3
                                      0.000
              0.000
                          -60.000 3
                                      0.000
4320 cl c3 c3 cl
                       0
                       0
4321 cl c3 c3 h1
              0.000
                           180.000 3
                                      0.000
              0.000 0
4322 cl c3 c3 h1
                           60.000 3
                                      0.000
      TOTAL TORSIONAL ENERGY = 0.000 kJ/mol
4323
4324
4325 IMPROPER TORSIONAL
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 VAN DER WAALS
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 cl
           2.792
                  0.356
           2.400
4340 h1 h1
                  0.030
4341 h1 h1
           2.400
                  0.030
           3.499
4342 h1 cl
                 -0.127
           3.499 -0.127
4343
    cl h1
4344 cl h1
           2.792
                  0.356
4345 cl cl
           3.087
                  4.588
    TOTAL VAN DER WAALS ENERGY = 5.105 kJ/mol
4346
4347
4348 ELECTROSTATIC INTERACTIONS
4349
4350 ATOM TYPES
           Rij 332.17*QiQj ENERGY
```

```
4352 -----
4353
    h1 h1
             2.400
                     1.352
                              0.563
                     1.352 0.466
4354 h1 h1
             2.903
4355 h1 cl
             2.792
                     -3.809 -1.364
             2.400
                              0.563
4356
    h1 h1
                     1.352
    h1 h1
             2.400
                     1.352
                              0.563
4357
4358 h1 cl
             3.499
                     -3.809 -1.089
4359
    cl h1
             3.499
                             -1.089
                     -3.809
                    -3.809 -1.364
4360 cl h1
             2.792
4361 cl cl
             3.087
                     10.728
                              3.476
        TOTAL ELECTROSTATIC ENERGY = 0.726 kJ/mol
4362
4363
4364 TOTAL ENERGY = 88.891 kJ/mol
4365
4366
    ATOM TYPES
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
    6 5 NO
4374
4375 7 5 NO
4376 8 12 NO
4377
4378 FORMAL CHARGES
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 PARTIAL CHARGES
4391
4392
    IDX CHARGE
4393 1 0.290000
4394 2 0.290000
4395
    3 0.000000
4396 4 0.000000
4397 5 -0.290000
    6 0.000000
4398
4399 7 0.000000
4400 8 -0.290000
```

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4401
4402
     SETTING UP CALCULATIONS
4403
4404 SETTING UP BOND CALCULATIONS...
4405
     SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
     SETTING UP TORSION CALCULATIONS...
4406
4407
     SETTING UP OOP CALCULATIONS...
4408
     SETTING UP VAN DER WAALS CALCULATIONS...
     SETTING UP ELECTROSTATIC CALCULATIONS...
4409
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
     4 h1 NO
4417
4418
     5 cl NO
     6 h1 NO
4419
4420 7 h1 NO
4421
     8 cl NO
4422
4423 C H A R G E S
4424
4425 IDX CHARGE
4426 1 0.036009
     2 0.036009
4427
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 SETTING UP CALCULATIONS
4436
4437
     SETTING UP BOND CALCULATIONS...
4438 SETTING UP ANGLE CALCULATIONS...
4439
     SETTING UP TORSION CALCULATIONS...
     SETTING UP IMPROPER TORSION CALCULATIONS...
4440
4441
     SETTING UP VAN DER WAALS CALCULATIONS...
4442
     SETTING UP ELECTROSTATIC CALCULATIONS...
4443
4444
     ENERGY
4445
4446
4447 BOND STRETCHING
4448
4449
    ATOM TYPES FF BOND IDEAL
                                      FORCE
```

							ONSTANT		
451							4.766		
							4.766		
1454			0			.773			
1455			0			.508			
1456			0			.093			
							2.974		
							4.766		
1459							29 kcal/mol		010,0
1460									
461	A N	G L E	BE	יד מת	V G				
462	21 11	0 1 1		., , ,					
1463	ΔπΩм	י ייעסד	!S	ਬਬ	WALENCE.	TDEAT.	FORCE		
							CONSTANT	חבו תא	FNFDCV
1465									
							0.636		
1467							0.516		
					109.442			1.280	
1469			5			110.549		-1.049	
1470		1		0	109.500			0.821	
1471		1			109.300			1.280	
			12 5					1.280	
1473		1			109.500			-1.049	
474					109.442			0.606	
1475			12		109.500			0.821	
							0.698		
							0.636	-1.049	0.015
478		mom v	II ANGTH	RENDII	NG ENERGY	= 0.20058	KCal/MOl		
170		TOTA							
				D F N I) T N C				
1480			СН	BENI) I N G				
1480	ST	RET	СН			DEITA	FODCE	CONSTANT	
480 481 482	S T	R E T	C H	FF	VALENCE		FORCE		FNFDCV
1480 1481 1482 1483	S T ATOM I	R E T I TYPE J	C H	FF CLASS	VALENCE ANGLE	ANGLE	ΙJ	J K	ENERGY
1480 1481 1482 1483	S T ATOM I	RETITYPE	C H	FF CLASS	VALENCE ANGLE	ANGLE	I J	J K	
1480 1481 1482 1483 1484 1485	S T ATOM I 1	R E T I TYPE J 1	С Н К ——————5	FF CLASS 	VALENCE ANGLE	ANGLE 	I J 0.227	J К 	-0.002
1480 1481 1482 1483 1484 1485	S T ATOM I 1 5	RETITYPE J 1	C H SS K 5 5	FF CLASS 0 0	VALENCE ANGLE 109.500 109.442	ANGLE -1.049 0.606	0.227 0.115	J K 0.070 0.115	-0.002 -0.033
1480 1481 1482 1483 1484 1485 1486	S T ATOM I 1 5 5	RETITYPE J 1 1	C H S K 5 5 12	FF CLASS 0 0	VALENCE ANGLE 109.500 109.442	ANGLE -1.049 0.606 1.280	0.227 0.115 -0.018	J K 0.070 0.115 0.380	-0.002 -0.033 -0.121
1480 1481 1482 1483 1484 1485 1486 1487	S T ATOM I 1 5 5	RETITYPE J 1 1 1	C H SS K 5 12 5	FF CLASS 0 0 0	VALENCE ANGLE 109.500 109.442 109.442	ANGLE -1.049 0.606 1.280 -1.049	0.227 0.115 -0.018 0.227	J K 0.070 0.115 0.380 0.070	-0.002 -0.033 -0.121 -0.002
1480 1481 1482 1483 1484 1485 1486 1487 1488	S T ATOM I 1 5 1 1	R E T I TYPE J 1 1 1 1	C H S K 5 5 12 5 12	FF CLASS 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500	ANGLE -1.049 0.606 1.280 -1.049 0.821	0.227 0.115 -0.018 0.227 0.176	J K 0.070 0.115 0.380 0.070 0.386	-0.002 -0.033 -0.121 -0.002 -0.070
1480 1481 1482 1483 1484 1485 1486 1487 1488 1489	S T ATOM I 1 5 1 1 5 5	R E T I TYPE J 1 1 1 1 1 1	C H SS K 5 5 12 5 12	FF CLASS 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500 109.442	-1.049 0.606 1.280 -1.049 0.821 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018	J K 0.070 0.115 0.380 0.070 0.386 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121
1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490	S T ATOM I 1 5 1 1 5 5 1	R E T I TYPE J 1 1 1 1 1	C H SS K 5 5 12 5 12 12 12	FF CLASS 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500 109.442 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121
1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491	S T ATOM I 1 5 1 1 5 1 1	R E T I TYPE J 1 1 1 1 1 1 1 1	C H SS K 5 5 12 5 12 12 12 12	FF CLASS 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 1.280 -1.049	0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.070	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121 -0.002
1479 1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493	S T ATOM I 1 5 5 1 1 5 5 1	R E T I TYPE J 1 1 1 1 1 1 1	C H SS K 5 5 12 5 12 12 5 5 5 5 6 6 7 7 8 8 8 8 8 8 8 8 8 8 8	FF CLASS 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 1.280 -1.049 0.606	0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.070 0.115	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121 -0.002 -0.033
1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493	S T ATOM I 1 5 5 1 1 5 1 1 5 1	R E T I TYPE J 1 1 1 1 1 1 1 1 1 1	C H SS K 5 5 12 5 12 12 12 12 12	FF CLASS 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.442 109.500 109.442	ANGLE	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.070 0.115 0.386	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121 -0.002 -0.033 -0.070
1480 1481 1482 1483 1484 1485 1486 1487 1488 1490 1491 1492 1493 1494	S T ATOM I 1 5 1 1 5 1 1 5 1 5 1 5 1	R E T I TYPE J 1 1 1 1 1 1 1 1 1 1 1 1	C H SS K 5 5 12 5 12 12 12 12 12	FF CLASS 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.442 109.500 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 -1.049 0.606 0.821 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176 -0.018	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.070 0.115 0.386 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121 -0.002 -0.033 -0.070 -0.121
1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493	S T ATOM I 1 5 1 1 5 1 1 5 1 5 1 5 1	R E T I TYPE J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	C H SS K 5 5 12 5 12 12 12 12 5 5 12	FF CLASS 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.500 109.442 109.500 109.442	ANGLE	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.070 0.115 0.386 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121 -0.002 -0.033 -0.070 -0.121

ATOM	TYPES			FF	TORSION	F	ORCE CONS	STANT	
I	J	K	L	CLASS	ANGLE		V1 V2	V3	ENERGY
			 5		-40.000	0.284	-1.386	0.314	 1 -0.24
									3 -0.08
					-160.000				
					80.000				
					-160.000				3 0.05
					-40.000				1 -0.24
					-160.000				3 0.05
									3 0.22
									3 -0.08
					= -1.51155				
						,			
O U T	- 0	F - P	LAN	Е В	ENDIN	G			
MOTA	TYPES			FF	OOP	FORCE			
					ANGLE			IERGY	
	D :	E R	OF-PLAI		DING ENERGY	z = 0.0	 00000 kcal	 ./mol	
V A N	D :	E R	W A A	L S				./mol	
V A N	D :	E R	W A A	L S	DING ENERGY	LON E		 ./mol	
V A N ATOM '	D : TYPES J	E R	W A A	L S R*	IJ EPSII	JON E	NERGY	 ./mol	
V A N ATOM '	D : TYPES J 5	E R I	W A A	L S R* 2.	IJ EPSII 970 0.0	LON E	NERGY	 ./mol	
V A N ATOM	D: TYPES J 5	E R	W A A	L S R* 2.	IJ EPSII 970 0.0	GON E 022 022 -	ENERGY 0.215	./mol	
V A N ATOM	D: TYPES J 5 5	E R	W A A Rij 2.300 2.885	L S R* 2. 2. 3.	IJ EPSI] 970 0.0 970 0.0	LON E 022 022 -	CNERGY 0.215 -0.021 0.331	./mol	
V A N ATOM 5 5 5 5	D: TYPES J 5 5	E R	W A A Rij 2.300 2.885 2.960	L S R* 2. 2. 3.	IJ EPSII 970 0.0 970 0.0	CON E 022 022 - 053	ENERGY 0.215 0.021 0.331 0.036	./mol	
V A N ATOM I 5 5 5 5	D: TYPES J 5 5 12	E R	W A A Rij 2.300 2.885 2.960 2.518	R* 2. 2. 3. 2.	IJ EPSII 	LON E 022 022 - 053 022	ENERGY 0.215 0.021 0.331 0.036	./mol	
V A N ATOM 5 5 5 5 5 5	D: TYPES J 5 5 12 5 5 12	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300	L S R* 2. 2. 3. 2. 3.	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0	GON E 022 022 - 053 022 022	ENERGY 0.215 0.021 0.331 0.036 0.215	./mol	
V A N ATOM 5 5 5 5 5 12	D: TYPES J5 5 5 12 5 5 5	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474	R* 2. 2. 3. 2. 3. 3.	IJ EPSII 	CON E 022 022 - 053 022 022 053 - 053 -	CNERGY 0.215 0.021 0.331 0.036 0.215 0.041	./mol	
V A N ATOM 5 5 5 5 12	D: TYPES J 5 5 12 5 5 12 5	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960	L S R* 2. 2. 3. 2. 3. 3.	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0 713 0.0 713 0.0	CON E 022 022 - 053 022 053 - 053 -	0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331	./mol	
V A N ATOM 5 5 5 12 12 12	D: TYPES J 5 5 12 5 12 5 12	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865	L S R* 2. 2. 3. 2. 3. 4.	IJ EPSII 	LON E 022 022 - 053 022 053 - 053 - 053	SNERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331 9.664	./mol	
V A N ATOM 5 5 5 12 12 12	D: TYPES J 5 5 12 5 12 5 12	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865	L S R* 2. 2. 3. 2. 3. 4.	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0 713 0.0 713 0.0 713 0.0	LON E 022 022 - 053 022 053 - 053 - 053	SNERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331 9.664	./mol	
V A N ATOM I 5 5 5 12 12	D: TYPES J 5 5 12 5 12 5 12 5 12 5 TOTAL	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865 DER WA	R* 2. 2. 3. 2. 3. 4. ALS EN	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0 713 0.0 713 0.0 713 0.0	LON E 022 022 - 053 022 053 - 053 - 053 276 69051 kc	SNERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331 9.664 eal/mol	./mol	
V A N ATOM I 5 5 5 12 12	D: TYPES J 5 5 12 5 12 5 12 5 12 5 TOTAL	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865 DER WA	R* 2. 2. 3. 2. 3. 4. ALS EN	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0 ERGY = 10.6	LON E 022 022 - 053 022 053 - 053 - 053 276 69051 kc	SNERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331 9.664 eal/mol	./mol	
V A N ATOM I 5 5 5 12 12 12	D: TYPES J 5 5 12 5 12 5 12 C T:	E R I	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865 DER WA	R* 2. 2. 3. 2. 3. 4. ALS EN	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0 ERGY = 10.6	LON E 022 022 - 053 022 053 - 053 - 053 276 69051 kc	SNERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331 9.664 eal/mol	./mol	
V A N ATOM I 5 5 5 12 12 12 12	TYPES J 5 5 12 5 12 5 12 TOTAL C T	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865 DER WAD	R* 2. 3. 2. 3. 3. 4. ALS EN	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0 713 0.0 713 0.0 713 0.0 ERGY = 10.6 INTER	CON E 022 022 - 053 022 053 - 053 - 053 276 69051 kc	O.215 O.021 O.331 O.036 O.215 O.041 O.041 O.331 9.664 al/mol	./mol	
V A N ATOM I 5 5 5 5 12 12 12 12	D: TYPES J 5 5 12 5 12 5 12 TOTAL C T: TYPES J	E R	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865 DER WAN	L S R* 2. 2. 3. 3. 4. ALS EN	IJ EPSII 970 0.0 970 0.0 713 0.0 970 0.0 713 0.0 713 0.0 713 0.0 713 0.0 ERGY = 10.6	GON E 022 022 022 053 022 053 - 053 276 69051 kc	ENERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331 9.664 al/mol	./mol	
V A N ATOM I 5 5 5 5 12 12 12 12 12	D: TYPES J 5 5 12 5 12 5 12 TOTAL C T: TYPES J	E R I VAN I R O S	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865 DER WAD T A T	L S R* 2. 2. 3. 3. 3. 4. ALS EN	IJ EPSII 	CON E 022 022 022 022 053 022 053 - 053 276 69051 kc	CNERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.041 0.331 9.664 cal/mol	./mol	
V A N ATOM I 5 5 5 12 12 12 12 12 ATOM I 12	D: TYPES J 5 5 12 5 12 5 12 TOTAL C T: TYPES J 12	ER I VAN I R O S	W A A Rij 2.300 2.885 2.960 2.518 2.300 3.474 3.474 2.960 2.865 DER WAI	L S R* 2. 2. 3. 3. 3. 4. ALS EN I C	IJ EPSII	GON E 022 022 022 053 022 053 - 053 276 69051 kc	ENERGY 0.215 0.021 0.331 0.036 0.215 0.041 0.031 9.664 cal/mol CONS ENERGY	./mol	

ENERG:	Y						
BOND	STRETC	HING					
ATOM TYPES	DOND	TDEAT	FORCE				
			CONSTANT	DEI	.πа	FNFDC	!V
			1406.346				
			1406.346				
			1168.117				
			1269.019				
			1406.346				
c3 cl	1.670	1.786	1168.117	-0.116	15	.718	
c3 h1	1.000	1.093	1406.346	-0.093	12	1.163	
TOTAL	BOND STRET	CHING ENER	RGY = 80.1	22 kJ/mol	_		
ANGLE	BENDI	N G					
			EAL FO				
			IGLE CON				
			104 100				
			194.100				
	109.442			-0.0			
n1 c3 cl	109.442)10		
c3 c3 h1	109.500			-0.0			
	109.300			0.0			
	109.442			0.0			
c3 c3 h1					10		
h1 c3 h1	109.442	109.550			002		
c3 c3 cl	109.500	110.330	260.419	-0.0)14	0.055	
	109.442			0.0	061		
			194.100				
TOTAL	ANGLE BEND	OING ENERGY	2.938	kJ/mol			
T O R S I O	ONAL						
ATOM T	YPES	FORCE		TORSION			
			S				
	1 0.651	. 0					
h1 c3 c3 h			80 000	3	0.000		
h1 c3 c3 c	0.000				0 00-		
h1 c3 c3 c3 h1 c3 c3 h3	1 0.000 1 0.651	. 0	-160.000	3	0.326		
h1 c3 c3 c3 h1 c3 c3 h1 h1 c3 c3 h1	1 0.000 1 0.651 1 0.651	0 0	-160.000 80.000	3	0.326		
h1 c3 c3 c h1 c3 c3 h h1 c3 c3 h h1 c3 c3 c	1 0.000 1 0.651 1 0.651 1 0.000	0 0 0	-160.000 80.000 -160.000	3 3 3	0.326		
h1 c3 c3 c1 h1 c3 c3 h1 h1 c3 c3 h1 h1 c3 c3 c1 h1 c3 c3 h1	1 0.000 1 0.651 1 0.651 1 0.000 1 0.651	0 0 0	-160.000 80.000 -160.000 -40.000	3 3 3 3	0.326 0.000 0.326		
h1 c3 c3 c3 h1 c3 c3 h1 h1 c3 c3 h1	1 0.000 1 0.651 1 0.651 1 0.000 1 0.651 1 0.000	0 0 0 0	-160.000 80.000 -160.000	3 3 3 3 3	0.326		

```
4597 cl c3 c3 hl 0.000 0 80.000 3 0.000
4598
       TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
4599
4600 IMPROPER TORSIONAL
4601
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
4602
    I J K L CONSTANT S ANGLE n ENERGY
4603
4604
    ______
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
4605
4606
4607 VAN DER WAALS
4608
4609 ATOM TYPES
4610
    I J
            Rij kij ENERGY
4611
           2.300
4612 h1 h1
                   0.109
4613 h1 h1
           2.885
                  -0.031
4614 h1 cl
           2.960
                  0.012
           2.518
4615 h1 h1
                  -0.013
4616 h1 h1
           2.300
                  0.109
4617 h1 cl
           3.474 -0.129
           3.474
4618 cl h1
                  -0.129
4619 cl h1
           2.960
                  0.012
           2.865 15.169
4620 cl cl
     TOTAL VAN DER WAALS ENERGY = 15.111 kJ/mol
4621
4622
4623 ELECTROSTATIC INTERACTIONS
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
4630 h1 cl
           2.960 -3.809 -1.287
4631 h1 h1
           2.518
                  1.352
                         0.537
4632 h1 h1
           2.300
                  1.352
                          0.588
4633 h1 cl
           3.474 -3.809 -1.097
           3.474 -3.809 -1.097
4634 cl h1
4635 cl h1
           2.960
                  -3.809 -1.287
                          3.745
4636 cl cl
           2.865
                  10.728
    TOTAL ELECTROSTATIC ENERGY = 1.160 kJ/mol
4637
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
```

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4646 3 5 NO
4647 4 5 NO
4648 5 12 NO
4649 6 5 NO
4650 7 5 NO
4651 8 12 NO
4652
4653 FORMAL CHARGES
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 PARTIAL CHARGES
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 SETTING UP CALCULATIONS
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 ATOM TYPES
4687
4688 IDX TYPE RING
4689
     1 c3 NO
4690 2 c3 NO
4691 3 h1 NO
     4 h1 NO
4692
4693 5 cl NO
4694
     6 hl NO
```

```
4695 7 hl NO
4696
    8 cl NO
4697
4698 C H A R G E S
4699
4700 IDX CHARGE
4701 1 0.036009
4702 2 0.036009
    3 0.044101
4703
4704 4 0.044101
4705 | 5 -0.124211
4706
    6 0.044101
4707 7 0.044101
4708
    8 -0.124211
4709
4710 SETTING UP CALCULATIONS
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...
    SETTING UP ELECTROSTATIC CALCULATIONS...
4717
4718
4719 E N E R G Y
4720
4721
4722
    BOND STRETCHING
4723
4724 ATOM TYPES FF BOND IDEAL FORCE
     I J CLASS LENGTH
4725
                         LENGTH
                                  CONSTANT
                                            DELTA
                                                    ENERGY
4726
4727
    5 1
            0
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                     3.578
                          1.093
4728
    5
        1
             0
                  1.000
                                    4.766
                                            -0.093
                                                     3.578
                  1.540
                          1.508
                                    4.258
4729
    1
        1
             0
                                            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
    1 12
             0
                  1.670
                          1.773
                                    2.974
                                            -0.103
4732
                                                    2.795
    1 5
                                            -0.093
4733
                  1.000
                          1.093
                                    4.766
                                                    3.578
4734
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
4735
4736 ANGLE BENDING
4737
    ATOM TYPES FF VALENCE IDEAL FORCE
4738
    I J K
                CLASS ANGLE
                              ANGLE
4739
                                     CONSTANT
                                                DELTA
                                                        ENERGY
4740
    ______
               0 109.500 110.549
                                       0.636
                                               -1.049
4741
    1
        1 5
                                                         0.015
                 0 109.442 108.836
    5 1 5
                                       0.516
                                                0.606
4742
                                                        0.004
                0 109.442 108.162
4743
    5 1 12
                                     0.698
                                                1.280
                                                         0.025
```

	_									
1	1	5	0	109.500	110.5	49	0.636	5 –1	.049	0.01
1	1	12	0	109.500	108.6	79	1.056	5 0	.821	0.01
5 5	1	12	0	109.442	108.1	62	0.698	3 1	.280	0.02
1	1	5	0	109.500	110.5	49	0.636	5 –1	.049	0.01
5	1	12	0	109.442	108.1	62	0.698	3 1	.280	0.02
5	1	5	0	109.442	108.8	36	0.516	5 0	.606	0.00
1	1	12	0	109.500	108.6	79	1.056	5 0	.821	0.01
1	1	5	0	109.500	110.5	49	0.636	5 –1	.049	0.01
5	1	12	0	109.442	108.1	62	0.698	3 1	.280	0.02
3	TOTA	AL ANG	GLE BENDI	NG ENERGY	7 = 0.20	058 kc	cal/mol			
ł.										
ST	R E I	г с н	B E N	D I N G						
5										
ATOM	1 TYPE	ES	FF	VALENCE	E DEL	TA	FORCE	E CONSTA	NT	
3 I	J	K	CLASS	ANGLE	ANG	LE	ΙJ	J	K	ENERGY
1	1	5	0	109.500	-1.0	49	0.227	0.0	70 -	-0.002
. 5	1	5	0	109.442	0.6	06	0.115	0.1	15 -	-0.033
5	1	12	0	109.442	1.2	80	-0.018	0.3	80 -	-0.121
1	1	5	0	109.500	-1.0	49	0.227	0.0	70 -	-0.002
1	1	12	0	109.500	0.8	21	0.176	0.3	86 -	-0.070
5	1	12	0	109.442	1.2	80	-0.018	0.3	80 -	-0.121
1	1	5	0	109.500	-1.0	49	0.227	0.0	70 -	-0.002
5	1	12	0	109.442	1.2	80	-0.018	0.3	80 -	-0.121
5	1	5	0	109.442	0.6	06	0.115	0.1	15 -	-0.033
1	1	12	0	109.500	0.8	21	0.176	0.3	86 -	-0.070
1	1	5	0	109.500	-1.0	49	0.227	0.0	70 -	-0.002
. 5	1	12	0	109.442	1.2	80	-0.018	0.3	80 -	-0.121
_			RETCH BEN	IDING ENE	RGY = -0.	69593	kcal/mol			
	TOTA	AL STF								
2	TOTA	AL STE								
3		AL STR	A L							
2 3 4 T O			A L							
2 3 4 T O	R S I	ON		FF :	PORSION	F	FORCE CONS	STANT		
T O ATOM	R S I	I O N		FF CLASS			FORCE CONS		ENERGY	
T O ATOM	R S I	I O N							ENERGY	
T O ATOM	R S I I TYPE J	ON ES K	L	CLASS	ANGLE			V3).349
T O ATOM	R S I 1 TYPE J 1	EON ES K 1	L 5	CLASS	ANGLE 		V1 V2 	V3	4 (
T O ATOM	R S I I TYPE J 1 1	ES K	L 5	CLASS 0 -20 0 100	ANGLE	 0.284	V1 V2 -1.386 -0.602	V3 	 4 (8 –(0.005
T O ATOM T S 5 5 5 5 5 5 5 5	R S I I TYPE J 1 1	ES K	L 5 12	0 -20 0 100 0 -140	ANGLE 0.000 0.000	 0.284 0.678	V1 V2 	0.31 0.39 0.31	4 (8 – (4 – (4	0.005
T O ATOM 5	R S I M TYPE J 1 1 1	ES K 1 1 1	L 5 12 5	0 -20 0 100 0 -140 0 100	ANGLE 0.000 0.000 0.000 0.000	 0.284 0.678 0.284	V1 V2 -1.386 -0.602 -1.386 -1.386	0.31 0.39 0.31	4 (8 – (4 – (4 – (4 – (4 – (4 – (4 – (4	0.005 0.304 0.991
T O ATOM 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	R S I M TYPE J 1 1 1	ES K 1 1 1 1 1	L 5 12 5 5	0 -20 0 100 0 -140 0 100 0 -140	ANGLE 0.000 0.000 0.000 0.000 0.000	0.284 0.678 0.284 0.284	V1 V21.386 -0.602 -1.386 -1.386 -0.602	V3 0.31 0.39 0.31 0.31 0.39	4 (8 – (4 – (4 – (4 – (4 – (4 – (4 – (4	0.005 0.304 0.991 0.129
T O S ATOM S S S S S S S S S S S S S S S S S S S	R S I M TYPE J 1 1 1 1 1	I O N ES K 1 1 1 1	L 5 12 5 5 12	0 -20 0 100 0 -140 0 100 0 -140 0 -20	ANGLE 0.000 0.000 0.000 0.000 0.000 0.000	0.284 0.678 0.284 0.284 0.678	V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386	V3 0.31 0.39 0.31 0.31 0.39	4 (6) 4 (7) 4 (8) 4 (4) 6 (4) 6 (4)	0.005 0.304 0.991 0.129 0.349
T O ATOM 5	R S I 1 TYPE 1 1 1 1 1 1	ES K 1 1 1 1 1	L 5 12 5 5 12 5 5	0 -20 0 100 0 -140 0 100 0 -140 0 -140 0 -140	ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000	 0.284 0.678 0.284 0.678 0.284 0.678	V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386	V3 0.314 0.399 0.314 0.399 0.314 0.399	4 (0 8 - (0 4 - (0 4 - (0 8 (0 4 (0 8 (0	0.005 0.304 0.991 0.129 0.349 0.129
T O ATOM I S 5 5 5 5 5 5 6 7 1 8 7 1 8 7 1 8 7 1 8 7 1 8 8 8 8 8 8 8 8 8 8 8 8	R S I 1 TYPE 1 1 1 1 1 1 1 1	I O N ES K 1 1 1 1 1	L 5 12 5 12 5 12 5 12 5 12	CLASS 0 -20 0 100 0 -140 0 100 0 -140 0 -20 0 -140 0 -20	ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000	0.284 0.678 0.284 0.284 0.678 0.284 0.678	V1 V21.386 -0.602 -1.386 -0.602 -1.386 -0.602	V3 0.31 0.39 0.31 0.39 0.31 0.39 0.39 0.39 0.39	4 (0 8 -0 4 -0 4 -0 8 (0 4 (0 8 (0 3 (0)	0.005 0.304 0.991 0.129 0.349 0.129
T O ATOM I S 5 5 5 5 5 5 12 12 12	R S I 1 TYPE J 1 1 1 1 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1	L 5 12 5 12 5 12 5 12 5 5 5	CLASS 0 -20 0 100 0 -140 0 100 0 -140 0 -20 0 -140 0 -20	ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	 0.284 0.678 0.284 0.678 0.284 0.678 0.000 0.678	V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 0.31 0.39 0.31 0.39 0.31 0.39 0.39 0.39 0.39	4 (0 8 -0 4 -0 4 -0 8 (0 4 (0 8 (0 3 (0)	0.005 0.304 0.991 0.129 0.349 0.129
T O ATOM I S 5 5 5 5 5 7 1 1 1 1 1 1 1 1 1 1 1 1	R S I 1 TYPE J 1 1 1 1 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1	L 5 12 5 12 5 12 5 12 5 5 5	CLASS 0 -20 0 100 0 -140 0 -140 0 -20 0 -140 0 -20 0 100	ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	 0.284 0.678 0.284 0.678 0.284 0.678 0.000 0.678	V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 0.31 0.39 0.31 0.39 0.31 0.39 0.39 0.39 0.39	4 (0 8 -0 4 -0 4 -0 8 (0 4 (0 8 (0 3 (0)	0.005 0.304 0.991 0.129 0.349 0.129
T O ATOM I S 5 5 5 5 5 12 12 12 12	R S I 1 TOTA	ES K 1 1 1 1 1 1 1 1 1 THE TOP	L 5 12 5 12 5 12 5 12 5 8 12 5	CLASS 0 -20 0 100 0 -140 0 -140 0 -20 0 -140 0 -20 0 100	ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	0.284 0.678 0.284 0.678 0.284 0.678 0.000 0.678 kcal/n	V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 0.31 0.39 0.31 0.39 0.31 0.39 0.39 0.39 0.39	4 (0 8 -0 4 -0 4 -0 8 (0 4 (0 8 (0 3 (0)	0.005 0.304 0.991 0.129 0.349 0.129
T O ATOM I S 5 5 5 5 5 5 12 12 12 12	R S I 1 TOTA	ES K 1 1 1 1 1 1 1 1 1 THE TOP	L 5 12 5 12 5 12 5 12 5 8 12 5	CLASS 0 -20 0 100 0 -140 0 -140 0 -20 0 -140 0 -20 0 -140 0 -20 0 100 CNERGY =	ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	0.284 0.678 0.284 0.678 0.284 0.678 0.000 0.678 kcal/n	V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 0.31 0.39 0.31 0.39 0.31 0.39 0.39 0.39 0.39	4 (0 8 -0 4 -0 4 -0 8 (0 4 (0 8 (0 3 (0)	0.005 0.304 0.991 0.129 0.349 0.129

	TAL OUT-OF-PI	LANE BENDIN	G ENERGY = (0.00000 kcal	./mol
V A N	DER WA	ALS			
ATOM TYP					
	Rij 		EPSILON	ENERGY	
			0.022	0.328	
			0.022		
			0.053		
5 5	2.638	3 2.970	0.022	0.001	
5 5	2.232	2.970	0.022	0.328	
5 12	3.399	3.713	0.053	-0.028	
12 5	3.399	3.713	0.053	-0.028	
12 5	3.129	3.713	0.053	0.104	
12 12	2.71	1 4.089	0.276	16.993	
TOT	TAL VAN DER 1	WAALS ENERG	Y = 17.78153	kcal/mol	
E L E C	T R O S T A	TICII	NTERAC	r I O N S	
ATOM TYP					
I J	Rij	Qi	Qj	ENERGY	
			-0.290		
TOT	TAL ELECTROS	PATIC ENERG	Y = 7.58721	kcal/mol	
MOMAT EN	VEDCV - 4F 20	2046 11/	-1		
TOTAL EN	NERGY = 45.38	3946 kcal/m	ol		
		3946 kcal/m	ol		
TOTAL EN		3946 kcal/m	ol		
		3946 kcal/m	ol		
ENER	G Y		ol		
ENER			ol		
E N E R B O N D	G Y	CHING			
E N E R B O N D	G Y S T R E T PES BOND	C H I N G		DELTA	ENERGY
ENER BOND ATOM TYPE I J	G Y S T R E T PES BOND	C H I N G	FORCE CONSTANT	DELTA	ENERGY
ENER BOND ATOM TYP	G Y S T R E T PES BOND LENGTH	C H I N G IDEAL LENGTH	FORCE CONSTANT		
ENER BOND ATOM TYP I J	G Y S T R E T PES BOND LENGTH	C H I N G IDEAL LENGTH 1.093	FORCE CONSTANT	-0.093	12.163
ENER BOND ATOM TYP I J	S T R E T PES BOND LENGTH 1.000 1.000	C H I N G IDEAL LENGTH 1.093	FORCE CONSTANT	-0.093 -0.093	12.163 12.163
ENER BOND ATOM TYP I J	S T R E T PES BOND LENGTH 1.000 1.000 1.540	CHING IDEAL LENGTH 1.093 1.093	FORCE CONSTANT 1406.346 1406.346	-0.093 -0.093 0.005	12.163 12.163 0.032
ENER BOND ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1	S T R E T PES BOND LENGTH 1.000 1.000 1.540 1.000	C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093	FORCE CONSTANT 1406.346 1406.346 1269.019	-0.093 -0.093 0.005 -0.093	12.163 12.163 0.032
E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1	S T R E T PES BOND LENGTH 1.000 1.000 1.540 1.000 1.670	C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346	-0.093 -0.093 0.005 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718
E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1	S T R E T PES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670	C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117	-0.093 -0.093 0.005 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718

I J K ANGLE ANGLE CONSTANT DELTA ENERGY 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 h1 109.442 109.550 164.039 -0.002 0.001 2 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 1 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.500 110.330 260.419 -0.002 0.001 3 c3 c1 109.500 110.330 260.419 -0.0014 0.055 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY	2	ATOM '	TYPE	S	VALE	ICE	IDEAL	FC	RCE			
1 c3 h1 109.442 109.550 164.039 -0.002 0.001 1 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 1 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.500 110.070 194.100 -0.010 0.019 2 c3 c1 109.442 105.930 183.005 0.061 0.688 2 c3 h1 109.442 109.550 164.039 -0.002 0.001 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688		I	J	K	ANGI	LΕ	ANGLE	CON	STANT	DEL'	га Е	NERGY
1 c3 h1 109.442 109.550 164.039 -0.002 0.001 1 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 1 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.500 110.070 194.100 -0.010 0.019 2 c3 c1 109.442 105.930 183.005 0.061 0.688 2 c3 h1 109.442 109.550 164.039 -0.002 0.001 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688												
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3 c3 h1 109.500 110.070 194.100 -0.010 0.019 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 1 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.500 110.070 194.100 -0.002 0.001 3 c3 c1 109.442 109.550 164.039 -0.002 0.001 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688		h1 c3	h1	109.	442	109.550		164.039	-	-0.002	0.001	
3 c3 cl 109.500 110.330 260.419 -0.014 0.055 1 c3 cl 109.442 105.930 183.005 0.061 0.688 3 c3 hl 109.500 110.070 194.100 -0.010 0.019 1 c3 cl 109.442 105.930 183.005 0.061 0.688 1 c3 hl 109.442 105.930 183.005 0.061 0.688 1 c3 hl 109.442 109.550 164.039 -0.002 0.001 3 c3 cl 109.500 110.330 260.419 -0.014 0.055 3 c3 hl 109.500 110.070 194.100 -0.010 0.019 1 c3 cl 109.442 105.930 183.005 0.061 0.688		h1 c3	cl									
1 c3 c1 109.442 105.930 183.005 0.061 0.688 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.442 109.550 164.039 -0.002 0.001 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY		c3 c3	h1	109.	500	110.070		194.100	-	-0.010	0.019	
3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 1 c3 h1 109.442 109.550 164.039 -0.002 0.001 3 c3 c1 109.500 110.330 260.419 -0.014 0.055 3 c3 h1 109.500 110.070 194.100 -0.010 0.019 1 c3 c1 109.442 105.930 183.005 0.061 0.688 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol ORSIONAL ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY 1 c3 c3 h1 0.651 0 -20.000 3 0.977 1 c3 c3 c1 0.000 0 100.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.651 0 -20.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.651 0 -20.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.651 0 -20.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.051 N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY												
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ORSIONAL ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY											0.000	
ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY			TOTA	יי בווטוי	רמאמר ב	THE CHEK	.01 –	2.930	NO / IIIC	/ 1		
ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY		TOR	ST	ONA	L							
I J K L CONSTANT S ANGLE N ENERGY			. I	, , , A	_							
I J K L CONSTANT S ANGLE N ENERGY		A'	TOM	TYPES-		FORCE			TORSIC	ON		
1 c3 c3 h1											ENERGY	
1 c3 c3 cl 0.000 0 100.000 3 0.000 1 c3 c3 hl 0.651 0 -140.000 3 0.977 1 c3 c3 hl 0.651 0 100.000 3 0.977 1 c3 c3 cl 0.000 0 -140.000 3 0.000 1 c3 c3 hl 0.651 0 -20.000 3 0.977 1 c3 c3 hl 0.651 0 0 0.000 3 0.977 1 c3 c3 hl 0.000 0 -140.000 3 0.000 1 c3 c3 hl 0.000 0 -20.000 3 0.000 1 c3 c3 hl 0.000 0 100.000 3 0.000 1 c3 c3 hl 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY												
1 c3 c3 h1 0.651 0 -140.000 3 0.977 1 c3 c3 h1 0.651 0 100.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.651 0 -20.000 3 0.977 1 c3 c3 h1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.000 0 -20.000 3 0.000 1 c3 c3 h1 0.000 0 100.000 3 0.000 1 c3 c3 h1 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY		h1 c3	c 3	h1	0.651		0 -	-20.000	3	0.977		
1 c3 c3 h1 0.651 0 100.000 3 0.977 1 c3 c3 c1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.651 0 -20.000 3 0.977 1 c3 c3 h1 0.000 0 -140.000 3 0.000 1 c3 c3 h1 0.000 0 -20.000 3 0.000 1 c3 c3 c1 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY		h1 c3	c 3	cl	0.000		0	100.000	3	0.000		
1 c3 c3 cl 0.000 0 -140.000 3 0.000 1 c3 c3 hl 0.651 0 -20.000 3 0.977 1 c3 c3 hl 0.000 0 -140.000 3 0.000 1 c3 c3 cl 0.000 0 -20.000 3 0.000 1 c3 c3 hl 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY		h1 c3	c 3	h1	0.651		0 -	140.000	3	0.977		
1 c3 c3 h1 0.651 0 -20.000 3 0.977 1 c3 c3 h1 0.000 0 -140.000 3 0.000 1 c3 c3 c1 0.000 0 -20.000 3 0.000 1 c3 c3 h1 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY		h1 c3	c 3	h1	0.651		0 :	100.000	3	0.977		
1 c3 c3 h1 0.000 0 -140.000 3 0.000 1 c3 c3 c1 0.000 0 -20.000 3 0.000 1 c3 c3 h1 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY		h1 c3	c 3	cl	0.000		0 -	140.000	3	0.000		
l c3 c3 cl 0.000 0 -20.000 3 0.000 l c3 c3 hl 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT s ANGLE n ENERGY		h1 c3	c 3	h1	0.651		0 -	-20.000	3	0.977		
1 c3 c3 h1 0.000 0 100.000 3 0.000 TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT s ANGLE n ENERGY		cl c3	c 3	h1	0.000		0 -	140.000	3	0.000		
TOTAL TORSIONAL ENERGY = 3.908 kJ/mol M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY		cl c3	c3	cl	0.000		0 -	-20.000	3	0.000		
MPROPER TORSIONAL ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY		cl c3	c3	h1	0.000		0	100.000	3	0.000		
ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT s ANGLE n ENERGY			TOTA	L TORS	IONAL E	ENERGY =	3	.908 kJ/	mol			
ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT s ANGLE n ENERGY												
I J K L CONSTANT s ANGLE n ENERGY		I M P	R O	PER	ТО	R S I O	N A I	L				
I J K L CONSTANT s ANGLE n ENERGY												
			IOTA	THEK	OFER-I(MOTONAL	писк(31 -	0.000	VO / IIIOT		
TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol		77 7\ NT	D	FD	Ta7 7\ 7\	T. C						
		V A IV	D	, r. K	WAA	цъ						
TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol A N D E R W A A L S		ΣπОм	TVDE	25								
AN DER WAALS					Rii	kii		ENERGV				
TAN DER WAALS												
AN DER WAALS TOM TYPES I J Rij kij ENERGY												
TAN DER WAALS TOM TYPES I J Rij kij ENERGY												
TAN DER WAALS TOM TYPES I J Rij kij ENERGY												
TOM TYPES I J Rij kij ENERGY												
TAN DER WAALS TOM TYPES I J Rij kij ENERGY				2,00	-							

```
4891 h1 h1 2.232 0.205
4892 h1 cl
            3.399
                    -0.133
4893 cl h1
            3.399 -0.133
4894 cl h1
             3.129 -0.106
             2.711
4895 cl cl
                    33.340
     TOTAL VAN DER WAALS ENERGY = 33.209 kJ/mol
4896
4897
4898 ELECTROSTATIC INTERACTIONS
4899
4900 ATOM TYPES
4901
    I J
                Rij 332.17*QiQj ENERGY
4902
             2.232
4903 h1 h1
                    1.352
                             0.606
4904 h1 h1
            2.831
                    1.352
                            0.478
            3.129 -3.809 -1.217
4905 h1 cl
4906 h1 h1
            2.638
                    1.352
                            0.513
4907 h1 h1
            2.232
                    1.352
                            0.606
            3.399 -3.809 -1.121
4908 h1 cl
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
     TOTAL ELECTROSTATIC ENERGY = 1.484 kJ/mol
4912
4913
4914 TOTAL ENERGY = 121.662 kJ/mol
4915
4916 ATOM TYPES
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 FORMAL CHARGES
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 PARTIAL CHARGES
4941
4942 IDX CHARGE
4943 1 0.290000
     2 0.290000
4944
4945 3 0.000000
4946
     4 0.000000
4947
     5 -0.290000
     6 0.000000
4948
4949 7 0.000000
4950
     8 -0.290000
4951
     SETTING UP CALCULATIONS
4952
4953
4954
     SETTING UP BOND CALCULATIONS...
4955 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4956
     SETTING UP TORSION CALCULATIONS...
     SETTING UP OOP CALCULATIONS...
4957
     SETTING UP VAN DER WAALS CALCULATIONS...
4958
4959
     SETTING UP ELECTROSTATIC CALCULATIONS...
4960
     ATOM TYPES
4961
4962
     IDX TYPE RING
4963
4964 1 c3 NO
     2 c3 NO
4965
     3 h1 NO
4966
4967
     4 h1 NO
     5 cl NO
4968
4969
     6 hl NO
4970
     7 h1 NO
4971
     8 cl NO
4972
4973
     CHARGES
4974
4975
     IDX CHARGE
4976
     1 0.036009
     2 0.036009
4977
4978
     3 0.044101
     4 0.044101
4979
     5 -0.124211
4980
4981 6 0.044101
4982 7 0.044101
4983
     8 -0.124211
4984
4985
     SETTING UP CALCULATIONS
4986
     SETTING UP BOND CALCULATIONS...
4987
4988
     SETTING UP ANGLE CALCULATIONS...
```

```
4989 SETTING UP TORSION CALCULATIONS...
    SETTING UP IMPROPER TORSION CALCULATIONS...
4990
    SETTING UP VAN DER WAALS CALCULATIONS...
4991
4992
    SETTING UP ELECTROSTATIC CALCULATIONS...
4993
4994
    ENERGY
4995
4996
    BOND STRETCHING
4997
4998
4999
    ATOM TYPES FF BOND
                         IDEAL
                                  FORCE
                         LENGTH
                                 CONSTANT
           CLASS LENGTH
5000
       J
                                           DELTA
5001
5002
     5
        1
              0
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                     3.578
        1
             0
                  1.000
                          1.093
                                   4.766
                                           -0.093
5003
     5
                                                     3.578
                                            0.032
5004
    1
        1
             0
                  1.540
                          1.508
                                   4.258
                                                    0.294
    1 5
5005
             0
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                    3.578
                  1.670
5006
      12
             0
                          1.773
                                    2.974
                                           -0.103
                                                    2.795
     1
    1 5
5007
              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
    ANGLE BENDING
5012
5013
    ATOM TYPES
                 FF VALENCE
                              IDEAL
                                      FORCE
5014
    I J K
               CLASS ANGLE
                              ANGLE CONSTANT
                                               DELTA
                                                       ENERGY
5015
    ______
5016
            5
                     109.500
                            110.549
                                        0.636
                                                -1.049
                                                        0.015
        1 5
                 0 109.442 108.836
                                       0.516
5017
    5
                                               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
                 0 109.500 108.679
5020
    1
        1 12
                                        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
                 0 109.442 108.836
5023
    5
        1 5
                                        0.516
                                               0.606
                                                        0.004
                                       0.698
                                                1.280
5024
     5
        1 12
                 0 109.442
                            108.162
                                                        0.025
           5
5025
                    109.500
                            110.549
                                        0.636
                                               -1.049
                                                        0.015
     1
        1
                 0
                    109.500 108.679
        1 12
                 0
                                        1.056
5026
    1
                                               0.821
                                                        0.016
5027
        1 12
                 0
                    109.442
                            108.162
                                       0.698
                                                1.280
                                                       0.025
5028
       TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
5029
5030
    STRETCH BENDING
5031
    ATOM TYPES FF VALENCE DELTA FORCE CONSTANT
5032
               CLASS ANGLE
5033
    I J K
                                       ΙJ
                                               JК
                              ANGLE
                                                      ENERGY
5034
                                      0.227
                                              0.070
5035
     1
        1 5
                0 109.500 -1.049
                                                     -0.002
                 0 109.442
                              0.606
                                      0.115
5036
    5
           5
                                              0.115
        1
                                                      -0.033
5037
     5 1 12
                0 109.442 1.280 -0.018 0.380
                                                      -0.121
```

038	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
039	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
040	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
041	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
)42	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
043	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
)44	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
)45	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
046	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
)47		TOTA	L STR	RETCH BEN	DING ENERGY	r = -0.6959	3 kcal/mol		
)48									
)49	Т О	RSI	O N	A L					
)50									
)51	ATOM	TYPE	S		FF TOF	RSION	FORCE CON	STANT	
)52	I	J	K	L	CLASS AN	IGLE	V1 V2	V3 ENE	RGY
)53									
54	5	1	1	5	0 0.0	0.28	4 -1.386	0.314	0.598
55	5	1	1	5	0 -120.0	0.28	4 -1.386	0.314	-0.655
56	5	1	1	12	0 120.0	0.67	8 -0.602	0.398	0.116
)57	5	1	1	5	0 120.0	0.28	4 -1.386	0.314	-0.655
)58	5	1	1	5	0.0	0.28	4 -1.386	0.314	0.598
)59	5	1	1	12	0 -120.0	0.67	8 -0.602	0.398	0.116
060	12	1	1	5	0 -120.0	0.67	8 -0.602	0.398	0.116
61	12	1	1	5	0 120.0	0.67	8 -0.602	0.398	0.116
62	12	1	1	12	0 -0.0	0.00	0.000	0.893	0.893
)63		TOTA	L TOR	RSIONAL E	NERGY = 1.	24400 kcal	/mol		
064									
)65	OU	Т – О	F -	PLAN	E BEND) I N G			
)66									
		TYPE			FF C				
					CLASS AN		TANT E	NERGY	
)69									
70		TOTA	L OUI	-OF-PLAN	E BENDING E	NERGY = 0	.00000 kca	1/mol	
71					T 0				
	VA.	N D	ER	WAA	L S				
73	3 most		a						
		TYPE			D.1.T.T.				
					R*IJ		ENERGY		
76									
		5			2.970				
		5			2.970				
79	5				3.713				
		5			2.970				
	5				2.970				
082	5				3.713				
083		5			3.713				
084		5			3.713				
085	12	12			4.089 LS ENERGY =	0.276			

```
5087
    ELECTROSTATIC INTERACTIONS
5088
5089
5090 ATOM TYPES
5091
    I J
             Rij Qi Qj ENERGY
5092
    ______
    12 12 2.705 -0.290 -0.290
5093
                                  7.743
       TOTAL ELECTROSTATIC ENERGY = 7.74347 kcal/mol
5094
5095
5096 TOTAL ENERGY = 50.10353 kcal/mol
5097
5098
    ENERGY
5099
5100
5101 BOND STRETCHING
5102
5103 ATOM TYPES BOND
                   IDEAL
                            FORCE
                   LENGTH CONSTANT DELTA ENERGY
    I J
5104
           LENGTH
5105 | -----
5106 h1 c3
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
                                          12.163
5107 h1 c3
          1.000
                  1.093
                         1406.346
                                  -0.093
          1.540
                  1.535
                         1269.019
                                   0.005
                                           0.032
5108 c3 c3
5109 c3 h1
          1.000
                  1.093
                                          12.163
                         1406.346
                                  -0.093
5110 c3 cl
          1.670
                  1.786
                         1168.117
                                  -0.116
                                          15.718
5111 c3 h1
          1.000
                  1.093
                         1406.346
                                   -0.093
                                          12.163
5112 c3 c1 1.670 1.786 1168.117 -0.116 15.718
    TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
5113
5114
5115 ANGLE BENDING
5116
                        IDEAL
5117 ATOM TYPES
               VALENCE
                               FORCE
                ANGLE ANGLE
                               CONSTANT DELTA ENERGY
5118
    I J K
5119
5120 c3 c3 h1 109.500
                   110.070
                            194.100
                                     -0.010
                                             0.019
5121 h1 c3 h1 109.442 109.550
                            164.039 -0.002
                                             0.001
5122 h1 c3 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
5123 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                             0.019
                            260.419
5124 c3 c3 cl 109.500 110.330
                                     -0.014
                                             0.055
                                     0.061
5125 h1 c3 cl 109.442
                   105.930
                            183.005
                                             0.688
5126 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                             0.019
           109.442 109.550
                            164.039
                                     -0.002
5127 h1 c3 h1
                                             0.001
5128 h1 c3 cl 109.442
                   105.930
                            183.005
                                     0.061
                                             0.688
    c3 c3 h1 109.500 110.070
5129
                            194.100
                                     -0.010
                                             0.019
                                     -0.014
    c3 c3 cl 109.500 110.330
                            260.419
5130
                                             0.055
5131 h1 c3 cl 109.442
                            183.005
                                     0.061
                   105.930
                                             0.688
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
5132
5133
5134 TORSIONAL
5135
```

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

```
5185 cl h1 3.280 -3.809 -1.161

5186 cl cl 2.655 10.728 4.041

5187 TOTAL ELECTROSTATIC ENERGY = 1.607 kJ/mol

5188

5189 TOTAL ENERGY = 134.023 kJ/mol
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