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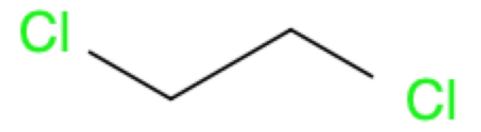
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BIM2005: Homework I

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

Preparation

• Structure of $C_2H_4Cl_2$ (For reference)



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

```
1
2
 3
   C2H4Cl2
4
5
   0 1
 6
 7
    C 1 1.54
    н 1 1.0 2 109.5
 8
9
     Н 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/BIM2005-HWK1</u> (github.com).

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

- 1. We added the headers to the code manually for it to be recognised by OpenBabel
- 2. We modify the code in order to change $\tau(Cl^8-C^2-C^1-Cl^5)$ by $20\times N^\circ$. (As the reference plane, which is the 2-1-5 plane, is the same for the last three definitions of atoms, we only need to change the dihedral angles of the last three lines by an increment of 20° .)
- 3. We convert the code from the .gzmat format to the .xyz. one via <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 <u>Seaborn</u>. For details, please refer to <u>Result III</u>

GitHub Repo File Hierarchy

```
1
 2
      - C2H4Cl2_structure.png
                                       // the 2D molecule structure overview
 3
    CODE
                                       // the directory containing all the .xyz and
    .gzmat file
 4
        — C2H4Cl2 0 degrees.gzmat
 5
          - C2H4Cl2 0 degrees.xyz
          — C2H4Cl2 100 degrees.gzmat
 6
 7
          — C2H4Cl2_100_degrees.xyz
          - C2H4Cl2_120_degrees.gzmat
 8
9
         C2H4Cl2_120_degrees.xyz
          — C2H4Cl2_140_degrees.gzmat
10
          - C2H4Cl2 140 degrees.xyz
11
          — C2H4Cl2 160 degrees.gzmat
12
13
          - C2H4Cl2 160 degrees.xyz
          — C2H4Cl2_180_degrees.gzmat
14
15
          — C2H4Cl2_180_degrees.xyz
          — C2H4Cl2_200_degrees.gzmat
16
          — C2H4Cl2_200_degrees.xyz
17
18
          — C2H4Cl2_20_degrees.gzmat
          - C2H4Cl2 20 degrees.xyz
19
          - C2H4Cl2 220 degrees.gzmat
20
          - C2H4Cl2_220_degrees.xyz
21
           - C2H4Cl2_240_degrees.gzmat
22
```

```
23
         - C2H4Cl2 240 degrees.xyz
24
          - C2H4Cl2 260 degrees.gzmat
2.5
          - C2H4Cl2 260 degrees.xyz
26
        — C2H4Cl2 280 degrees.gzmat
2.7
         — C2H4Cl2_280_degrees.xyz
          — C2H4Cl2_300_degrees.gzmat
28
29
        C2H4Cl2_300_degrees.xyz
          — C2H4Cl2_320_degrees.gzmat
30
         — C2H4Cl2 320 degrees.xyz
31
         — C2H4Cl2_340_degrees.gzmat
32
          - C2H4Cl2 340 degrees.xyz
33
34
        — C2H4Cl2_360_degrees.gzmat
35
         — C2H4Cl2_360_degrees.xyz
          — C2H4Cl2_40_degrees.gzmat
36
         — C2H4Cl2 40 degrees.xyz
37
          — C2H4Cl2_60_degrees.gzmat
38
        — C2H4Cl2 60 degrees.xyz
39
40
         — C2H4Cl2_80_degrees.gzmat
        C2H4Cl2_80_degrees.xyz
41
42
    — DATA
                                        // .csv table file containing all the energy
    data
       — data.csv
43
          data in KJ.csv
44
        ___ data_in_Kcal.csv
45
     — README.md
                                       // This file you are in
47
     — XYZ_GAMAT_SUMMARY.md
                                       // (Not Important)
48
    - code2mkdoc.py
                                       // The script used to facilitate the processing
    of the documentation
     — 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
51
     — rel_energy.png
                                      // Lineplot of the relative energy in kcal/mol
52
    torsion_angle.py
                                     // The main program to process the molecule
53
54
    2 directories, 49 files
```

Results

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

Torsion Angle at $0\,^\circ$

• ./CODE/C2H4Cl2_0_degrees.gzmat

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

• ./CODE/C2H4Cl2_0_degrees.xyz

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

Torsion Angle at $20\,^\circ$

• ./CODE/C2H4Cl2_20_degrees.gzmat

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

./CODE/C2H4Cl2_20_degrees.xyz

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

Torsion Angle at $40\,^\circ$

./CODE/C2H4Cl2_40_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-40-degrees
 5
   0 1
 6
 7
   C 1 1.54
 8
    H 1 1.0 2 109.5
9
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 -80.0
13 H 2 1.0 1 109.5 5 160.0
   Cl 2 1.67 1 109.5 5 40.0
14
15
16
```

• ./CODE/C2H4Cl2_40_degrees.xyz

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

Torsion Angle at $60\,^\circ$

• ./CODE/C2H4Cl2_60_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-60-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 -60.0
   н 2 1.0 1 109.5 5 180.0
13
14
   Cl 2 1.67 1 109.5 5 60.0
15
16
```

• ./CODE/C2H4Cl2_60_degrees.xyz

```
1
   8
   ./CODE/C2H4Cl2_60_degrees.gzmat
2
           0.00000
                        0.00000
                                      0.00000
3
                        0.00000
4
           1.54000
                                      0.00000
5
  Н
           -0.33381
                        0.0000
                                     -0.94264
                       -0.81635
6
  H
           -0.33381
                                     0.47132
          -0.55746
7
                        1.36331
                                     0.78711
           1.87381
                        0.81635
                                     -0.47132
8
  Η
           1.87381
                       -0.81635
                                     -0.47132
9
           2.09746 -0.00000
   Cl
                                     1.57421
10
11
```

Torsion Angle at $80\,^\circ$

• ./CODE/C2H4Cl2_80_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-80-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```
10 H 1 1.0 2 109.5 3 120.0

11 Cl 1 1.67 2 109.5 4 120.0

12 H 2 1.0 1 109.5 5 -40.0

13 H 2 1.0 1 109.5 5 200.0

14 Cl 2 1.67 1 109.5 5 80.0
```

./CODE/C2H4Cl2_80_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 80 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
                         -0.81635
            -0.33381
                                        0.47132
6
7
           -0.55746
                         1.36331
                                        0.78711
   Cl
            1.87381
                          0.92832
                                       -0.16369
8
   Η
9
            1.87381
                         -0.60592
                                       -0.72211
            2.09746
10
  Cl
                         -0.53841
                                        1.47927
11
```

Torsion Angle at $100\,^\circ$

• ./CODE/C2H4Cl2_100_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-100-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 -20.0
12
13 H 2 1.0 1 109.5 5 220.0
   Cl 2 1.67 1 109.5 5 100.0
14
15
16
```

• ./CODE/C2H4Cl2_100_degrees.xyz

```
1
    8
 2
    ./CODE/C2H4Cl2_100_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
                              0.92832
 8
                                                0.16369
9
    Η
               1.87381
                              -0.32240
                                               -0.88579
    Cl
                2.09746
                              -1.01188
                                                1.20592
10
11
```

Torsion Angle at $120\,^\circ$

• ./CODE/C2H4Cl2_120_degrees.gzmat

```
1
 2
 3
 4
    C2H4Cl2-120-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
11
    Cl 1 1.67 2 109.5 4 120.0
12
    н 2 1.0 1 109.5 5 0.0
    н 2 1.0 1 109.5 5 240.0
13
14
    Cl 2 1.67 1 109.5 5 120.0
15
16
```

• ./CODE/C2H4Cl2_120_degrees.xyz

```
8
 1
    ./CODE/C2H4Cl2_120_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
                               0.00000
                                               -0.94264
 9
               1.87381
                2.09746
                              -1.36331
                                                0.78711
10
    Cl
11
```

Torsion Angle at $140\,^\circ$

• ./CODE/C2H4Cl2_140_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-140-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 20.0
   н 2 1.0 1 109.5 5 260.0
13
14
   Cl 2 1.67 1 109.5 5 140.0
15
16
```

• ./CODE/C2H4Cl2_140_degrees.xyz

```
1
   8
   ./CODE/C2H4Cl2_140_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
                        1.36331
7
                                      0.78711
           1.87381
8
   H
                        0.60592
                                      0.72211
           1.87381
                        0.32240
                                     -0.88579
9
           2.09746 -1.55030
   Cl
                                      0.27336
10
11
```

Torsion Angle at $160\,^\circ$

• ./CODE/C2H4Cl2_160_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-160-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```
10 H 1 1.0 2 109.5 3 120.0

11 Cl 1 1.67 2 109.5 4 120.0

12 H 2 1.0 1 109.5 5 40.0

13 H 2 1.0 1 109.5 5 280.0

14 Cl 2 1.67 1 109.5 5 160.0
```

./CODE/C2H4Cl2_160_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 160 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
                         -0.81635
            -0.33381
                                        0.47132
6
7
           -0.55746
   Cl
                         1.36331
                                        0.78711
                          0.32240
                                        0.88579
8
   Η
            1.87381
9
            1.87381
                          0.60592
                                       -0.72211
10
  Cl
            2.09746
                        -1.55030
                                       -0.27336
11
```

Torsion Angle at $180\,^\circ$

• ./CODE/C2H4Cl2_180_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-180-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
   н 2 1.0 1 109.5 5 60.0
12
13 H 2 1.0 1 109.5 5 300.0
   Cl 2 1.67 1 109.5 5 180.0
14
15
16
```

• ./CODE/C2H4Cl2_180_degrees.xyz

```
1
    8
 2
    ./CODE/C2H4Cl2_180_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
                              -0.00000
                                               0.94264
 8
9
    Η
               1.87381
                               0.81635
                                              -0.47132
    Cl
                2.09746
                              -1.36331
                                              -0.78711
10
11
```

Torsion Angle at $200\,^\circ$

• ./CODE/C2H4Cl2_200_degrees.gzmat

```
1
 2
 3
 4
    C2H4Cl2-200-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
11
    Cl 1 1.67 2 109.5 4 120.0
12
    н 2 1.0 1 109.5 5 80.0
    н 2 1.0 1 109.5 5 320.0
13
14
    Cl 2 1.67 1 109.5 5 200.0
15
16
```

• ./CODE/C2H4Cl2_200_degrees.xyz

```
8
 1
    ./CODE/C2H4Cl2_200_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
                               0.92832
                                              -0.16369
 9
               1.87381
                2.09746
                              -1.01188
                                              -1.20592
10
    Cl
11
```

Torsion Angle at $220\,^\circ$

• ./CODE/C2H4Cl2_220_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-220-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 5 340.0
13
14
   Cl 2 1.67 1 109.5 5 220.0
15
16
```

• ./CODE/C2H4Cl2_220_degrees.xyz

```
8
1
  ./CODE/C2H4Cl2_220_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
                                    0.72211
           1.87381
                       -0.60592
8
  H
           1.87381
                       0.92832
                                    0.16369
9
          2.09746 -0.53841
   Cl
                                    -1.47927
10
11
```

Torsion Angle at $240\,^\circ$

• ./CODE/C2H4Cl2_240_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-240-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```
10 H 1 1.0 2 109.5 3 120.0

11 Cl 1 1.67 2 109.5 4 120.0

12 H 2 1.0 1 109.5 5 120.0

13 H 2 1.0 1 109.5 5 0.0

14 Cl 2 1.67 1 109.5 5 240.0
```

./CODE/C2H4Cl2_240_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 240 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
                         -0.81635
                                         0.47132
8
   Η
            1.87381
9
            1.87381
                          0.81635
                                         0.47132
                          0.00000
10
  Cl
            2.09746
                                        -1.57421
11
```

Torsion Angle at $260\,^\circ$

• ./CODE/C2H4Cl2_260_degrees.gzmat

```
1
 2
   #
 3
 4
   C2H4Cl2-260-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 5 140.0
12
13 H 2 1.0 1 109.5 5 20.0
   Cl 2 1.67 1 109.5 5 260.0
14
15
16
```

• ./CODE/C2H4Cl2_260_degrees.xyz

```
1
    8
 2
    ./CODE/C2H4Cl2_260_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
                              -0.92832
 8
               1.87381
                                                0.16369
9
    Η
               1.87381
                               0.60592
                                               0.72211
    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
    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 5 160.0
    н 2 1.0 1 109.5 5 40.0
13
14
    Cl 2 1.67 1 109.5 5 280.0
15
16
```

• ./CODE/C2H4Cl2_280_degrees.xyz

```
8
 1
    ./CODE/C2H4Cl2_280_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
                              -0.92832
 8
               1.87381
                                              -0.16369
    Η
                               0.32240
                                               0.88579
 9
               1.87381
                2.09746
                               1.01188
                                              -1.20592
10
    Cl
11
```

Torsion Angle at $300\,^\circ$

• ./CODE/C2H4Cl2_300_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-300-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 5 180.0
   н 2 1.0 1 109.5 5 60.0
13
14
   Cl 2 1.67 1 109.5 5 300.0
15
16
```

• ./CODE/C2H4Cl2_300_degrees.xyz

```
1
   8
   ./CODE/C2H4Cl2_300_degrees.gzmat
2
           0.00000
                        0.00000
                                      0.00000
3
                        0.00000
4
           1.54000
                                      0.00000
5
  Н
           -0.33381
                        0.0000
                                     -0.94264
                       -0.81635
6
  H
           -0.33381
                                     0.47132
          -0.55746
                        1.36331
7
                                     0.78711
           1.87381
                        -0.81635
8
  Η
                                     -0.47132
           1.87381
                        -0.00000
                                     0.94264
9
                        1.36331
   Cl
           2.09746
                                     -0.78711
10
11
```

Torsion Angle at $320\,^\circ$

• ./CODE/C2H4Cl2_320_degrees.gzmat

```
1
2 #
3
4 C2H4Cl2-320-degrees
5
6 0 1
7 C
8 C 1 1.54
9 H 1 1.0 2 109.5
```

```
10 H 1 1.0 2 109.5 3 120.0

11 Cl 1 1.67 2 109.5 4 120.0

12 H 2 1.0 1 109.5 5 200.0

13 H 2 1.0 1 109.5 5 80.0

14 Cl 2 1.67 1 109.5 5 320.0
```

./CODE/C2H4Cl2_320_degrees.xyz

```
1
   8
2
   ./CODE/C2H4Cl2 320 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
                         -0.60592
                                       -0.72211
8
   Η
            1.87381
                        -0.32240
9
            1.87381
                                        0.88579
            2.09746
10
  Cl
                         1.55030
                                       -0.27336
11
```

Torsion Angle at $340\,^\circ$

• ./CODE/C2H4Cl2_340_degrees.gzmat

```
1
 2
 3
 4
   C2H4Cl2-340-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 5 220.0
13 H 2 1.0 1 109.5 5 100.0
   Cl 2 1.67 1 109.5 5 340.0
14
15
16
```

• ./CODE/C2H4Cl2_340_degrees.xyz

```
1
    8
 2
    ./CODE/C2H4Cl2_340_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
                              -0.32240
                                              -0.88579
 8
9
    Η
               1.87381
                              -0.60592
                                                0.72211
    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
    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 5 240.0
    н 2 1.0 1 109.5 5 120.0
13
14
    Cl 2 1.67 1 109.5 5 0.0
15
16
```

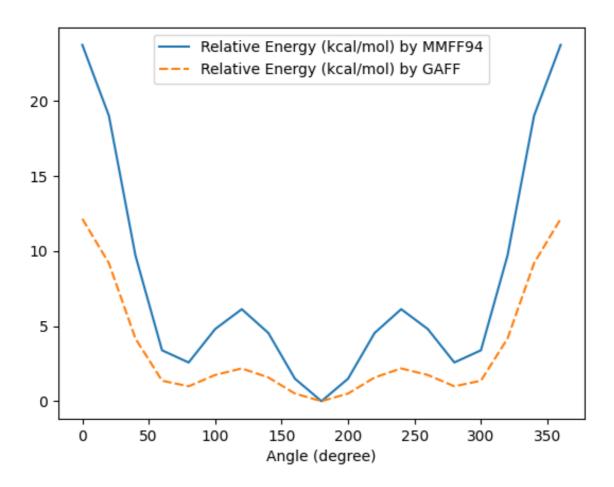
• ./CODE/C2H4Cl2_360_degrees.xyz

```
8
 1
    ./CODE/C2H4Cl2_360_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
                               0.00000
                                               -0.94264
    Η
                               -0.81635
                                                0.47132
 9
               1.87381
                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

```
1
    # This the main program to process the molecule.
 2
 3
    from openbabel import openbabel
    import numpy as np
 5
    import pandas as pd
    import seaborn as sns
7
    import matplotlib.pyplot as plt
8
9
    # Set the constant used to convert kCal/mol to kJ/mol
10
    KCAL2KJ_CONSTANT = 4.184
11
12
    \# The C2H4Cl2 molecule with the torsion angle at 0 degree
13
    gzmat code = """
14
15
    C2H4C12
16
17
```

```
18
    0 1
19
20
   C 1 1.54
   H 1 1.0 2 109.5
21
   н 1 1.0 2 109.5 3 120.0
22
23
    Cl 1 1.67 2 109.5 4 120.0
24
   H 2 1.0 1 109.5 5 -120.0
   H 2 1.0 1 109.5 5 120.0
2.5
    Cl 2 1.67 1 109.5 5 0.0
26
27
28
29
    # Store the code of the 18 modified molecules as a list
30
    code_list = []
31
    for n in range(0, 19):
32
        \# Count the reference number of the atoms to determine which atom to
33
    manipulate
34
        atom_counter = 0
35
36
        # .xyz code after conversion
        code_aft_cnv = ""
37
        for line in gzmat code.split("\n"):
38
            words = line.split()
39
40
41
            # if the line is empty, do not make modifications
42
            if len(words) == 0:
43
                pass
44
            # if the title is met, rename the title to mark it with the torsion angle
45
46
            elif line.startswith("C2H4Cl2"):
47
                words.append(str(20 * n))
48
                words.append("degrees")
49
                code_aft_cnv = code_aft_cnv + "-".join(words) + "\n"
50
                continue
51
            elif words[0].isalpha() and len(words[0]) in [1, 2]:
52
5.3
                atom_counter = atom_counter + 1
54
                if atom_counter in [6, 7, 8]:
55
56
57
                    words[-1] = str(float(words[-1]) + 20 * n)
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
    # Write the code to the .gzmat format
64
    for code, angle in zip(code_list, range(0, 380, 20)):
```

```
66
         with open(f"./CODE/C2H4Cl2 {angle} degrees.gzmat", "w") as gzmat file:
 67
             gzmat file.write(code)
 68
 69
     # Set the input format to gzmat and the output format to xyz
 70
     OB_converter = openbabel.OBConversion()
 71
     OB converter.SetInAndOutFormats("gzmat", "xyz")
 72
 73
     MMFF94_abs_energy_in_Kcal_list = []
 74
     GAFF abs energy in KJ list = []
 75
     # Convert the .gzmat files to .xyz file via OpenBabel
 76
     for angle in range(0, 380, 20):
 77
 78
         mol_C2H4Cl2 = openbabel.OBMol()
 79
         # Use MMFF94 and GAFF to calculate the absolute energy
 80
         OB_converter.ReadFile(mol_C2H4Cl2, f"./CODE/C2H4Cl2_{angle}_degrees.gzmat")
 81
 82
 83
         MMFF94 forcefield = openbabel.OBForceField.FindForceField("MMFF94")
         GAFF forcefield = openbabel.OBForceField.FindForceField("GAFF")
 84
 85
         # Redirect the log output to std::cout
 86
         MMFF94 forcefield.SetLogToStdOut()
 87
         GAFF forcefield.SetLogToStdOut()
 88
 89
         # Set the priority of log to high
 90
 91
         MMFF94_forcefield.SetLogLevel(openbabel.OBFF_LOGLVL_HIGH)
         GAFF forcefield.SetLogLevel(openbabel.OBFF LOGLVL HIGH)
 92
 93
         # Specify the molecule we calculate the energy of
 94
 95
         MMFF94 forcefield.Setup(mol C2H4Cl2)
 96
         GAFF forcefield.Setup(mol C2H4Cl2)
 97
98
         # Energy of C 2H 4Cl 2 with Torsion Angle at `angle` Degrees Starts
99
         # by MMFF94
100
         MMFF94 abs energy in Kcal = MMFF94 forcefield.Energy()
         # by GAFF
101
102
         GAFF_abs_energy_in_KJ = GAFF_forcefield.Energy()
103
104
         MMFF94_abs_energy_in_Kcal_list.append(MMFF94_abs_energy_in_Kcal)
105
         GAFF_abs_energy_in_KJ_list.append(GAFF_abs_energy_in_KJ)
106
107
         OB_converter.WriteFile(mol_C2H4Cl2, f"./CODE/C2H4Cl2_{angle}_degrees.xyz")
108
109
     # Construct a table containing the information required by the question
     ref MMFF94 energy in Kcal = min(MMFF94 abs energy in Kcal list)
110
     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)
     GAFF_abs_energy_in_KJ_vec = np.array(GAFF_abs_energy_in_KJ_list)
114
```

```
115
116
     MMFF94_abs_energy_in_KJ_vec = KCAL2KJ_CONSTANT * MMFF94_abs_energy_in_Kcal_vec
117
     GAFF abs energy in Kcal vec = GAFF abs energy in KJ vec / KCAL2KJ CONSTANT
118
119
     MMFF94_rel_energy_in_Kcal_vec = MMFF94_abs_energy_in_Kcal_vec -
     ref MMFF94 energy in Kcal
120
     GAFF_rel_energy_in_KJ_vec = GAFF_abs_energy_in_KJ_vec - ref_GAFF_energy_in_KJ
121
122
     MMFF94 rel energy in KJ vec = MMFF94 abs energy in KJ vec - KCAL2KJ CONSTANT *
     ref_MMFF94_energy_in_Kcal
     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 = {
         "Absolute Energy (kcal/mol) by MMFF94" :
126
     MMFF94_abs_energy_in_Kcal_vec.tolist(),
         "Absolute Energy (kcal/mol) by GAFF" : GAFF abs energy in Kcal vec.tolist(),
127
128
         "Relative Energy (kcal/mol) by MMFF94" :
     MMFF94 rel energy in Kcal vec.tolist(),
129
         "Relative Energy (kcal/mol) by GAFF" : GAFF_rel_energy_in_Kcal_vec.tolist()
130
     data in KJ dict = {
131
         "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(),
135
         "Relative Energy (kJ/mol) by GAFF" : GAFF_rel_energy_in_KJ_vec.tolist()
136
137
     data_in_Kcal_df = pd.DataFrame(data_in_Kcal_dict,index=[angle for angle in
138
     range(0, 380, 20)])
139
     data in KJ df = pd.DataFrame(data in KJ dict,index=[angle for angle in range(0,
     380, 20)])
140
141
     data_in_Kcal_df.to_csv("./DATA/data_in_Kcal.csv")
142
     data_in_KJ_df.to_csv("./DATA/data_in_KJ.csv")
143
144
     data dict = {
         "Absolute Energy (kcal/mol) by MMFF94":
145
     np.round(MMFF94_abs_energy_in_Kcal_vec.tolist(), 3),
146
         "Absolute Energy (kcal/mol) by GAFF":
     np.round(GAFF abs energy in Kcal vec.tolist(), 3),
147
         "Relative Energy (kcal/mol) by MMFF94":
     np.round(MMFF94 rel energy in Kcal vec.tolist(), 3),
         "Relative Energy (kcal/mol) by GAFF":
148
     np.round(GAFF rel energy in Kcal vec.tolist(), 3),
         "Absolute Energy (kJ/mol) by MMFF94":
149
     np.round(MMFF94_abs_energy_in_KJ_vec.tolist(), 3),
150
         "Absolute Energy (kJ/mol) by GAFF":
     np.round(GAFF_abs_energy_in_KJ_vec.tolist(), 3),
```

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

code2mkdoc.py

```
# This script aims to facilitate the gerneration of the documentation
 2
   # which is not part of the main program.
   # For the homework solution,
 3
   # pls refer to torsion angle.py
 4
5
   import sys
 6
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
    # Wrap the code to make it be recognised by the Markdown parser
14
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:
2.1
        for angle in range(0, 380, 20):
22
23
            mkdoc heading(f"Torsion Angle at {angle}$\degree$", level= 4)
24
            print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.gzmat\n")
25
            with open(f"./CODE/C2H4Cl2 {angle} degrees.gzmat", "r") as gzmat:
2.6
                wrap_code(gzmat.read(), lang="gzmat")
2.7
28
29
            print(f"\n- ./CODE/C2H4Cl2_{angle}_degrees.xyz\n")
```

```
with open(f"./CODE/C2H4C12_{angle}_degrees.xyz", "r") as xyz:
wrap_code(xyz.read(), lang="xyz")
```

II Analysis of the Energy

```
1
 2
  ATOM
            TYPES
 3
4 IDX TYPE RING
5 1 1 NO
6 2 1 NO
7 3 5 NO
   4 5 NO
9 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
36 8 -0.290000
37
38 SETTING UP CALCULATIONS
39
40 SETTING UP BOND CALCULATIONS...
41 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
42
   SETTING UP TORSION CALCULATIONS...
43
   SETTING UP OOP CALCULATIONS...
```

```
44
   SETTING UP VAN DER WAALS CALCULATIONS...
45
   SETTING UP ELECTROSTATIC CALCULATIONS...
46
47 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
   8 cl NO
57
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
   6 0.044101
67
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
    I J
86
            CLASS LENGTH
                           LENGTH
                                    CONSTANT
                                               DELTA
                                                         ENERGY
87
       1
             0
88
    5
                   1.000
                            1.093
                                       4.766
                                                -0.093
                                                          3.578
    5
       1
                   1.000
                            1.093
                                      4.766
                                               -0.093
                                                         3.578
89
             0
                   1.540
                                      4.258
90
   1
       1
             0
                            1.508
                                                0.032
                                                         0.294
   1 5
                   1.000
                                      4.766
91
              0
                            1.093
                                                -0.093
                                                         3.578
92
   1 12
              0
                   1.670
                            1.773
                                       2.974
                                                -0.103
                                                          2.795
```

93 1 5 0 1.000 1.093 4.766 -0.093 3.578 2.974 -0.103 94 0 1.670 1.773 2.795 95 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol 96 ANGLE BENDING 97 98 99 ATOM TYPES FF VALENCE IDEAL FORCE CONSTANT 100 I J K CLASS ANGLE ENERGY ANGLE DELTA 101 ______ 102 1 1 5 0 109.500 110.549 0.636 -1.0490.015 5 5 0 109.442 108.836 0.516 0.606 0.004 103 1 109.442 108.162 104 5 1 12 0 0.698 1.280 0.025 105 1 1 5 0 109.500 110.549 0.636 -1.0490.015 1 12 0 109.500 108.679 1.056 0.821 0.016 106 1 109.442 108.162 107 5 1 12 0 0.698 1.280 0.025 1 5 0 109.500 110.549 0.636 -1.049 0.015 108 1 5 1 5 109 0 109.442 108.836 0.516 0.606 0.004 109.442 108.162 5 1 12 0 0.698 1.280 0.025 110 1 5 0 109.500 110.549 0.636 -1.049 0.015 111 1 1 1 12 0 109.500 108.679 1.056 0.821 0.016 112 0.698 5 1 12 0 109.442 108.162 1.280 0.025 113 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol 114 115 STRETCH BENDING 116 117 118 ATOM TYPES FF VALENCE DELTA FORCE CONSTANT IJ JK I J K 119 CLASS ANGLE ANGLE ENERGY 120 1 5 0 109.500 -1.049 0.227 121 1 0.070 -0.002122 5 1 5 0 109.442 0.606 0.115 0.115 -0.033 123 5 1 12 0 109.442 1.280 -0.018 0.380 -0.1211 5 0 109.500 124 1 -1.049 0.227 0.070 -0.002 125 1 1 12 0 109.500 0.821 0.176 0.386 -0.070 -0.018 126 5 1 12 0 109.442 1.280 0.380 -0.1211 5 0 109.500 127 1 -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 -0.1211 5 109.500 -1.049 0.227 130 1 0 0.070 -0.002 131 1 1 12 0 109.500 0.821 0.176 0.386 -0.070 -0.018 0.380 5 109.442 1.280 -0.121132 1 12 0 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol 133 134 135 TORSIONAL 136 ATOM TYPES FF TORSION FORCE CONSTANT 137 V1 V2 V3 138 I J K L CLASS ANGLE ENERGY 139 ______ 0.314 0.598 1 5 0 0.000 0.284 -1.386 5 1 140 5 1 1 5 0 -120.000 0.284 -1.386 0.314 -0.655

```
142 5 1 1 12 0 120.000 0.678 -0.602 0.398 0.116
143
              5
                     120.000
                             0.284 - 1.386
                                        0.314
    5
       1
          1
                  0
                                               -0.654
144
    5
       1
          1
             5
                  0
                      0.000 0.284 -1.386
                                        0.314
                                                0.598
145
    5
       1 1 12
                  0 -120.000 0.678 -0.602
                                        0.398
                                                0.116
                  0 -120.000 0.678 -0.602
                                        0.398
146 12
       1 1
              5
                                                0.116
    12
       1
          1
             5
                  0 120.000 0.678 -0.602 0.398
147
                                                0.116
148 12
       1
          1 12
                  0
                      -0.000 0.000 0.000 0.893
                                                0.893
      TOTAL TORSIONAL ENERGY = 1.24400 kcal/mol
149
150
151 OUT-OF-PLANE BENDING
152
                  FF OOP FORCE
153
    ATOM TYPES
    I J K
154
             L
                 CLASS ANGLE CONSTANT
                                     ENERGY
155
    _____
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
156
157
158 VAN DER WAALS
159
160 ATOM TYPES
    I J
           Rij R*IJ EPSILON ENERGY
161
    _____
162
              2.208
    5 5
                           0.022
163
                    2.970
                                 0.377
                          0.022 -0.014
164
    5 5
             2.746
                   2.970
                                 0.009
165
    5 12
             3.280
                   3.713
                          0.053
    5 5
                    2.970
                          0.022
166
             2.746
                                -0.014
167
    5 5
             2.208
                    2.970
                          0.022
                                0.377
             3.280
                    3.713
168
    5 12
                          0.053
                                 0.009
    12 5
169
             3.280
                    3.713
                          0.053
                                 0.009
    12 5
             3.280
                   3.713
                          0.053
                                 0.009
170
171
    12 12
             2.655
                    4.089
                          0.276 20.655
172
      TOTAL VAN DER WAALS ENERGY = 21.41512 kcal/mol
173
174
    ELECTROSTATIC INTERACTIONS
175
176
    ATOM TYPES
    I J
             Rij Qi Qj ENERGY
177
178
    _____
    12 12 2.705 -0.290 -0.290 7.743
179
     TOTAL ELECTROSTATIC ENERGY = 7.74347 kcal/mol
180
181
182
    TOTAL ENERGY = 50.10353 kcal/mol
183
184
    ENERGY
185
186
187
    BOND STRETCHING
188
189 ATOM TYPES BOND
                  IDEAL
                          FORCE
    I J LENGTH LENGTH CONSTANT DELTA ENERGY
 190
```

		1 000			1 4 0 5	246				1.60	
				1.093							
				1.093							
				1.535							
				1.093							
				1.786							
				1.093							
				1.786					15	. /18	
	TOTA	AL BOND	STRET	CHING EN	ERGY =	80.1	.22 KJ/	/mol			
. 37	a		N. D. T	N. C							
7 IV (G L 1	E BE	NDI	N G							
шом	my/DI	7.C	573\ T 121	ICE	TDEAT	EC	ND CE				
				NCE					DET m	7	ENED CIT
				LE .							
				110.070							
				10.070							
				109.550							
	3 cl 3 h1			105.930							
	3 ni 3 cl			110.070		194.100 260.419					
	3 cl			10.330							
	3 h1			110.070							
	3 h1			10.070		164.100					
	3 cl			105.930		183.005					
	3 h1			110.070				-0.010			
	3 cl			110.330							
				105.930							
				ING ENER						01000	
	_ 0 11				-	,,	-20 / 1110				
0 1	R S I	IONA	L								
	ATOM	TYPES-		FORCE			TORSI	ON			
I	J	K	L	CONSTAN	T s	S	ANGLE	E n	ı 1	ENERGY	
1 c	3 c3	h1	0.651		0	0.000	3	1.	303		
									303		
1 c	3 c3	cl	0.000		0 12	20.000	3	0.	000		
									303		
1 c	3 c3	h1	0.651		0	0.000	3	1.	303		
ı1 c	3 c3	cl	0.000		0 -12	20.000	3	0.	000		
:1 c	3 c3	h1	0.000		0 -12	20.000	3	0.	000		
:1 c	3 c3	h1	0.000		0 12	20.000	3	0.	000		
cl c	3 c3	cl	0.000		0 -	-0.000	3	0.	000		
	TOTA	AL TORS	IONAL I	ENERGY =	5.2	210 kJ/	mol				
. M .	PRO	O P E R	ТО	R S I O	N A L						
	ATOM	TYPES-		FORCE	IMI	PROPER_	TORSI	ON			
I	J	K	L	CONSTAN	T s	S	ANGLI	E n	1]	ENERGY	

```
240 -----
241
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2.42
243 VAN DER WAALS
244
245 ATOM TYPES
246 I J Rij kij ENERGY
2.47
    _____
           2.208
248 h1 h1
                  0.251
249 h1 h1
           2.746
                  -0.033
250 h1 cl
           3.280
                  -0.134
           2.746
251 h1 h1
                  -0.033
252 h1 h1
           2.208
                  0.251
253 h1 cl
           3.280
                  -0.134
                 -0.134
254 cl h1
           3.280
255 cl h1
           3.280
                  -0.134
256 cl cl
           2.655
                  44.245
257
     TOTAL VAN DER WAALS ENERGY = 44.146 kJ/mol
258
259 ELECTROSTATIC INTERACTIONS
260
261 ATOM TYPES
               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
           2.746
                  1.352
267 h1 h1
                         0.493
268 h1 h1
           2.208
                  1.352
                         0.613
269 h1 cl
           3.280 -3.809 -1.161
270 cl h1
           3.280
                  -3.809
                        -1.161
           3.280 -3.809 -1.161
271 cl h1
272 cl cl
           2.655
                 10.728
                         4.041
273
      TOTAL ELECTROSTATIC ENERGY = 1.607 kJ/mol
274
275 TOTAL ENERGY = 134.023 kJ/mol
2.76
277 ATOM TYPES
278
279 IDX TYPE RING
280
    1 1 NO
281 2 1 NO
282 | 3 5 NO
    4 5 NO
283
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
    4 0.000000
295
296 5 -0.290000
    6 0.000000
297
298 7 0.000000
    8 -0.290000
299
300
301 PARTIAL CHARGES
302
303
    IDX CHARGE
304 1 0.290000
    2 0.290000
305
    3 0.000000
306
    4 0.000000
307
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
321
    6 hl NO
322
    7 h1 NO
323
    8 cl NO
324
325
    FORMAL CHARGES
326
327 IDX CHARGE
328 1 0.036009
    2 0.036009
329
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
```

```
339 IDX CHARGE
340 1 0.036009
341 2 0.036009
342 3 0.044101
   4 0.044101
343
344 5 -0.124211
345
   6 0.044101
   7 0.044101
346
347
   8 -0.124211
348
349
   ENERGY
350
351
   BOND STRETCHING
352
353
354
   ATOM TYPES FF BOND
                        IDEAL
                                 FORCE
                        LENGTH
                                CONSTANT
                                          DELTA
355
    I J CLASS LENGTH
                                                  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
       1
                 1.540
                         1.508
                                          0.032
    1
            0
                                  4.258
359
                                                   0.294
    1 5
360
            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
362
    1
             0
                 1.000
                         1.093
                                   4.766
                                           -0.093
                                                   3.578
                         1.773 2.974 -0.103
363
    1 12
            0
                 1.670
                                                  2.795
     TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
364
365
366 ANGLE BENDING
367
368
   ATOM TYPES
                FF VALENCE
                             IDEAL
                                     FORCE
369
    I J K
               CLASS ANGLE
                             ANGLE CONSTANT
                                              DELTA ENERGY
370
371
       1
           5
                0
                   109.500 110.549
                                       0.636
                                              -1.049
                                                       0.015
    1
                0 109.442 108.836
   5
       1 5
                                      0.516
                                              0.606
                                                      0.004
372
                0 109.442 108.162
                                      0.698
                                              1.280
                                                      0.025
373
   5
       1 12
374
           5
                0 109.500 110.549
                                       0.636
                                              -1.049
                                                       0.015
    1
       1
                0 109.500 108.679
       1 12
                                       1.056
375
    1
                                              0.821
                                                       0.016
376
   5
       1 12
                0 109.442 108.162
                                      0.698
                                              1.280
                                                       0.025
       1 5
                                              -1.049
377
                0 109.500 110.549
                                       0.636
                                                       0.015
    1
       1 5
                0 109.442 108.836
378
    5
                                       0.516
                                              0.606
                                                       0.004
379
    5
       1 12
                0 109.442 108.162
                                      0.698
                                              1.280
                                                       0.025
       1 5
                0 109.500 110.549
380
    1
                                       0.636
                                              -1.049
                                                       0.015
                   109.500 108.679
       1
           12
381
    1
                0
                                       1.056
                                              0.821
                                                       0.016
                   109.442
                                              1.280
382
   5
       1 12
                0
                           108.162
                                      0.698
                                                      0.025
      TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
383
384
   STRETCH BENDING
385
```

338

T J K CLASS ANGLE ANGLE I J J K ENERGY 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 5 0 109.442 0.606 0.115 0.115 -0.033 5 1 12 0 109.500 -1.049 0.227 0.070 -0.002 1 1 12 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 0 109.500 -1.049 0.227 0.070 -0.002 1 1 12 0 109.500 -1.049 0.227 0.070 -0.002 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 5 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 0 109.442 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 0 109.442 1.280 -0.018 0.380 -0.121 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol **CORSIONAL** **TOM TYPES*** **FF** **FF** **TORSION** **FORCE CONSTANT** I J K L CLASS** **ANGLE** V1 V2 V3 ENERGY* **5 1 1 5 0 140.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 140.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 140.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 140.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 140.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 0 140.000 0.678 -0.602 0.398 -0.005 2 1 1 5 0 0 140.000 0.678 -0.602 0.398 -0.005 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	T J K CLASS ANGLE ANGLE I J J K ENERGY 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 5 0 109.442 0.606 0.115 0.115 -0.033 5 1 12 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.442 1.280 -0.018 0.386 -0.070 5 1 12 0 109.442 1.280 -0.018 0.386 -0.070 5 1 12 0 109.442 1.280 -0.018 0.386 -0.070 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 5 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 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 1 2 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.442 1.280 -0.018 0.380 -0.121 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol FOR S I O N A L **TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol	7\ ITI	OM MVDI	E.C.	DD.	MATENCE	DELUA	EODGE	CONCEANE	
1 1 5 0 109.402 1.280 -0.018 0.380 -0.121 1 12 0 109.402 1.280 -0.018 0.380 -0.121 1 15 0 109.402 1.280 -0.018 0.380 -0.121 1 15 0 109.402 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 0.821 0.176 0.386 -0.070 5 1 12 0 109.402 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 12 0 109.402 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 1 2 0 109.402 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 1 1 1 2 0 109.402 0.606 0.115 0.115 -0.033 1 1 2 0 109.402 0.606 0.115 0.115 -0.033 1 1 2 0 109.402 0.606 0.115 0.115 -0.033 1 1 2 0 109.402 0.606 0.115 0.115 -0.033 1 1 2 0 109.402 0.821 0.176 0.386 -0.070 0.821 0.176 0.386 -0.070 0.821 0.176 0.386 -0.070 0.821 0.176 0.386 -0.070 0.821 0.176 0.386 -0.070 0.821 0.176 0.386 -0.070 0.821 0.176 0.386 0.314 0.349 0.380 0.121 0.380 0.380 0.121 0.380 0.380 0.121 0.380 0.380 0.121 0.380 0.380 0.121 0.380 0.380 0.121 0.380	1 1 5 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.442 0.606 0.115 0.115 -0.002 1 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 0 109.442 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 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 5 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.442 1.280 -0.018 0.380 -0.121 1 1 5 0 109.500 -1.049 0.227 0.070 -0.002 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121 1 1 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 0 109.500 0.821 0.176 0.386 -0.070 5 1 12 0 109.500 0.821 0.176 0.386 -0.070 5 1 12 0 109.442 1.280 -0.018 0.380 -0.121 **TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol **POR S I O N A L** **TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol **TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol **TOTAL STRETCH BENDING ENERGY = -0.602 0.398 0.129 5 1 1 5 0 140.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 20.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 20.000 0.284 -1.386 0.314 0.349 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 0 140.000 0.678 -0.602 0.398 0.129 5 1 1 5 0 0 140.000 0.678 -0.602 0.398 0.129 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0									ENEDCY
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12 1 1 5 0 -100.000 0.678 -0.602 0.398 -0.005 12 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 12 1 1 12 0 20.000 0.000 0.000 0.893 0.670 10 TOTAL TORSIONAL ENERGY = 0.31978 kcal/mol O U T - O F - P L A N E B E N D I N G ATOM TYPES FF OOP FORCE	1									
2 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 2 1 1 12 0 20.000 0.000 0.000 0.893 0.670 TOTAL TORSIONAL ENERGY = 0.31978 kcal/mol U T - O F - P L A N E B E N D I N G TOM TYPES FF OOP FORCE	2 1 1 5 0 140.000 0.678 -0.602 0.398 0.129 2 1 1 12 0 20.000 0.000 0.000 0.893 0.670 TOTAL TORSIONAL ENERGY = 0.31978 kcal/mol U T - O F - P L A N E B E N D I N G TOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY									
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NTOM TYPES FF OOP FORCE	ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY		1011			.,,	1013,0 11001	-,o <u>-</u>		
NTOM TYPES FF OOP FORCE	ATOM TYPES FF OOP FORCE I J K L CLASS ANGLE CONSTANT ENERGY)	υт – (0 F -	PTANI	EBEN	DING			
	I J K L CLASS ANGLE CONSTANT ENERGY			-						
	I J K L CLASS ANGLE CONSTANT ENERGY	ΥР	OM TYPI	ES		FF	OOP FOR	RCE		
									ERGY	
			1011	.11 001	01 111111	DENDING		, cood and a	7 1110 1	
	TOTAL OUT-OF-FLANE BENDING ENERGY - 0.00000 RCAT/MOT		A N I	DEB	W 7 7 7	r. S				
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol			-1 -1 I	ИП	" A A I					
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol	7 A N DER WAALS	\ m	רעעייי אר	FC						
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol	7AN DER WAALS				Dii	D*TT	EDCTI ON	FNFDCV		
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol VAN DER WAALS	7 AN DER WAALS ATOM TYPES									
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol AN DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY	7 A N DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY									
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol A N DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY	7 A N DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY									
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol 7 A N D E R W A A L S ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.232 2.970 0.022 0.328	7 A N DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.232 2.970 0.022 0.328									
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol A N DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.232 2.970 0.022 0.328 5 5 2.638 2.970 0.022 0.001	7 A N DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.232 2.970 0.022 0.328 5 5 2.638 2.970 0.022 0.001									
TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol 7 A N D E R W A A L S ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.232 2.970 0.022 0.328 5 5 2.638 2.970 0.022 0.001 5 12 3.399 3.713 0.053 -0.028	7 A N DER WAALS ATOM TYPES I J Rij R*IJ EPSILON ENERGY 5 5 2.232 2.970 0.022 0.328 5 5 2.638 2.970 0.022 0.001 5 12 3.399 3.713 0.053 -0.028	5	5		2.831	2.970	0.022	-0.019		

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436 5 5 2.232 2.970 0.022 0.328
                            0.053
437
    5 12
              3.129
                     3.713
                                   0.104
438 12 5
              3.129
                     3.713
                            0.053
                                   0.104
439 12 5
              3.399
                     3.713
                            0.053
                                   -0.028
440 12 12
              2.711
                     4.089
                            0.276 16.993
441
      TOTAL VAN DER WAALS ENERGY = 17.78153 kcal/mol
442
443 ELECTROSTATIC INTERACTIONS
444
445 ATOM TYPES
446
    I J
             Rij Qi
                          Qj
                                  ENERGY
447
    ______
             2.761
                   -0.290
                          -0.290
448 12 12
                                  7.587
       TOTAL ELECTROSTATIC ENERGY = 7.58721 kcal/mol
449
450
451 TOTAL ENERGY = 45.38946 kcal/mol
452
453 ENERGY
454
455
456 BOND STRETCHING
457
458 ATOM TYPES BOND
                   IDEAL
                           FORCE
                   IDEAL FORCE
LENGTH CONSTANT DELTA ENERGY
459
    I J
           LENGTH
460
                  1.093
          1.000
461 h1 c3
                         1406.346
                                  -0.093
                                          12.163
462 hl c3
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
                  1.535
463 c3 c3
          1.540
                         1269.019
                                   0.005
                                          0.032
                                         12.163
464 c3 h1
          1.000
                  1.093
                         1406.346
                                  -0.093
465 c3 cl
          1.670
                  1.786
                         1168.117
                                  -0.116
                                          15.718
466
    c3 h1
           1.000
                  1.093
                         1406.346
                                   -0.093
                                          12.163
    c3 cl 1.670 1.786 1168.117 -0.116 15.718
467
     TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
468
469
470 ANGLE BENDING
471
472 ATOM TYPES
               VALENCE
                        IDEAL
                               FORCE
    I J K
                ANGLE
                       ANGLE
                              CONSTANT DELTA ENERGY
473
474
    ______
    c3 c3 h1 109.500 110.070
475
                            194.100
                                    -0.010
                                             0.019
    h1 c3 h1 109.442 109.550
                            164.039
                                    -0.002
                                             0.001
476
477 h1 c3 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
478
    c3 c3 h1 109.500 110.070
                            194.100
                                    -0.010
                                             0.019
                            260.419
    c3 c3 cl 109.500 110.330
                                    -0.014
479
                                             0.055
                   105.930
                                     0.061
480 h1 c3 cl 109.442
                            183.005
                                             0.688
481 c3 c3 h1 109.500 110.070
                            194.100
                                    -0.010
                                             0.019
482 h1 c3 h1 109.442 109.550
                            164.039
                                    -0.002
                                             0.001
                                     0.061
 483 h1 c3 cl 109.442 105.930
                            183.005
                                             0.688
 484 c3 c3 h1 109.500 110.070 194.100 -0.010
                                            0.019
```

```
485 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055
486 h1 c3 cl 109.442 105.930
                           183.005 0.061
                                           0.688
487
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
488
489 TORSIONAL
490
                                TORSION
491 ----ATOM TYPES---- FORCE
492
    I J K
              L
                  CONSTANT
                               ANGLE n ENERGY
                           S
    ______
493
494 h1 c3 c3 h1
                           20.000 3
              0.651
                       0
                                      0.977
495 h1 c3 c3 h1
              0.651
                       0 -100.000 3
                                      0.977
496 h1 c3 c3 cl 0.000
                       0 140.000 3
                                      0.000
                       0 140.000 3
497 h1 c3 c3 h1
              0.651
                                      0.977
498 h1 c3 c3 h1
                       0
                           20.000 3
              0.651
                                      0.977
499 h1 c3 c3 cl 0.000
                       0 -100.000 3
                                      0.000
500 cl c3 c3 h1
              0.000
                       0 -100.000 3
                                      0.000
501 cl c3 c3 h1
                       0
              0.000
                          140.000 3
                                      0.000
              0.000 0
                           20.000 3
502 cl c3 c3 cl
                                      0.000
     TOTAL TORSIONAL ENERGY = 3.908 kJ/mol
503
504
505 IMPROPER TORSIONAL
506
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
507
    I J K L CONSTANT S ANGLE n ENERGY
508
509
510
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
511
    512
513
514 ATOM TYPES
    I J Rij kij ENERGY
515
516
517 h1 h1 2.232
                 0.205
518 h1 h1
           2.638
                 -0.029
519 h1 cl
           3.399 -0.133
520 h1 h1
           2.831
                 -0.032
521 h1 h1
           2.232
                 0.205
           3.129 -0.106
522 h1 cl
523 cl h1
           3.129
                 -0.106
524 cl h1
           3.399
                 -0.133
    cl cl
           2.711 33.340
525
526
     TOTAL VAN DER WAALS ENERGY = 33.209 kJ/mol
527
528 ELECTROSTATIC INTERACTIONS
529
530 ATOM TYPES
    I J
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
535 h1 cl
             3.399
                     -3.809 -1.121
536 h1 h1
             2.831
                     1.352
                             0.478
537 h1 h1
             2.232
                     1.352
                             0.606
538 h1 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
541
     cl cl
                     10.728
                             3.958
             2.711
      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
     2 0.290000
574
575 3 0.000000
576 4 0.000000
    5 -0.290000
577
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
595 2 c3 NO
596 3 h1 NO
597
    4 h1 NO
598 5 cl NO
    6 hl NO
599
    7 h1 NO
600
    8 cl NO
601
602
603 C H A R G E S
604
605 IDX CHARGE
606 1 0.036009
607 2 0.036009
    3 0.044101
608
    4 0.044101
609
610
    5 -0.124211
    6 0.044101
611
612 7 0.044101
613
    8 -0.124211
614
615 SETTING UP CALCULATIONS
616
617
    SETTING UP BOND CALCULATIONS...
618 SETTING UP ANGLE CALCULATIONS...
619
    SETTING UP TORSION CALCULATIONS...
    SETTING UP IMPROPER TORSION CALCULATIONS...
620
621
    SETTING UP VAN DER WAALS CALCULATIONS...
    SETTING UP ELECTROSTATIC CALCULATIONS...
622
623
624
    ENERGY
625
626
627 BOND STRETCHING
628
629 ATOM TYPES FF BOND IDEAL FORCE
     I J
              CLASS LENGTH
                              LENGTH
                                        CONSTANT
                                                    DELTA
630
                                                               ENERGY
```

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
	TOT	AL BONI	D STRETCH	HING ENERG	SY = 20.1962	29 kcal/mol		
A N	GLE	Е В 1	ENDI	N G				
ATOM	TYPE	ES	FF	VALENCE	IDEAL	FORCE		
I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERO
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
5	1	5	0	109.442	108.836	0.516	0.606	0.004
5	1	12	0	109.442	108.162	0.698	1.280	0.025
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
1	1	12	0	109.500	108.679	1.056	0.821	0.016
5	1	12	0	109.442	108.162	0.698	1.280	0.025
5	1	5	0	109.442	108.836	0.516	0.606	0.004
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
5	1	12	0	109.442	108.162	0.698	1.280	0.025
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
5	1	12	0	109.442	108.162	0.698	1.280	0.025
1	1	12	0	109.500	108.679	1.056	0.821	0.016
	TOT	AL ANG	LE BENDI	NG ENERGY	= 0.20058	kcal/mol		
ST	RE 7	ГСН	BENI	O I N G				
						FORCE		
						ΙJ		
						0 227		
						0.227		
						0.115		
						-0.018		
Τ		5				0.227		
1	Τ		0			0.176		
1	1		()	109.442	1.280	-0.018	0.380	
5				100 440	0.606	0 115	0 115	
5 5	1	5	0			0.115		
5 5 1	1 1	5 5	0	109.500	-1.049	0.227	0.070	-0.002
5 5 1 5	1 1 1	5 5 12	0 0 0	109.500 109.442	-1.049 1.280	0.227 -0.018	0.070 0.380	-0.002 -0.121
5 5 1 5	1 1 1	5 5 12 5	0 0 0	109.500 109.442 109.500	-1.049 1.280 -1.049	0.227 -0.018 0.227	0.070 0.380 0.070	-0.002 -0.121 -0.002
5 5 1 5 1 5	1 1 1 1	5 5 12 5 12	0 0 0 0	109.500 109.442 109.500 109.442	-1.049 1.280 -1.049 1.280	0.227 -0.018 0.227 -0.018	0.070 0.380 0.070 0.380	-0.002 -0.121 -0.002 -0.121
5 5 1 5 1 5	1 1 1 1 1	5 5 12 5 12	0 0 0 0 0	109.500 109.442 109.500 109.442 109.500	-1.049 1.280 -1.049 1.280 0.821	0.227 -0.018 0.227 -0.018 0.176	0.070 0.380 0.070 0.380	-0.002 -0.121 -0.002 -0.121
5 5 1 5 1 5	1 1 1 1 1	5 5 12 5 12	0 0 0 0 0	109.500 109.442 109.500 109.442 109.500	-1.049 1.280 -1.049 1.280 0.821	0.227 -0.018 0.227 -0.018	0.070 0.380 0.070 0.380	-0.002 -0.121 -0.002 -0.121
5 5 1 5 1	1 1 1 1 1	5 5 12 5 12	0 0 0 0 0	109.500 109.442 109.500 109.442 109.500	-1.049 1.280 -1.049 1.280 0.821	0.227 -0.018 0.227 -0.018 0.176	0.070 0.380 0.070 0.380	-0.002 -0.121 -0.002 -0.121

					TORSION					
					ANGLE					
					40.000					
					40.000					
					160.000					
					160.000					
					40.000				0.31	
			12		-80.000				0.31	
					-80.000					
					160.000					
					40.000					
					= -1.5115			000	0.07	5
	10	IAL IO	ROIONAL	пипиот	1.5115.	, KCGI	шот			
0	пт –	0 F -	Р Т. А 1	JE B	ENDIN	G				
	0 1	0 1		.,		C				
AT	OM TY	PES		FF	OOP	FORC	E.			
					ANGLE			ENE	RGY	
	TO'	TAL OU'	T-OF-PLA	ANE BENI	OING ENERG	Y = 0.	00000	kcal/	mol	
								,		
7.7	ΔNI	DER	WAA	A T. S						
•		р ц к	** 11 1	1 1 0						
AT	OM TY	PES								
			Rii	R*:	IJ EPSI	LON	ENERGY	7		
					970 0.					
					970 0.					
5	12		3.4/4		/13 0.0	053	-0.041	_		
						053 022				
5	5		2.885	2.9	970 0.	022	-0.021	_		
5 5	5 5		2.885 2.300	2.9	970 0.0 970 0.0	022	-0.021 0.215	- 5		
5	5 5 12		2.885 2.300 2.960	2.9	970 0.0 970 0.0 713 0.0	022 022 053	-0.021 0.215 0.331	- 5		
5 5 5 12	5 5 12 5		2.885 2.300 2.960 2.960	2.9 2.9 3.7	970 0.0 970 0.0 713 0.0 713 0.0	022 022 053 053	-0.021 0.215 0.331 0.331	- 5 -		
5 5 5 12 12	5 5 12 5 5		2.885 2.300 2.960 2.960 3.474	2.9 2.9 3.7 3.7	970 0.0 970 0.0 713 0.0 713 0.0	022 022 053 053	-0.021 0.215 0.331 0.331			
5 5 5 12	5 12 5 5 12		2.885 2.300 2.960 2.960 3.474 2.865	2.9 2.9 3.7 3.7 4.0	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0	022 022 053 053 053	-0.021 0.215 0.331 0.331 -0.041 9.664	- 5 - - -		
5 5 5 12 12	5 12 5 5 12		2.885 2.300 2.960 2.960 3.474 2.865	2.9 2.9 3.7 3.7 4.0	970 0.0 970 0.0 713 0.0 713 0.0	022 022 053 053 053	-0.021 0.215 0.331 0.331 -0.041 9.664	- 5 - - -		
5 5 12 12 12	5 5 12 5 5 12 TO	TAL VAI	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA	2.9 3.3 3.4.0 AALS END	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 989 0.2	022 022 053 053 053 076 69051 k	-0.021 0.215 0.331 0.331 -0.041 9.664			
5 5 12 12 12	5 5 12 5 5 12 TO	TAL VAI	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA	2.9 3.3 3.4.0 AALS END	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0	022 022 053 053 053 076 69051 k	-0.021 0.215 0.331 0.331 -0.041 9.664			
5 5 12 12 12	5 5 12 5 12 TO'	TAL VAI	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA	2.9 3.3 3.4.0 AALS END	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 989 0.2	022 022 053 053 053 076 69051 k	-0.021 0.215 0.331 0.331 -0.041 9.664			
5 5 12 12 12	5 12 5 12 TO' LE C	TAL VAI T R O PES	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA	2.9 3.7 3.7 4.0 AALS ENI	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 889 0.3 ERGY = 10.0)22)22)53)53)53 276 69051 k	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo			
5 5 12 12 12 12	5 5 12 5 12 TO' L E C	TAL VAI T R O PES	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA	2.9 3.7 3.7 4.0 AALS END	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 1089 0.3 ERGY = 10.0	022 022 053 053 053 276 69051 k	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo			
5 5 12 12 12 12	5 5 12 5 12 TO' LECOMTY: J	TAL VAI T R O PES	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA	2.9 2.9 3.7 3.7 4.0 AALS ENI	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 889 0.3 ERGY = 10.0 INTER	022 022 053 053 053 276 69051 k	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo			
5 5 5 12 12 12 12 E : ATC	5 5 12 5 12 TO' L E C OM TY: J	TAL VAI T R O PES	2.885 2.300 2.960 3.474 2.865 N DER WA	2.9 3.7 3.7 4.0 AALS END	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 889 0.3 ERGY = 10.0 INTER	022 022 053 053 053 276 69051 k A C T	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo	S S ERGY		
5 5 5 12 12 12 12 E : ATC	5 5 12 5 12 TO' L E C OM TY: J	TAL VAI T R O PES	2.885 2.300 2.960 3.474 2.865 N DER WA	2.9 3.7 3.7 4.0 AALS END	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 889 0.3 ERGY = 10.0 INTER	022 022 053 053 053 276 69051 k A C T	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo	S S ERGY		
5 5 5 12 12 12 E:: ATC I	5 5 12 5 12 TO' LECOMTY: J 12 TO'	TAL VAI T R O PES : TAL ELI	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA S T A S Rij 2.915 ECTROSTA	2.9 3.7 3.7 4.0 AALS END F I C	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 889 0.3 ERGY = 10.0 INTER i 0 -0.29 ERGY = 7.3	022 022 053 053 053 276 69051 k A C T	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo	S S ERGY		
5 5 5 12 12 12 E:: ATC I	5 5 12 5 12 TO' LECOMTY: J 12 TO'	TAL VAI T R O PES : TAL ELI	2.885 2.300 2.960 3.474 2.865 N DER WA	2.9 3.7 3.7 4.0 AALS END F I C	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 889 0.3 ERGY = 10.0 INTER i 0 -0.29 ERGY = 7.3	022 022 053 053 053 276 69051 k A C T	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo	S S ERGY		
5 5 5 12 12 12 12 E :: ATC I 12	5 5 12 5 12 TO' LECOMTY: J 12 TO'	TAL VAI T R O PES TAL ELI	2.885 2.300 2.960 2.960 3.474 2.865 N DER WA S T A S Rij 2.915 ECTROSTA	2.9 3.7 3.7 4.0 AALS END F I C	970 0.0 970 0.0 713 0.0 713 0.0 713 0.0 889 0.3 ERGY = 10.0 INTER i 0 -0.29 ERGY = 7.3	022 022 053 053 053 276 69051 k A C T	-0.021 0.215 0.331 0.331 -0.041 9.664 ccal/mo	S S ERGY		

B O N	ם ז	ст Б	э т т с	HING	<u>.</u>						
		0 1 1		11 11 10							
MOTA	TYPE	S BON	ID	IDEAL		FORCE					
I	J	LEN	IGTH	LENGTH	C	ONSTANT		DELTA	A	ENER	GY
				1.093							
				1.093							
				1.093		.346					
				1.535							
				1.093							
				1.786							
				1.786 CHING EN					15	0./10	
	IUIA	L BONL) SIKEI	CHING EN	EKGI -	80.1	22 N) / IIIOI			
ANG	LE	ВЕ	NDI	N G							
MOTA	TYPE	S	VALEI	NCE	IDEAL	FO	RCE				
I	J	K	ANGI	LE	ANGLE	CON	STANT	Г	DELT	'A	ENERGY
				110.070							
h1 c3	3 h1			109.550							
h1 c3				105.930							
c3 c3	3 h1			110.070							
c3 c3				110.330							
h1 c3				105.930							
h1 c3				109.550							
c3 c3				110.070							
				105.930		194.100					
c3 c3			500	110.070							
				105.930							
				110.330 ING ENER					•	0.03	
	1017				.51	2.750	110 / 1				
ГОБ	RSI	ONA	L								
<i>P</i>	MOTA	TYPES-		FORCE			TORS	ION			
I	J	K	L	CONSTAN	Т	S	ANGI	LE r	ì	ENERGY	
											_
h1 c3	3 c3	h1	0.651		0	40.000	3	0.	326		
						80.000	3		326		
						60.000	3		000		
						60.000	3		326		
						40.000	3		326		
		cl	0.000			80.000	3		000		
			0.000			80.000	3		000		
			0.000			60.000	3		000		
CT C3				ENEDCV -		40.000		0.	000		
	TOTA	TORS	TONAL I	ENERGY =	Ι.	303 kJ/	TOUT				

```
779
780
   IMPROPER TORSIONAL
781
782 ----ATOM TYPES---- FORCE IMPROPER_TORSION
                           s ANGLE n ENERGY
783
   I J K L CONSTANT
784
    ______
785
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
786
   VAN DER WAALS
787
788
789 ATOM TYPES
          Rij kij ENERGY
    I J
790
791 -----
792 h1 h1
         2.300
                 0.109
          2.518 -0.013
793
   h1 h1
794 h1 cl
          3.474
                 -0.129
795 h1 h1
          2.885
                 -0.031
796 h1 h1
          2.300
                 0.109
          2.960
                 0.012
797 h1 cl
798
   cl h1
          2.960
                 0.012
          3.474 -0.129
799 cl h1
800 cl cl
          2.865
                 15.169
801
     TOTAL VAN DER WAALS ENERGY = 15.111 kJ/mol
802
803
   ELECTROSTATIC INTERACTIONS
804
805 ATOM TYPES
    I J
806
           Rij 332.17*QiQj ENERGY
807
   _____
808 h1 h1
          2.300 1.352
                        0.588
                        0.537
          2.518
809 h1 h1
                 1.352
810 h1 cl
          3.474 -3.809 -1.097
811 h1 h1
          2.885
                 1.352
                        0.469
812 h1 h1
          2.300
                 1.352
                        0.588
          2.960 -3.809 -1.287
813 h1 cl
814 cl h1
          2.960 -3.809 -1.287
815
   cl h1
          3.474
                 -3.809
                        -1.097
   cl cl 2.865 10.728 3.745
816
    TOTAL ELECTROSTATIC ENERGY = 1.160 kJ/mol
817
818
819
   TOTAL ENERGY = 100.634 \text{ kJ/mol}
820
821 ATOM TYPES
822
823 IDX TYPE RING
824 | 1 1 NO
825 2 1 NO
826 3 5 NO
827 4 5 NO
```

```
828 5 12 NO
 829
     6 5 NO
830 7 5 NO
831 8 12 NO
 832
833 FORMAL CHARGES
834
 835 IDX CHARGE
 836 1 0.290000
 837 2 0.290000
 838 3 0.000000
     4 0.000000
 839
 840 5 -0.290000
 841 6 0.000000
     7 0.000000
 842
 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
     3 h1 NO
 862
 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
 872 1 0.036009
     2 0.036009
 873
     3 0.044101
 874
 875 4 0.044101
 876 5 -0.124211
```

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877 6 0.044101
    7 0.044101
878
879 8 -0.124211
880
881 PARTIAL CHARGES
882
883 IDX CHARGE
884
    1 0.036009
    2 0.036009
885
886 3 0.044101
887
    4 0.044101
888
    5 -0.124211
889
    6 0.044101
890 7 0.044101
    8 -0.124211
891
892
893 ENERGY
894
895
896 BOND STRETCHING
897
898 ATOM TYPES FF BOND IDEAL
                                 FORCE
            CLASS LENGTH
                         LENGTH
899
                                 CONSTANT
                                           DELTA
                                                   ENERGY
900
    ______
              0
901
     5
                  1.000
                          1.093
                                    4.766
                                           -0.093
                                                    3.578
902
    5
        1
             0
                  1.000
                          1.093
                                   4.766
                                          -0.093
                                                   3.578
    5
                  1.000
                                   4.766
903
        1
             0
                          1.093
                                           -0.093
                                                   3.578
904
     1
        1
              0
                  1.540
                          1.508
                                   4.258
                                           0.032
                                                   0.294
905
    1 5
                                   4.766
              0
                  1.000
                          1.093
                                           -0.093
                                                   3.578
906
    1 12
            0
                  1.670
                          1.773
                                   2.974
                                           -0.103
                                                   2.795
907
     1 12
              0
                  1.670
                          1.773
                                   2.974
                                           -0.103
                                                   2.795
908
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
909
910 ANGLE BENDING
911
912 ATOM TYPES
                FF VALENCE IDEAL
                                     FORCE
913
     I J K
               CLASS ANGLE
                             ANGLE
                                    CONSTANT
                                              DELTA
                                                      ENERGY
914
915
    1
        1 5
                0 109.500
                            110.549
                                       0.636
                                              -1.049
                                                       0.015
916
     5
        1
           5
                0 109.442 108.836
                                       0.516
                                              0.606
                                                       0.004
        1 12
                0 109.442 108.162
917
     5
                                       0.698
                                               1.280
                                                       0.025
918
        1 5
                0 109.500
                            110.549
                                       0.636
                                               -1.049
                                                       0.015
    1
                0 109.500 108.679
                                       1.056
919
    1
        1 12
                                               0.821
                                                       0.016
                    109.442 108.162
920
        1 12
                0
                                       0.698
                                               1.280
                                                       0.025
     5
        1 5
                    109.442
921
    5
                0
                            108.836
                                        0.516
                                               0.606
                                                       0.004
           5
922
    1
        1
                0
                    109.500 110.549
                                        0.636
                                               -1.049
                                                       0.015
923
     5
        1 12
                0 109.442 108.162
                                       0.698
                                               1.280
                                                       0.025
        1 5
                0 109.500 110.549
    1
                                       0.636
                                              -1.049
                                                       0.015
924
925
    5
        1 12
                0 109.442 108.162
                                        0.698
                                               1.280
                                                       0.025
```

	тОт≀				108.679 $t = 0.20058$		0.821	0.01
	1017	אוא עני.	TINNIIG TIL	ТОЛИНИ СК	- 0.20038	reat/IIIOT		
S Т	RET	гсн	BENI	OING				
		- 11	1, 1	_ 1. 0				
ATOM	1 TYPI	ES	FF	VALENCE	DELTA	FORCE	CONSTANT	
I					ANGLE			ENERGY
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
5	1	5	0	109.442	0.606	0.115	0.115	-0.033
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5	1	12	0		1.280			-0.121
5			0		0.606			
1		5	0	109.500		0.227		
5			0		1.280			
1					-1.049			
5					1.280			
1	1 TOT:				0.821 $6GY = -0.6959$		0.386	-0.070
	1017	ALC UL	CLICII DENI	ATMG DMEK	0.0939	J KCal/IIIOI		
т О	R C	I O N	Δ Т.					
1 0	1. 0 .	IA						
ATOM	1 TYPI	ES		FF T	ORSION	FORCE CONST	ANT	
					ORSION ANGLE			RGY
I	J	K	L (CLASS		V1 V2	V3 ENE	RGY
I 	J	K	L (CLASS	ANGLE	V1 V2	V3 ENE	
I 5	J 1	К 1	L (CLASS 0 60	ANGLE	V1 V2 4 -1.386	V3 ENE 0.314	 -0.827
I 5	J 1	К 1	L (CLASS 0 60 0 -60	ANGLE	V1 V2 4 -1.386 4 -1.386	V3 ENE 0.314 0.314	 -0.827
5 5	J 1 1	K 1 1	L (CLASS 0 60 0 -60 0 -180	ANGLE .000 0.28 .000 0.28	V1 V2 4 -1.386 4 -1.386 8 -0.602	V3 ENE 0.314 0.314 0.398	 -0.827 -0.826 0.000
5 5 5 5 5	J 1 1 1	1 1 1 1 1	L (5 5 12 5 5	CLASS 0 60 0 -60 0 -180 0 -180 0 60	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28	V1 V2 4 -1.386 4 -1.386 8 -0.602 4 -1.386 4 -1.386	V3 ENE 0.314 0.314 0.398 0.314 0.314	 -0.827 -0.826 0.000 0.000 -0.827
5 5 5 5 5	J 1 1 1 1 1 1 1 1	1 1 1 1 1 1	L (0 60 0 -60 0 -180 0 -180 0 60 0 -60	ANGLE .000 0.28 .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67	V1 V2 	V3 ENE 0.314 0.314 0.398 0.314 0.314 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057
5 5 5 5 5 5 5	J 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1	L (5 5 12 5 12 5 5 5 5 5 7 7 8 7 8 8 8 8 8 8 8 8 8	CLASS 0 60 0 -60 0 -180 0 -180 0 60 0 -60 0 -60	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.67 .000 0.67 .000 0.67	V1 V2 4 -1.386 4 -1.386 8 -0.602 4 -1.386 4 -1.386 8 -0.602 8 -0.602	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057
5 5 5 5 5 5 5 12	J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1	L (0 60 0 -60 0 -180 0 -180 0 -60 0 -60 0 180	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67 .000 0.67	V1 V2 4 -1.386 4 -1.386 8 -0.602 4 -1.386 4 -1.386 8 -0.602 8 -0.602 8 -0.602	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
5 5 5 5 5 5 5	J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	L (5 5 12 5 12 5 12 5 12	CLASS 0 60 0 -60 0 -180 0 -180 0 -60 0 -60 0 180 0 60	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
5 5 5 5 5 5 5 12	J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	L (5 5 12 5 12 5 12 5 12	CLASS 0 60 0 -60 0 -180 0 -180 0 -60 0 -60 0 180 0 60	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67 .000 0.67	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
5 5 5 5 5 5 5 12 12	J 1 1 1 1 1 1 1 1 TOTA	1 1 1 1 1 1 1 1 1 1	L (CLASS 0 60 0 -60 0 -180 0 -180 0 -60 0 -60 0 -60 0 -60 NERGY = -	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
5 5 5 5 5 5 5 12 12	J 1 1 1 1 1 1 1 1 TOTA	1 1 1 1 1 1 1 1 1 1	L (5 5 12 5 12 5 12 5 12	CLASS 0 60 0 -60 0 -180 0 -180 0 -60 0 -60 0 -60 0 -60 NERGY = -	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
5 5 5 5 5 5 12 12	J 1 1 1 1 1 1 1 TOTA	1 1 1 1 1 1 1 1 1 1 0 F -	L (5 5 12 5 12 5 12 5 12 7 12 8 RSIONAL EN	CLASS 0 60 0 -60 0 -180 0 -180 0 -60 0 -60 0 -60 0 -60 NERGY = -	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
5 5 5 5 5 5 12 12	J 1 1 1 1 1 1 1 TOTA T - (1 1 1 1 1 1 1 1 1 TOP	L 0 5 5 12 5 12 5 12 5 12 8 PLANE	CLASS 0 60 0 -60 0 -180 0 -60 0 -60 0 -60 0 -60 ERGY = -	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 FOR	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
I 5 5 5 5 5 5 12 12 12 12 12 12	J 1 1 1 1 1 1 1 TOTA T - (1 1 1 1 1 1 1 1 COF -	L (CLASS 0 60 0 -60 0 -180 0 -180 0 -60 0 -60 0 -60 0 -60 NERGY = -	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.398	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
I 5 5 5 5 5 5 12 12 12 12 12 12	J 1 1 1 1 1 1 1 TOTA T - (1 1 1 1 1 1 1 1 1 1 1 TOF	L (CLASS 0 60 0 -60 0 -180 0 -60 0 -60 0 -60 0 -60 ERGY = - E B E N FF	ANGLE .0000 0.28 .0000 0.67 .0000 0.28 .0000 0.67 .0000 0.67 .0000 0.67 .0000 0.67 .0000 0.67 .0000 0.67 .0000 0.67 .0000 0.67 .0000 FOR	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.893	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
I 5 5 5 5 5 5 12 12 12 12 12 12	J 1 1 1 1 1 1 1 TOTA T - (1 1 1 1 1 1 1 1 1 1 1 TOF	L (CLASS 0 60 0 -60 0 -180 0 -60 0 -60 0 -60 0 -60 ERGY = - E B E N FF	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 FORMANGLE CONST	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.893	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057
I 5 5 5 5 5 5 12 12 12 12 O U ATOM I	J 1 1 1 1 1 1 1 TOTA T - (K 1 1 1 1 1 1 1 1 COF - ES K AL OUT	L (CLASS 0 60 0 -60 0 -180 0 -60 0 -60 0 -60 0 -60 0 FF CLASS E BENDING	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 FORMANGLE CONST	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.893	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057 0.000
I 5 5 5 5 5 5 12 12 12 12 O U ATOM I	J 1 1 1 1 1 1 1 TOTA T - (K 1 1 1 1 1 1 1 1 COF - ES K AL OUT	L (CLASS 0 60 0 -60 0 -180 0 -60 0 -60 0 -60 0 -60 0 FF CLASS E BENDING	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 FORMANGLE CONST	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.893	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057 0.000
I 5 5 5 5 5 5 12 12 12 12 V A	J 1 1 1 1 1 1 1 TOTA T - (K 1 1 1 1 1 1 1 1 COF - ES K AL OUT	L (CLASS 0 60 0 -60 0 -180 0 -60 0 -60 0 -60 0 -60 0 FF CLASS E BENDING	ANGLE .000 0.28 .000 0.67 .000 0.28 .000 0.28 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 0.67 .000 FORMANGLE CONST	V1 V2	V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.893	 -0.827 -0.826 0.000 0.000 -0.827 0.057 0.057

5			2.970		0.107		
			2.970		0.107		
			3.713		-0.044		
	5	2.903			-0.021		
5	5	2.400	2.970	0.022	0.107		
5	12	2.792	3.713	0.053	0.792		
12	5	2.792	3.713	0.053	0.792		
12	5	3.499	3.713	0.053	-0.044		
12	12	3.087	4.089	0.276	3.947		
	TOTAL	VAN DER W	AALS ENERG	Y = 5.74158	kcal/mol		
E L	ECTE	ROSTA	TICI	N T E R A C	TIONS		
ATOM	TYPES						
Ι	J	Rij	Qi	Qj	ENERGY	Z	
						-	
12	12	3.137	-0.290	-0.290	6.678		
	TOTAL	ELECTROST	ATIC ENERG	Y = 6.67788	kcal/mol		
тОпл	L ENERG	SY = 29.75	490 kcal/m	ol			
TOTA							
101A							
	E R G Y	Ĭ					
		Z.					
		7					
E N	ERGY	on the second se	C H I N G				
E N	ERGY ND S	STRET					
E N B O ATOM	ERGY NDS	S T R E T	IDEAL	FORCE			
E N B O ATOM	ERGY NDS	STRET	IDEAL	FORCE CONSTANT	. DELTA	A ENER	GY
E N B O ATOM I	ERGY NDS TYPES J	S T R E T BOND LENGTH	IDEAL LENGTH	CONSTANT			GY
E N B O ATOM I h1 c	ERGY NDS TYPES J 3 1	BOND LENGTH	IDEAL LENGTH	CONSTANT	-0.093	12.163	GY
E N B O ATOM I h1 c	ERGY NDS TYPES J 3 1 3 1	BOND LENGTH	IDEAL LENGTH 	CONSTANT 1406.346 1406.346	-0.093 -0.093	12.163 12.163	GY
E N B O ATOM I h1 c h1 c	ERGY NDS TYPES J 3 1 3 1 3 1	BOND LENGTH L.000 L.000	IDEAL LENGTH 1.093 1.093 1.093	CONSTANT 1406.346 1406.346 1406.346	-0.093 -0.093 -0.093	12.163 12.163 12.163	GY
E N B O ATOM I h1 c h1 c h1 c c3 c	E R G Y N D S TYPES J 3 1 3 1 3 1	BOND LENGTH 1.000 1.000 1.000	IDEAL LENGTH 1.093 1.093 1.093 1.535	CONSTANT 1406.346 1406.346 1406.346 1269.019	-0.093 -0.093 -0.093 0.005	12.163 12.163 12.163 0.032	GY
E N B O ATOM I h1 c h1 c h1 c c3 c c3 h	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1	BOND LENGTH 1.000 1.000 1.000 1.000	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346	-0.093 -0.093 -0.093 0.005 -0.093	12.163 12.163 12.163 0.032 12.163	GY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1	BOND LENGTH 1.000 1.000 1.000 1.540 1.000	IDEAL LENGTH 	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117	-0.093 -0.093 -0.093 0.005 -0.093 -0.116	12.163 12.163 12.163 0.032 12.163 15.718	GY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1 1 1	BOND LENGTH 1.000 1.000 1.000 1.000 1.540 1.000	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 12.163 0.032 12.163 15.718	GY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1 1 1	BOND LENGTH 1.000 1.000 1.000 1.000 1.540 1.000	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 12.163 0.032 12.163 15.718	GY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c c3 c	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1 1 1 1 1 TOTAL	BOND LENGTH	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 12.163 0.032 12.163 15.718	GY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c c3 c	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1 1 1 1 1 TOTAL	BOND LENGTH 1.000 1.000 1.000 1.000 1.540 1.000	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 12.163 0.032 12.163 15.718	GY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c c3 c	E R G Y N D S TYPES J 3 1 3 1 1 1 1 1 TOTAL	BOND LENGTH 1.000 1.000 1.000 1.540 1.000 1.670 1.670 BOND STRE	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 12.163 0.032 12.163 15.718	GY ————
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c c3 c	ERGY NDS TYPES J 3 1 3 1 1 1 1 1 TOTAL GLE	BOND LENGTH 1.000 1.000 1.000 1.540 1.000 1.670 1.670 BOND STRE B E N D VAL	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE I N G ENCE I	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 12.163 0.032 12.163 15.718	
E N B O ATOM I h1 c h1 c c3 c c3 c c3 c A N ATOM I	ERGY NDS TYPES J 3 1 3 1 1 1 1 1 TOTAL GLE TYPES J	BOND LENGTH 1.000 1.000 1.000 1.670 1.670 BOND STRE BEND VAL K AN	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 -0.095 -0.093 -0.116 -0.116	12.163 12.163 12.163 0.032 12.163 15.718 15.718	ENERGY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c c3 c	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1 1 1 TOTAL G L E TYPES J	BOND LENGTH 1.000 1.000 1.000 1.000 1.670 1.670 BOND STRE BEND VAL K AN	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE I N G ENCE I	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 0.032 12.163 15.718	ENERGY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c c3 c A N ATOM I c3 c	ERGY NDS TYPES J 3 1 3 1 1 1 1 1 TOTAL GLE TYPES J 3 h1	BOND LENGTH 1.000 1.000 1.000 1.000 1.670 1.670 BOND STRE BEND VAL KAN 109.500	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE I N G ENCE I GLE A 110.070	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -22 kJ/mol	12.163 12.163 12.163 0.032 12.163 15.718 15.718	ENERGY
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c C3 c A N ATOM I c3 c h1 c	E R G Y N D S TYPES J 3 1 3 1 3 1 1 1 1 1 TOTAL G L E TYPES J 3 h1 3 h1	BOND LENGTH 1.000 1.000 1.000 1.000 1.540 1.000 1.670 1.670 BOND STRE BEND VAL KAN 109.500 109.442	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE I N G ENCE I GLE A 110.070 109.550	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -22 kJ/mol	12.163 12.163 12.163 0.032 12.163 15.718 15.718	ENERGY 9
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c c3 c A N ATOM I c3 c h1 c h1 c	E R G Y N D S TYPES J 3 1 3 1 1 1 1 1 TOTAL G L E TYPES J TYPES J TOTAL 3 h1 3 h1 3 c1	BOND LENGTH 1.000 1.000 1.000 1.540 1.000 1.670 1.670 BOND STRE B E N D VAL K AN 109.500 109.442 109.442	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE I N G ENCE I GLE A 110.070 109.550 105.930	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -22 kJ/mol	12.163 12.163 12.163 0.032 12.163 15.718 15.718 DELTA DELTA 0.01 0.00 0.68	ENERGY 9 1
E N B O ATOM I h1 c h1 c c3 c c3 h c3 c A N ATOM I c3 c h1 c h1 c c3 c	E R G Y N D S TYPES J 3 1 3 1 1 1 1 1 TOTAL G L E TYPES J TYPES J TOTAL 3 h1 3 h1 3 c1	BOND LENGTH 1.000 1.000 1.000 1.540 1.000 1.670 1.670 BOND STRE B E N D VAL K AN 109.500 109.442 109.442	IDEAL LENGTH 1.093 1.093 1.093 1.535 1.093 1.786 1.786 TCHING ENE I N G ENCE I GLE A 110.070 109.550	CONSTANT 1406.346 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 RGY = 80.1	-0.093 -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -22 kJ/mol	DELTA DELTA DELTA 0.01 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03 0.03	ENERGY 9 1 8

```
1024 h1 c3 cl 109.442 105.930 183.005 0.061 0.688
1025 h1 c3 h1 109.442
                   109.550
                            164.039
                                    -0.002
                                            0.001
1026 c3 c3 h1 109.500 110.070
                           194.100
                                    -0.010
                                            0.019
1027 h1 c3 cl 109.442 105.930
                           183.005
                                    0.061
                                            0.688
1028 c3 c3 h1 109.500 110.070
                            194.100
                                   -0.010
                                            0.019
1029 h1 c3 cl 109.442 105.930
                           183.005
                                    0.061
                                            0.688
1030 c3 c3 cl 109.500 110.330
                           260.419 -0.014
                                            0.055
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
1031
1032
1033 T O R S I O N A L
1034
1035
    ----ATOM TYPES---- FORCE
                                TORSION
1036 I J K L CONSTANT
                                ANGLE n ENERGY
                           S
1037
    _____
    h1 c3 c3 h1 0.651 0 60.000 3 0.000
1038
1039 h1 c3 c3 h1
              0.651
                       0 -60.000 3
                                      0.000
              0.000
1040 h1 c3 c3 cl
                       0 -180.000 3
                                      0.000
1041 h1 c3 c3 h1 0.651
                       0 -180.000 3
                                      0.000
                       0
                           60.000 3
1042 h1 c3 c3 h1
              0.651
                                      0.000
1043 h1 c3 c3 cl
              0.000
                       0 -60.000 3
                                      0.000
              0.000
1044 cl c3 c3 h1
                       0 -60.000 3
                                      0.000
                       0
                           180.000 3
1045 cl c3 c3 h1
              0.000
                                      0.000
              0.000 0
                           60.000 3
1046 | cl c3 c3 cl
                                      0.000
      TOTAL TORSIONAL ENERGY = 0.000 kJ/mol
1047
1048
1049 IMPROPER TORSIONAL
1050
1051
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
    I J K L CONSTANT S ANGLE n ENERGY
1052
    _____
1053
1054
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
1055
1056 VAN DER WAALS
1057
1058 ATOM TYPES
    I J
             Rij kij ENERGY
1059
1060
    _____
           2.400
1061 h1 h1
                 0.030
1062 h1 h1
           2.400
                  0.030
1063 h1 cl
           3.499 -0.127
    h1 h1
           2.903 -0.031
1064
1065 h1 h1
           2.400
                  0.030
1066 h1 cl
           2.792
                  0.356
                  0.356
    cl h1
           2.792
1067
1068 cl h1
           3.499
                 -0.127
1069
    cl cl
           3.087
                  4.588
    TOTAL VAN DER WAALS ENERGY = 5.105 kJ/mol
1070
1071
1072 ELECTROSTATIC INTERACTIONS
```

```
1073
1074 ATOM TYPES
             Rij 332.17*QiQj ENERGY
1075
     I J
1076
1077 h1 h1
                     1.352
                              0.563
            2.400
1078 h1 h1 2.400 1.352 0.563
1079 h1 cl
             3.499 -3.809 -1.089
1080 h1 h1
             2.903
                     1.352
                              0.466
1081 h1 h1
             2.400
                     1.352
                              0.563
1082 h1 cl
             2.792
                     -3.809 -1.364
1083 cl h1
             2.792 -3.809 -1.364
             3.499 -3.809 -1.089
1084 cl h1
             3.087 10.728
1085 cl cl
                              3.476
      TOTAL ELECTROSTATIC ENERGY = 0.726 kJ/mol
1086
1087
1088 TOTAL ENERGY = 88.891 kJ/mol
1089
1090 A T O M T Y P E S
1091
1092 IDX TYPE RING
1093 | 1 1 NO
1094 2 1 NO
1095 | 3 5 NO
1096 | 4 5 NO
1097 5 12 NO
1098 | 6 5 NO
1099 7 5 NO
1100 8 12 NO
1101
1102 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
1158 6 0.044101
1159 7 0.044101
1160 8 -0.124211
1161
1162 ENERGY
1163
1164
1165 BOND STRETCHING
1166
1167 ATOM TYPES FF BOND IDEAL
                                       FORCE
                             LENGTH
                                      CONSTANT DELTA ENERGY
     I J CLASS LENGTH
1168
1169
1170
    5 	 1 	 0 	 1.000 	 1.093 	 4.766 	 -0.093
```

1171	5	1	0	1.0	000	1.093		-0.093	3.578
1172	5	1	0	1.0	000	1.093		-0.093	3.578
1173	1	1	0	1.	540	1.508	4.258	0.032	0.294
L174	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
175	1	12	0	1.0	570	1.773	2.974	-0.103	2.795
176	1	12	0	1.0	570	1.773	2.974	-0.103	2.795
177		TOT	AL BOND	STRETCI	HING ENER	GY = 20.1962	29 kcal/mol		
178									
179	A N	G L I	E BE	NDII	N G				
180									
181	ATON	4 TYPI	ES	FF	VALENCE	IDEAL	FORCE		
182	I	J	K	CLASS	ANGLE	ANGLE	CONSTANT	DELTA	ENERGY
183									
184	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
185	5	1	5	0	109.442	108.836	0.516	0.606	0.004
186	5	1	12	0	109.442	108.162	0.698	1.280	0.025
187	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
188	1	1	12	0	109.500	108.679	1.056	0.821	0.016
L189	5	1	12	0	109.442	108.162	0.698	1.280	0.025
1190	5	1	5	0	109.442	108.836	0.516	0.606	0.004
1191	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
L192	5	1	12	0	109.442	108.162	0.698	1.280	0.025
193	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
194	5	1	12	0	109.442	108.162	0.698	1.280	0.025
.195	1	1	12	0	109.500	108.679	1.056	0.821	0.016
.196		TOT	AL ANGL	E BENDII	NG ENERGY	= 0.20058	kcal/mol		
197									
198	ST	RE!	гсн	BENI	O I N G				
199									
200	ATON	4 TYPI	ES	FF	VALENCE	DELTA	FORCE	CONSTANT	
201								JК	
202									
.203	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
204	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
205	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
206	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
207	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
L208	5	1	12	0	109.442	1.280			-0.121
	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
L209		1		0	100 500	-1.049	0.227	0.070	-0.002
	1	1	5	0					
1210	1 5		12	0		1.280			-0.121
1210						1.280	-0.018 0.227		
L210 L211 L212	5	1 1	12 5	0	109.442 109.500	1.280 -1.049		0.070	-0.002
1210 1211 1212 1213	5 1	1 1 1	12 5	0 0 0	109.442 109.500 109.442	1.280 -1.049 1.280	0.227 -0.018	0.070	-0.002 -0.121
1209 1210 1211 1212 1213 1214 1215	5 1 5	1 1 1	12 5 12 12	0 0 0	109.442 109.500 109.442 109.500	1.280 -1.049 1.280	0.227 -0.018 0.176	0.070 0.380	-0.002 -0.121
1210 1211 1212 1213 1214	5 1 5	1 1 1	12 5 12 12	0 0 0	109.442 109.500 109.442 109.500	1.280 -1.049 1.280 0.821	0.227 -0.018 0.176	0.070 0.380	-0.002 -0.121
1210 1211 1212 1213 1214 1215	5 1 5 1	1 1 1 TOTA	12 5 12 12	0 0 0 0 TCH BENI	109.442 109.500 109.442 109.500	1.280 -1.049 1.280 0.821	0.227 -0.018 0.176	0.070 0.380	-0.002 -0.121
1210 1211 1212 1213 1214	5 1 5 1	1 1 1 TOTA	12 5 12 12 AL STRE	0 0 0 0 TCH BENI	109.442 109.500 109.442 109.500	1.280 -1.049 1.280 0.821	0.227 -0.018 0.176	0.070 0.380	-0.002 -0.121

	J	K	L	CLASS	ANGLE		V1	V2	V3	ENERGY	
221											
										-1.09	
										-0.24	
										98 0.050	
										-0.07	
										-1.09	
					-40.000					0.449	
										0.449	
										0.05	
30 12	1	1	12	0	80.000	0.000	0.	000	0.89	0.22	3
1	TOTA	L TORS	SIONAL	ENERGY	= -1.2953	4 kcal/	mol				
2											
3 O U	T - O) F – I	PLAN	IE B	ENDIN	G					
4											
ATO:	M TYPE	S		FF	OOP	FORC	EE				
I	J	K	L	CLASS	ANGLE	CONST	ANT	EN	ERGY		
3	TOTA	L OUT-	-OF-PLA	ANE BEND	ING ENERG	Y = 0.	00000	kcal	/mol		
V A	N D	ER	WAA	ALS							
2 ATO	M TYPE	S									
I	J		Rij	R*I	J EPSI	LON	ENERGY				
1											
5 5	5		2.518	2.9	70 0.	022	0.036				
5	5		2.300	2.9	70 0.	022	0.215				
5	12		3.474	3.7	13 0.	053	-0.041				
			2.885	2.9	70 0.	022	-0.021				
5	5		2.518	2.9	70 0.	022	0.036				
5	12		2.647	3.7	13 0.	053	1.520				
1 12	5		2.647	3.7	13 0.	053	1.520				
2 12	5		3.474	3.7	13 0.	053	-0.041				
3 12	12		3.338	4.0	89 0.	276	1.129				
Į.	TOTA	L VAN	DER WA	AALS ENE	RGY = 4.3	35500 k	cal/mo	1			
5											
6 E L	ЕСТ	ROS	вт а т	IC	INTER	A C T	I O N	S			
7											
8 ATO	M TYPE	S									
9 I	J		Rij	Qi	(Qj	ENE	RGY			
1 12	12	3.	.388	-0.290	-0.29	0 6	.182				
2	TOTA	L ELEC	CTROSTA	ATIC ENE	RGY = 6.	18170 k	cal/mo	1			
53											
	AL ENE	RGY =	28.942	230 kcal	/mol						
5		_			-						
	ERG	Y									
7	_ 10 0	-									
8											

ATOM TYPES BOND 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 12 c3 1.540 1.535 1269.019 0.005 0.032 12 c3 c3 1.540 1.535 1269.019 0.005 0.032 12 c3 c3 1.670 1.786 1168.117 -0.116 15.718 13 c1 1.670 1.786 1168.117 -0.116 15.718 13 c1 1.670 1.786 1168.117 -0.116 15.718 14 c3 c1 1.670 1.786 1168.117 -0.116 15.718 15 c1 1.670 1.786 1168.117 -0.116 15.718 16 c3 c1 1.670 1.786 168.117 -0.0116 15.718 17 AN G L E B E N D I N G 18 c3 c1 1.690 \$10.070 194.100 -0.010 0.019 16 c3 c1 109.442 109.550 164.039 -0.002 0.001 17 c3 c1 109.442 105.930 183.005 0.061 0.688 18 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 18 c3 c3 c1 109.442 105.930 183.005 0.061 0.688 19 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 19 c3 c3 c1 109.442 105.930 183.005 0.061 0.688 19 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 10 c3 c1 109.442 105.930 183.005 0.061 0.688 19 c3 c3 c1 109.442 105.930 183.005 0.061 0.688 19 c3 c3 c1 109.442 105.930 183.005 0.061 0.688 19 c3 c3 c1 109.500 110.070 194.100 -0.010 0.019 10 c3 c1 109.442 105.930 183.005 0.061 0.688 10 c3 c1 109.500 110.070 194.100 -0.010 0.019 10 c3 c1 109.500 110.070 194.100 -0.010 0.019 11 c3 c1 109.442 105.930 183.005 0.061 0.688 11 c3 c1 109.500 110.070 194.100 -0.010 0.019 11 c3 c1 109.400 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0							
I J LENGTH LENGTH CONSTANT DELTA ENERGY 11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 13 c3 1.540 1.535 1269.019 0.005 0.032 13 h1 1.000 1.093 1406.346 -0.093 12.163 13 c1 1.670 1.786 1168.117 -0.116 15.718 13 c1 1.670 1.786 1168.117 -0.116 15.718 15 c1 1.670 1.786 1168.117 -0.116 15.718 16 c1 1.670 1.786 1168.117 -0.116 15.718 17 OTAL BOND STRETCHING ENERGY = 80.122 kJ/mol A N G L E B E N D I N G AN G	B O N D	STRET	CHING				
I J LENGTH LENGTH CONSTANT DELTA ENERGY 11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 13 c3 1.540 1.535 1269.019 0.005 0.032 13 h1 1.000 1.093 1406.346 -0.093 12.163 13 c1 1.670 1.786 1168.117 -0.116 15.718 13 c1 1.670 1.786 1168.117 -0.116 15.718 15 c1 1.670 1.786 1168.117 -0.116 15.718 16 c1 1.670 1.786 1168.117 -0.116 15.718 17 OTAL BOND STRETCHING ENERGY = 80.122 kJ/mol A N G L E B E N D I N G AN G	AMOM MAT	EC DOND	TDEAT	EODGE			
11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 12 c3 c3 1.540 1.535 1269.019 0.005 0.032 12 c3 h1 1.000 1.093 1406.346 -0.093 12.163 13 c1 1.670 1.786 1168.117 -0.116 15.718 13 c1 1.670 1.786 1168.117 -0.116 15.718 15 c1 1.670 1.786 1168.117 -0.116 15.718 16 c3 c1 1.670 1.786 1168.117 -0.116 15.718 17 OTAL BOND STRETCHING ENERGY = 80.122 kJ/mol ANGLE BENDING ANGLE BENDING ANGLE ANGLE CONSTANT DELTA ENERGY 10 J K ANGLE ANGLE CONSTANT DELTA ENERGY 11 c3 c1 109.500 110.070 194.100 -0.010 0.019 11 c3 c1 109.442 105.930 183.005 0.061 0.688 12 c3 c1 109.500 110.070 194.100 -0.010 0.019 13 c3 c1 109.500 110.330 260.419 -0.014 0.055 14 c3 c1 109.442 105.930 183.005 0.061 0.688 15 c3 c1 109.500 110.070 194.100 -0.010 0.019 16 c3 c1 109.442 105.930 183.005 0.061 0.688 16 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 17 c3 c1 109.442 105.930 183.005 0.061 0.688 18 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 18 c3 c3 c1 109.442 105.930 183.005 0.061 0.688 19 c3 c3 c1 109.500 110.070 194.100 -0.010 0.019 19 c1 c3 c1 109.442 105.930 183.005 0.061 0.688 19 c3 c3 c1 109.500 110.070 194.100 -0.010 0.019 10 c3 c1 109.442 105.930 183.005 0.061 0.688 10 c3 c3 c1 109.500 110.070 194.100 -0.010 0.019 10 c3 c1 109.442 105.930 183.005 0.061 0.688 10 c3 c3 c1 109.500 110.070 194.100 -0.010 0.019 10 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055 10 c3 c3 c1 109.500 110.000 0 -160.000 3 0.326 11 c3 c3 c1 10.651 0 80.000 3 0.326 11 c3 c3 c1 10.651 0 -160.000 3 0.326 11 c3 c3 c1 0.000 0 -40.000 3 0.326 11 c3 c3 c1 0.000 0 -40.000 3 0.326 11 c3 c3 c1 0.000 0 -40.000 3 0.000 11 c3 c3 c1 0.000 0 -40.000 3 0.000 12 c3 c3 c1 0.000 0 -40.000 3 0.000 13 c3 c3 c1 0.000 0 -40.000 3 0.000 14 c3 c3 c1 0.000 0 -40.000 3 0.000					חביו יו	רא ביאביב	OCV.
11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 11 c3 1.000 1.093 1406.346 -0.093 12.163 13 c3 1.540 1.535 1269.019 0.005 0.032 12 c3 c3 1 1.670 1.786 1168.117 -0.116 15.718 13 c1 1.670 1.786 1168.117 -0.116 15.718 13 c1 1.670 1.786 1168.117 -0.116 15.718 14							
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10.00	h1 c3	1.000	1.093	1406.346	-0.093	12.163	
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TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol A N G L E	c3 cl	1.670	1.786	1168.117	-0.116	15.718	
ANGLE BENDING ANGLE BENDING ANGLE BENDING ANGLE BENDING ANGLE CONSTANT DELTA ENERGY DO 0.010 D	c3 cl	1.670	1.786	1168.117	-0.116	15.718	
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11 c3 c3 h1 0.651 0 80.000 3 0.326 11 c3 c3 h1 0.651 0 -40.000 3 0.326 11 c3 c3 c1 0.000 0 -160.000 3 0.000 11 c3 c3 h1 0.651 0 -160.000 3 0.326 11 c3 c3 h1 0.651 0 80.000 3 0.326 11 c3 c3 c1 0.000 0 -40.000 3 0.000 12 c3 c3 h1 0.000 0 -40.000 3 0.000 13 c3 c3 c1 0.000 0 -160.000 3 0.000 14 c3 c3 c1 0.000 0 80.000 3 0.000	I J	K L	CONSTANT	S	ANGLE	n ENERGY	
11 c3 c3 h1 0.651 0 -40.000 3 0.326 11 c3 c3 c1 0.000 0 -160.000 3 0.000 11 c3 c3 h1 0.651 0 -160.000 3 0.326 11 c3 c3 h1 0.651 0 80.000 3 0.326 11 c3 c3 c1 0.000 0 -40.000 3 0.000 12 c3 c3 h1 0.000 0 -40.000 3 0.000 12 c3 c3 h1 0.000 0 -160.000 3 0.000 12 c3 c3 c1 0.000 0 80.000 3 0.000							-
n1 c3 c3 c1 0.000 0 -160.000 3 0.000 n1 c3 c3 h1 0.651 0 -160.000 3 0.326 n1 c3 c3 h1 0.651 0 80.000 3 0.326 n1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -160.000 3 0.000 c1 c3 c3 c1 0.000 0 80.000 3 0.000							
n1 c3 c3 h1 0.651 0 -160.000 3 0.326 n1 c3 c3 h1 0.651 0 80.000 3 0.326 n1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -160.000 3 0.000 c1 c3 c3 c1 0.000 0 80.000 3 0.000							
n1 c3 c3 h1 0.651 0 80.000 3 0.326 n1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -160.000 3 0.000 c1 c3 c3 c1 0.000 0 80.000 3 0.000							
n1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -160.000 3 0.000 c1 c3 c3 c1 0.000 0 80.000 3 0.000							
cl c3 c3 h1 0.000 0 -40.000 3 0.000 cl c3 c3 h1 0.000 0 -160.000 3 0.000 cl c3 c3 cl 0.000 0 80.000 3 0.000							
cl c3 c3 h1 0.000 0 -160.000 3 0.000 cl c3 c3 cl 0.000 0 80.000 3 0.000							
cl c3 c3 cl 0.000 0 80.000 3 0.000							
TOTAL TOTAL BILLION - 1.500 RO/ ROI							
	101	I TONDIONAL	. 11111101 -	1.303 KU/I			

```
1318 IMPROPER TORSIONAL
1319
1320 ----ATOM TYPES---- FORCE IMPROPER_TORSION
1321 I J K L CONSTANT s ANGLE n
1322
    _____
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
1323
1324
1325 VAN DER WAALS
1326
1327 ATOM TYPES
1328
    I J
            Rij kij ENERGY
1329
            2.518 -0.013
1330 h1 h1
1331 h1 h1
           2.300
                   0.109
            3.474 -0.129
1332 h1 cl
1333 h1 h1
            2.885
                  -0.031
1334 h1 h1
            2.518
                  -0.013
1335 h1 cl
            2.647
                   1.083
            2.647
                   1.083
1336 cl h1
1337 cl h1
            3.474
                  -0.129
1338 cl cl
            3.338
                   0.738
     TOTAL VAN DER WAALS ENERGY = 2.701 kJ/mol
1339
1340
1341 ELECTROSTATIC INTERACTIONS
1342
1343 ATOM TYPES
1344
    I J
            Rij 332.17*QiQj ENERGY
1345
          2.518 1.352 0.537
1346 h1 h1
1347 h1 h1
            2.300
                   1.352
                          0.588
1348 h1 cl
            3.474 -3.809 -1.097
            2.885
                   1.352
                          0.469
1349 h1 h1
1350 h1 h1
           2.518
                   1.352
                          0.537
1351 h1 cl
            2.647 -3.809 -1.439
            2.647 -3.809 -1.439
1352 cl h1
1353 cl h1
            3.474
                  -3.809 -1.097
1354 cl cl
                          3.214
            3.338
                  10.728
     TOTAL ELECTROSTATIC ENERGY = 0.273 kJ/mol
1355
1356
1357 TOTAL ENERGY = 87.337 \text{ kJ/mol}
1358
1359 ATOM TYPES
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
     7 h1 NO
1413
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
    6 0.044101
1424
1425 7 0.044101
1426 8 -0.124211
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...
1434
    SETTING UP VAN DER WAALS CALCULATIONS...
1435
    SETTING UP ELECTROSTATIC CALCULATIONS...
1436
1437 E N E R G Y
1438
1439
1440
    BOND STRETCHING
1441
1442
    ATOM TYPES FF BOND IDEAL
                                   FORCE
     I J CLASS LENGTH
                                             DELTA
1443
                          LENGTH
                                   CONSTANT
                                                      ENERGY
1444
1445
     5 1
             0
                   1.000
                           1.093
                                     4.766
                                             -0.093
                                                      3.578
1446
     5
        1
              0
                   1.000
                           1.093
                                     4.766
                                             -0.093
                                                      3.578
1447
    1
        1
             0
                   1.540
                           1.508
                                     4.258
                                             0.032
                                                      0.294
1448
    1 5
             0
                   1.000
                           1.093
                                     4.766
                                             -0.093
                                                      3.578
1449
    1 12
             0
                   1.670
                           1.773
                                     2.974
                                             -0.103
                                                      2.795
    1 5
1450
              0
                   1.000
                           1.093
                                     4.766
                                             -0.093
                                                      3.578
1451
                                             -0.103
    1 12
                   1.670
                           1.773
                                     2.974
                                                      2.795
1452
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
1453
1454 ANGLE BENDING
1455
    ATOM TYPES FF VALENCE IDEAL FORCE
1456
1457
    I J K
                CLASS ANGLE
                               ANGLE
                                      CONSTANT
                                                 DELTA
                                                          ENERGY
1458
    ______
                 0 109.500 110.549
         1
            5
                                                          0.015
1459
     1
                                         0.636
                                                 -1.049
            5
                     109.442
1460
    5
        1
                 0
                             108.836
                                         0.516
                                                 0.606
                                                         0.004
    5
1461
        1 12
                 0
                     109.442 108.162
                                         0.698
                                                 1.280
                                                          0.025
                                         0.636
1462
    1
        1 5
                 0 109.500 110.549
                                                 -1.049
                                                          0.015
                 0 109.500 108.679
    1
1463
        1 12
                                         1.056
                                                 0.821
                                                          0.016
1464
    5 1 12
                 0 109.442 108.162
                                          0.698
                                                 1.280
                                                          0.025
```

1	1	_							
		5	0	109.500	110.5	549	0.636	-1.049	0.01
5	1	5	0	109.442	108.8	836	0.516	0.606	0.00
5	1	12	0	109.442	108.	162	0.698	1.280	0.02
1	1	5	0	109.500	110.5	549	0.636	-1.049	0.01
1	1	12	0	109.500	108.	679	1.056	0.821	0.01
5	1	12	0	109.442	108.	162	0.698	1.280	0.02
	TOTA	AL ANO	GLE BENDI	NG ENERGY	Y = 0.20	0058 kc	al/mol		
S T	R E	гс н	BEN	DING					
ATOM	4 TYPI	ES	FF	VALENCI	E DEI	LTA	FORCE	CONSTANT	
I	J	K	CLASS	ANGLE	ANG	GLE	ΙJ	JК	ENERGY
1	1	5	0	109.500	-1.0	049	0.227	0.070	-0.002
5	1	5	0	109.442	0.0	606	0.115	0.115	-0.033
5	1	12	0	109.442	1.2	280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.0	049	0.227	0.070	-0.002
1	1	12	0	109.500	0.8	821	0.176	0.386	-0.070
5	1	12	0	109.442	1.2	280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.0	049	0.227	0.070	-0.002
5	1	5	0	109.442	0.0	606	0.115	0.115	-0.033
5	1	12	0	109.442	1.2	280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.0	049	0.227	0.070	-0.002
1	1	12	0	100 500	0 (
		12	U	109.500	0.0	821	0.176	0.386	-0.070
5	TOTA	12 AL STE	0 RETCH BEN	109.442	1.2	280	-0.018		
	TOTA	12 AL STF	0 RETCH BEN A L	109.442 DING ENEI	1.2 $RGY = -0$	280 .69593	-0.018 kcal/mol	0.380	
T O	TOTAR S :	12 AL STE I O N ES	0 RETCH BEN A L	109.442 DING ENE	1.2 $RGY = -0$ $TORSION$	280 .69593 F	-0.018 kcal/mol	0.380 FANT	-0.121
T O ATOM	TOTA R S : 4 TYPI J	12 AL STF I O N ES K	0 RETCH BEN A L L	109.442 DING ENER FF CLASS	1.2 RGY = -0 FORSION ANGLE	280 .69593 F	-0.018 kcal/mol ORCE CONS	0.380 FANT V3 ENE	-0.121
T O ATOM	TOTA R S : 4 TYP1 J	12 AL STF I O N ES K	0 RETCH BEN A L L	109.442 DING ENER FF CLASS	1.2 RGY = -0 TORSION ANGLE	280 .69593 F	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE	-0.121
T O ATOM I 5	TOTA R S : 4 TYP1 J 1	12 AL STF I O N ES K 1	O RETCH BEN A L L 5	109.442 DING ENER FF CLASS 0 -20	1.2 RGY = -0 FORSION ANGLE	280 .69593 F 	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314	-0.121 GRGY 0.349
T O ATOM I 5 5	TOTA R S : 4 TYPI J 1	12 AL STF I O N ES K 1	O RETCH BEN L 5 5	109.442 DING ENER FF CLASS 0 -20 0 100	1.2 RGY = -0 TORSION ANGLE 0.000	280 .69593 F 0.284 0.284	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314 0.314	-0.121 ERGY -0.349 -0.991
T O ATOM I 5 5	TOTA R S : 4 TYPP J 1 1	12 AL STF I O N ES K 1 1	ORETCH BEN	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140	1.2 RGY = -0 FORSION ANGLE 0.000 0.000	280 .69593 F 0.284 0.284 0.678	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398	-0.121 GRGY 0.349 -0.991 0.129
T O ATOM I 5 5 5	R S : 4 TYPI J 1 1	12 AL STF I O N ES K 1 1 1	0 RETCH BEN A L 5 5 12 5	FF CLASS	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.678 0.284	-0.018 kcal/mol ORCE CONS V1 V2 -1.386 -1.386 -0.602 -1.386	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314	-0.121 ERGY -0.349 -0.991 0.129 -0.991
T O ATOM I 5 5 5 5	TOTA R S : 4 TYP1 J 1 1 1	12 AL STF I O N ES K 1 1 1	0 RETCH BEN A L 5 5 12 5 5	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 100 0 -140	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.678 0.284 0.284	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.314	-0.121 ERGY -0.349 -0.991 0.129 -0.991 -0.304
T O ATOM I 5 5 5 5 5	TOTA R S : 4 TYPP 1 1 1 1 1	12 AL STF I O N ES K 1 1 1 1	0 RETCH BEN A L 5 5 12 5 12	FF CLASS 0 -20 0 100 0 -140 0 0 -140 0 -20	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.678 0.284 0.284 0.678	-0.018 kcal/mol ORCE CONS V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.314 0.398	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886
T O ATOM I 5 5 5 12	TOTA R S : 4 TYP1 J 1 1 1 1 1	12 AL STF I O N ES K 1 1 1 1 1	0 RETCH BEN A L L 5 5 12 5 12 5 12 5	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 0 -140 0 0 -140 0 -20 0 -140	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.284 0.284 0.678 0.678	-0.018 kcal/mol ORCE CONS V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398	-0.121 GRGY -0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129
T O ATOM I 5 5 5 12 12	TOTA R S : 4 TYPP 1 1 1 1 1 1 1 1	12 AL STF I O N ES	0 RETCH BEN A L 5 5 12 5 12 5 5 12 5	FF CLASS 0 -20 0 100 0 -140 0 0 -140 0 -20 0 -140 0 -20 0 -140	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.678 0.284 0.678 0.678	-0.018 kcal/mol ORCE CONS V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886
T O ATOM I 5 5 5 12 12	TOTA R S : 4 TYP1 1 1 1 1 1 1	12 AL STF I O N ES K 1 1 1 1 1 1 1	0 RETCH BEN A L L 5 5 12 5 12 5 12	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 0 -140 0 0 -140 0 0 -140 0 0 -140 0 100 0 100	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.284 0.284 0.678 0.678 0.678 0.678	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886
T O ATOM I 5 5 5 12 12	TOTA R S : 4 TYP1 1 1 1 1 1 1	12 AL STF I O N ES K 1 1 1 1 1 1 1	0 RETCH BEN A L 5 5 12 5 12 5 5 12 5	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 0 -140 0 0 -140 0 0 -140 0 0 -140 0 100 0 100	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.284 0.284 0.678 0.678 0.678 0.678	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886
T O ATOM I 5 5 5 12 12 12	TOTA R S : 4 TYPP 1 1 1 1 1 1 TOTA	12 AL STF I O N ES K 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0 RETCH BEN A L L 5 5 12 5 12 5 12 5 12 8 RSIONAL E	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 -20 0 -140 0 -20 0 100 NERGY =	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.678 0.284 0.678 0.678 0.678 0.678	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886
T O ATOM I 5 5 5 12 12 12	TOTA R S : 4 TYPP 1 1 1 1 1 1 TOTA	12 AL STF I O N ES K 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0 RETCH BEN A L L 5 5 12 5 12 5 12	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 -20 0 -140 0 -20 0 100 NERGY =	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.678 0.284 0.678 0.678 0.678 0.678	-0.018 kcal/mol ORCE CONS' V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886
T O ATOM I 5 5 5 12 12 12 O U	TOTA R S : 4 TYPP J 1 1 1 1 1 TOTA T - (12 AL STF I O N ES	ORETCH BEN A L L 5 5 12 5 12 5 12 7 PLAN	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 0 -140 0 0 -140 0 0 -20 0 100 NERGY =	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	280 .69593 F 0.284 0.284 0.678 0.678 0.678 0.678 0.678	-0.018 kcal/mol ORCE CONS V1 V21.386 -1.386 -0.602 -1.386 -0.602 -0.602 -0.602 0.000	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886
T O ATOM I 5 5 5 12 12 12 12 ATOM	TOTA R S : 4 TYP1 1 1 1 1 1 TOTA T - (12 AL STF I O N ES K 1 1 1 1 1 1 1 1 CON THE STF I O N	0 RETCH BEN A L L 5 5 12 5 12 5 12 7 12 8 P L A N	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 -20 0 -140 0 -20 0 100 NERGY = E B E I	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	FORCE	-0.018 kcal/mol ORCE CONST V1 V2	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.398 0.893	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886
T O ATOM I 5 5 5 12 12 12 12 12	TOTA R S : 4 TYPP 1 1 1 1 1 1 TOTA T - (4 TYPP) J	12 AL STF I O N ES	0 RETCH BEN A L L 5 5 12 5 12 5 12 7 12 8 P L A N	109.442 DING ENER FF CLASS 0 -20 0 100 0 -140 0 -20 0 -140 0 -20 0 100 NERGY = E B E I FF CLASS	1.2 RGY = -0 FORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.76131 N D I N O OOP ANGLE	280 .69593 F 0.284 0.284 0.678 0.678 0.678 0.678 0.678 0.678	-0.018 kcal/mol ORCE CONS V1 V21.386 -1.386 -0.602 -1.386 -0.602 -0.602 -0.602 0.000	0.380 FANT V3 ENE 0.314 0.314 0.398 0.314 0.398 0.398 0.398 0.398 0.398 0.893	-0.121 ERGY 0.349 -0.991 0.129 -0.991 -0.304 0.886 0.129 0.886

ATOM TYPE	ES					
I J	Rij	R*IJ	EPSILON	ENERGY		
	2.638					
	2.232					
	3.399		0.053			
	2.831					
5 5						
	2.547					
	2.547					
	3.399					
	3.587					
TOTA	AL VAN DER WAA	LS ENERGY	= 4.94916	kcal/mol		
ELEC	T R O S T A T	IC IN	TERAC	TIONS		
ATOM TYPE						
	Rij					
	3.637					
	AL ELECTROSTAT					
1011	TITIOOTICE INC.					
			3.73722	KCa1/MO1		
ΤΩΤΔΙ. ΕΝΙ	FRGV = 31 1706			KCCI/ MOI		
TOTAL ENI	ERGY = 31.1706			KGGI/ MOI		
				KCGI/ MOI		
				Real/ Mol		
				Real/ Mol		
ENERO		i4 kcal/mo		Real/ Mol		
ENERO	G Y	i4 kcal/mo		Real/ Mol		
ENER (G Y	64 kcal/mo	1	Real/ Mol		
ENER (BOND ATOM TYPE	G Y S T R E T C ES BOND LENGTH	64 kcal/mo H I N G IDEAL LENGTH	force Constant	DELTA		
ENER (BOND ATOM TYPE I J	STRETC ES BOND LENGTH	64 kcal/mo	FORCE CONSTANT	DELTA		
ENERO BOND ATOM TYPE I J h1 c3	S T R E T C ES BOND LENGTH 1.000 1	H I N G IDEAL LENGTH	FORCE CONSTANT	DELTA 	12.163	
ENER (BOND ATOM TYPE I J h1 c3 h1 c3	STRETC ES BOND LENGTH 1.000 1 1.000 1	H I N G IDEAL LENGTH .093	FORCE CONSTANT 1406.346	DELTA -0.093 -0.093	12.163 12.163	
ENER (BOND ATOM TYPE I J h1 c3 h1 c3 c3 c3	S T R E T C ES BOND LENGTH 1.000 1 1.000 1 1.540 1	H I N G IDEAL LENGTH .093 .093	FORCE CONSTANT 1406.346 1406.346 1269.019	DELTA -0.093 -0.093 0.005	12.163 12.163 0.032	
ENER O BOND ATOM TYPE I J h1 c3 h1 c3 c3 c3 c3 h1	S T R E T C ES BOND LENGTH 1.000 1 1.540 1 1.000 1	H I N G IDEAL LENGTH .093 .093 .535	FORCE CONSTANT 	DELTA -0.093 -0.093 0.005 -0.093	12.163 12.163 0.032 12.163	
E N E R (B O N D ATOM TYPH I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1	S T R E T C ES BOND LENGTH 1.000 1 1.540 1 1.000 1 1.670 1	H I N G IDEAL LENGTH .093 .093 .535 .093	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117	DELTA -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 TYPH I J	STRETC ES BOND LENGTH 1.000 1 1.540 1 1.000 1 1.670 1 1.000 1	H I N G IDEAL LENGTH .093 .093 .535 .093 .786	FORCE CONSTANT 	DELTA -0.093 -0.093 0.005 -0.093 -0.116 -0.093	12.163 12.163 0.032 12.163 15.718 12.163	
E N E R (B O N D ATOM TYPH I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 h1 c3 c1 c3 h1	S T R E T C ES BOND LENGTH 1.000 1 1.540 1 1.670 1 1.670 1	H I N G IDEAL LENGTH .093 .093 .535 .093 .786 .093	FORCE CONSTANT 	DELTA -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	
E N E R (B O N D ATOM TYPH I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 h1 c3 c1 c3 h1	STRETC ES BOND LENGTH 1.000 1 1.540 1 1.000 1 1.670 1 1.000 1	H I N G IDEAL LENGTH .093 .093 .535 .093 .786 .093	FORCE CONSTANT 	DELTA -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	
E N E R (B O N D ATOM TYPH I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 h1 c3 c1 c3 h1	S T R E T C ES BOND LENGTH 1.000 1 1.540 1 1.670 1 1.670 1 1.670 1 1.670 1	H I N G IDEAL LENGTH .093 .093 .093 .786 .093 .786 CHING ENERG	FORCE CONSTANT 	DELTA -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	
E N E R (B O N D ATOM TYPH I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 h1 c3 c1 c3 h1	S T R E T C ES BOND LENGTH 1.000 1 1.540 1 1.670 1 1.670 1	H I N G IDEAL LENGTH .093 .093 .093 .786 .093 .786 CHING ENERG	FORCE CONSTANT 	DELTA -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	
ENERO BOND ATOM TYPE I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 h1 c3 c1 c3 h1	S T R E T C ES BOND LENGTH 1.000 1 1.540 1 1.670 1 1.670 1 1.670 1 1.670 1	H I N G IDEAL LENGTH .093 .093 .535 .093 .786 .093 .786 CHING ENERG	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 1168.117 GY = 80.13	DELTA -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	

1563	c3 c3 h1	109.500	110.070	194.100	-0	.010	0.019
4	h1 c3 h1	109.442	109.550	164.039	-0	.002	0.001
5	h1 c3 cl	109.442	105.930	183.005	0	.061	0.688
66	c3 c3 h1	109.500	110.070	194.100	-0	.010	0.019
67	c3 c3 cl	109.500	110.330	260.419	-0	.014	0.055
58	h1 c3 cl	109.442	105.930	183.005	0	.061	0.688
59	c3 c3 h1	109.500	110.070	194.100	-0	.010	0.019
70	h1 c3 h1	109.442	109.550	164.039	-0	.002	0.001
1	h1 c3 cl	109.442	105.930	183.005	0	.061	0.688
72	c3 c3 h1	109.500	110.070	194.100	-0	.010	0.019
73	c3 c3 cl	109.500	110.330	260.419	-0	.014	0.055
4	h1 c3 cl	109.442	105.930	183.005	0	.061	0.688
5	TOTA	AL ANGLE BE	NDING ENERGY	= 2.938	kJ/mol		
6							
7	TORSI	ONAL					
8							
9	АТОМ	TYPES	FORCE		TORSION		
)	I J	K L	CONSTANT	s	ANGLE	n	ENERGY
_							
2	h1 c3 c3	h1 0.6	51 0	-20.000	3	0.977	
3	h1 c3 c3	h1 0.6	51 0	100.000	3	0.977	
34	h1 c3 c3	cl 0.0	0 0	-140.000	3	0.000	
35	h1 c3 c3	h1 0.6	51 0	100.000	3	0.977	
36	h1 c3 c3	h1 0.6	51 0	-140.000	3	0.977	
37	h1 c3 c3	cl 0.0	0 0	-20.000	3	0.000	
88	cl c3 c3	h1 0.0	0 0	-140.000	3	0.000	
39	cl c3 c3	h1 0.0	0 0	-20.000	3	0.000	
0	cl c3 c3	cl 0.0	0 0	100.000	3	0.000	
	TOTA	L TORSIONA	L ENERGY =	3.908 kJ/	mol		
2							
3	IMPRO	PER T	O R S I O N	A L			
4							
5	ATOM	TYPES	FORCE	IMPROPER_	TORSION		
	I J	K L	CONSTANT	S	ANGLE	n	ENERGY
	TOTA	L IMPROPER	-TORSIONAL E	NERGY =	0.000 k	J/mol	
)							
)	V A N D	E R W A	ALS				
1							
2	ATOM TYPE						
03	I J	Rij	kij	ENERGY			
) 4							
)5		2.638					
06	h1 h1	2.232	0.205				
07	h1 cl	3.399	-0.133				
8 0	h1 h1	2.831					
09							
		2.638					
LO	h1 cl	2.547	2.064				
	h1 cl		2.064				
	h1 cl	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
1619
               Rij 332.17*QiQj ENERGY
    I J
1620 -----
1621 h1 h1
            2.638
                    1.352
                            0.513
1622 h1 h1
            2.232
                   1.352
                           0.606
            3.399 -3.809 -1.121
1623 h1 cl
                    1.352
1624 h1 h1
            2.831
                           0.478
1625 h1 h1
            2.638
                    1.352
                           0.513
            2.547 -3.809 -1.495
1626 h1 cl
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
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 ATOM TYPES
1671
1672
     IDX TYPE RING
1673 | 1 c3 NO
1674
     2 c3 NO
1675
     3 h1 NO
1676
     4 h1 NO
1677
     5 cl NO
     6 hl NO
1678
     7 h1 NO
1679
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
1697
     1 0.036009
1698
     2 0.036009
1699 3 0.044101
1700
     4 0.044101
     5 -0.124211
1701
1702 6 0.044101
1703 7 0.044101
1704
     8 -0.124211
1705
1706
     ENERGY
1707
1708
1709
    BOND STRETCHING
```

л пом	my DE C		DOMD		E-3.T	FORGE		
	J				EAL NGTH (CONSTANT	DELTA	ENERGY
5	1	0	1.0	00 1	.093	4.766	-0.093	3.578
5	1	0	1.0	00 1	.093	4.766	-0.093	3.578
1	1	0	1.5	40 1	.508	4.258	0.032	0.294
1	5	0	1.0	00 1	.093	4.766	-0.093	3.578
1	12	0	1.6	70 1	.773	2.974	-0.103	2.795
1	5	0	1.0	00 1	.093	4.766	-0.093	3.578
1	12	0	1.6	70 1	.773	2.974	-0.103	2.795
	TOTAL	BOND ST	RETCH	ING ENERG	Y = 20.196	529 kcal/mol		
AN	GLE	B E N	DIN	G				
ATOM	TYPES		FF	VALENCE	IDEAL	FORCE		
I	J	K C	CLASS	ANGLE	ANGLE	CONSTANT	r 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	12	0	109.442	108.162	0.698	1.280	0.025
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
1	1	12	0	109.500	108.679	1.056	0.821	0.016
5	1	12	0	109.442	108.162		3 1.280	
1	1	5			110.549		-1.049	0.015
5				109.442	108.836		0.606	
5	1	12		109.442			3 1.280	
1		5		109.500			-1.049	
1		12				1.056		
						0.698		
						3 kcal/mol		
ST	RET	С Н В	E N D	I N G				
ATOM	TYPES		FF	VALENCE	DELTA	FORCE	E CONSTANT	
						I J		ENERGY
						0.227		
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	5	0	109.500	-1.049	0.227	0.070	-0.002
1		12	0	109.500	0.821	0.176	0.386	-0.070
1 1	1				1 000	-0.018	0.380	-0.121
		12	0	109.442	1.280	0.010		
1	1	12 5		109.442		0.227	0.070	-0.002
1 5	1 1		0	109.500	-1.049			
1 5 1	1 1 1	5	0	109.500 109.442	-1.049	0.227 0.115	0.115	-0.033
1 5 1 5	1 1 1	5 5	0 0 0	109.500 109.442 109.442	-1.049 0.606 1.280	0.227 0.115	0.115 0.380	-0.033 -0.121
1 5 1 5 5	1 1 1 1	5 5 12	0 0 0 0	109.500 109.442 109.442 109.500	-1.049 0.606 1.280 -1.049	0.227 0.115 -0.018	0.115 0.380 0.070	-0.033 -0.121 -0.002

```
1759 TOTAL STRETCH BENDING ENERGY = -0.69593 kcal/mol
1760
1761
    TORSIONAL
1762
   ATOM TYPES
1763
                  FF TORSION FORCE CONSTANT
    I J K L CLASS ANGLE
                                V1 V2 V3 ENERGY
1764
1765
    5 1 1 5
1766
                  0 0.000 0.284 -1.386 0.314
                                                0.598
                  0 120.000 0.284 -1.386 0.314 -0.654
   5 1 1 5
1767
       1
          1 12
                  0 -120.000 0.678 -0.602
                                                0.116
1768
   5
                                         0.398
   5 1 1
             5
                  0 120.000 0.284 -1.386 0.314
1769
                                                -0.655
          1 5
                  0 -120.000 0.284 -1.386 0.314
                                               -0.655
       1
1770
   5
                      0.000 0.678 -0.602
                                                1.076
1771
   5
       1 1 12
                  0
                                         0.398
              5
                  0 -120.000 0.678 -0.602 0.398
                                                0.116
1772 12
       1 1
             5
          1
                  0 -0.000 0.678 -0.602 0.398
    12
       1
                                                1.076
1773
1774 12 1
          1 12
                  0 120.000 0.000 0.000 0.893
                                                0.893
      TOTAL TORSIONAL ENERGY = 1.91150 kcal/mol
1775
1776
1777 OUT-OF-PLANE BENDING
1778
                  FF OOP FORCE
1779 ATOM TYPES
    I J K
                 CLASS ANGLE CONSTANT
             L
1780
                                      ENERGY
1781
1782
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
1783
1784 VAN DER WAALS
1785
1786
   ATOM TYPES
    I J Rij R*IJ EPSILON ENERGY
1787
    _____
1788
             2.746
1789
    5 5
                    2.970
                          0.022
                                 -0.014
1790 5 5
            2.208
                   2.970
                          0.022
                                 0.377
1791 5 12
             3.280
                    3.713
                          0.053
                                 0.009
1792
    5 5
             2.746
                    2.970
                          0.022 -0.014
   5 5
                    2.970
                          0.022 -0.014
1793
             2.746
1794
   5 12
             2.512
                    3.713
                          0.053
                                 2.649
1795 12 5
             2.512
                    3.713
                          0.053
                                 2.649
    12 5
             3.280
                   3.713
                          0.053
                                 0.009
1796
    12 12
1797
             3.806
                    4.089
                          0.276
                                 -0.201
1798
      TOTAL VAN DER WAALS ENERGY = 5.44875 kcal/mol
1799
1800 ELECTROSTATIC INTERACTIONS
1801
1802
   ATOM TYPES
    I J
             Rij Qi Qj ENERGY
1803
1804
    _____
    12 12 3.856 -0.290 -0.290 5.432
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
    I J LENGTH
                   LENGTH CONSTANT DELTA ENERGY
1816
1817
1818 h1 c3
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
                         1406.346 -0.093
                  1.093
    h1 c3
          1.000
                                          12.163
1819
1820 c3 c3
          1.540
                  1.535
                         1269.019
                                   0.005
                                           0.032
1821 c3 h1
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
                         1168.117 -0.116
1822 c3 cl
                                          15.718
          1.670
                  1.786
1823 c3 h1
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
                         1168.117 -0.116 15.718
1824
    c3 cl 1.670
                  1.786
     TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
1825
1826
1827 ANGLE BENDING
1828
                        IDEAL
               VALENCE
                               FORCE
1829 ATOM TYPES
1830
    I J K
                ANGLE
                       ANGLE
                               CONSTANT
                                        DELTA
                                                ENERGY
1831
    ______
    c3 c3 h1 109.500
1832
                   110.070
                             194.100
                                     -0.010
                                              0.019
                                     -0.002
1833 h1 c3 h1 109.442 109.550
                            164.039
                                             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
1837 h1 c3 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
1838 c3 c3 h1
           109.500
                   110.070
                            194.100
                                     -0.010
                                             0.019
1839 h1 c3 h1 109.442 109.550
                            164.039
                                     -0.002
                                             0.001
1840 h1 c3 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
                            260.419
1842 c3 c3 cl 109.500 110.330
                                     -0.014
                                             0.055
                                     0.061
1843 h1 c3 cl 109.442
                   105.930
                            183.005
                                             0.688
1844
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
1845
1846 TORSIONAL
1847
    ----ATOM TYPES---- FORCE
                                 TORSION
1848
1849
    I J K
              L
                  CONSTANT
                                  ANGLE
                                        n
                                           ENERGY
                            S
1850
    ______
                       0
                            0.000 3
    h1 c3 c3 h1 0.651
1851
                                       1.303
                        0
                           120.000 3
1852 h1 c3 c3 h1
               0.651
                                        1.303
1853 h1 c3 c3 cl
              0.000
                        0 -120.000 3
                                       0.000
              0.651
                        0
1854 h1 c3 c3 h1
                           120.000 3
                                       1.303
                       0 -120.000 3
              0.651
1855 h1 c3 c3 h1
                                       1.303
1856 h1 c3 c3 cl 0.000
                     0 0.000 3
                                      0.000
```

```
1857 cl c3 c3 hl 0.000 0 -120.000 3 0.000
1858 cl c3 c3 h1
               0.000
                         0
                             -0.000 3
                                         0.000
1859 cl c3 c3 cl 0.000 0 120.000 3
                                         0.000
     TOTAL TORSIONAL ENERGY = 5.210 kJ/mol
1860
1861
1862 IMPROPER TORSIONAL
1863
1864 ----ATOM TYPES----
                    FORCE IMPROPER_TORSION
    I J K L CONSTANT S ANGLE n ENERGY
1865
1866
1867
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
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
1877 h1 h1
           2.746 -0.033
           2.746
1878 h1 h1
                  -0.033
1879 h1 cl
           2.512
                   2.571
                   2.571
1880 cl h1
           2.512
            3.280
1881 cl h1
                   -0.134
1882 cl cl 3.806 -0.542
    TOTAL VAN DER WAALS ENERGY = 4.485 kJ/mol
1883
1884
1885 ELECTROSTATIC INTERACTIONS
1886
1887 ATOM TYPES
    I J
              Rij 332.17*QiQj ENERGY
1888
1889
          2.746
1890 h1 h1
                   1.352
                          0.493
1891 h1 h1
           2.208
                   1.352
                          0.613
1892 h1 cl
           3.280 -3.809 -1.161
1893 h1 h1
           2.746
                   1.352
                          0.493
           2.746
                   1.352
1894 h1 h1
                          0.493
1895 h1 cl
           2.512
                  -3.809 -1.516
1896 cl h1
           2.512 -3.809 -1.516
            3.280 -3.809 -1.161
1897
    cl h1
1898 cl cl
            3.806
                  10.728
                          2.819
      TOTAL ELECTROSTATIC ENERGY = -0.446 kJ/mol
1899
1900
1901 TOTAL ENERGY = 92.310 \text{ kJ/mol}
1902
1903 A T O M T Y P E S
1904
1905 IDX TYPE RING
```

```
1906 | 1 1 NO
1907 | 2 1 NO
1908 | 3 5 NO
1909 4 5 NO
1910 5 12 NO
1911 6 5 NO
1912 7 5 NO
1913 8 12 NO
1914
1915 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
     6 0.000000
1923
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
1935 6 0.000000
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...
1944 SETTING UP OOP CALCULATIONS...
1945
     SETTING UP VAN DER WAALS CALCULATIONS...
1946
     SETTING UP ELECTROSTATIC CALCULATIONS...
1947
1948
     ATOM TYPES
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
1956
    6 hl NO
1957 7 h1 NO
1958 8 cl NO
1959
1960
    CHARGES
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
    8 -0.124211
1970
1971
1972
    SETTING UP CALCULATIONS
1973
1974
    SETTING UP BOND CALCULATIONS...
1975
    SETTING UP ANGLE CALCULATIONS...
1976
    SETTING UP TORSION CALCULATIONS...
    SETTING UP IMPROPER TORSION CALCULATIONS...
1977
1978
    SETTING UP VAN DER WAALS CALCULATIONS...
1979
    SETTING UP ELECTROSTATIC CALCULATIONS...
1980
1981
    ENERGY
1982
1983
1984 BOND STRETCHING
1985
1986 ATOM TYPES FF BOND IDEAL FORCE
1987
    I J
            CLASS LENGTH
                          LENGTH
                                  CONSTANT
                                            DELTA
                                                    ENERGY
1988
    ______
     5 1
             0
1989
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                     3.578
1990
        1
             0
                  1.000
                           1.093
                                    4.766
                                            -0.093
    5
                                                     3.578
1991
    1
        1
             0
                  1.540
                           1.508
                                    4.258
                                            0.032
                                                     0.294
                  1.000
    1 5
             0
                           1.093
                                    4.766
                                            -0.093
                                                    3.578
1992
    1 12
             0
1993
                  1.670
                           1.773
                                    2.974
                                            -0.103
                                                     2.795
1994
    1 12
             0
                  1.670
                           1.773
                                    2.974
                                            -0.103
                                                     2.795
                           1.093 4.766 -0.093
     1 5
                   1.000
1995
             0
                                                    3.578
1996
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
1997
1998
    ANGLE BENDING
1999
2000
    ATOM TYPES
                 FF VALENCE
                              IDEAL
                                      FORCE
                              ANGLE CONSTANT
2001
    I J K
               CLASS ANGLE
                                                DELTA ENERGY
2002
2003
    1 1 5 0 109.500 110.549 0.636 -1.049
```

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		0.636	-1.049	0.015
2007	1	1	12	0	109.500	108.679	1.056	0.821	0.016
2008	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2009	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2010	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2011	5	1	5	0	109.442	108.836	0.516	0.606	0.004
2012	1	1	12	0	109.500	108.679	1.056	0.821	0.016
2013	1	1	5	0	109.500	110.549	0.636	-1.049	0.015
2014	5	1	12	0	109.442	108.162	0.698	1.280	0.025
2015		TOTA	AL ANG	LE BENDI	NG ENERGY	a = 0.20058	3 kcal/mol		
2016									
2017	ST	R E	гсн	BEN	DING				
2018									
2019	ATOM	I TYPI	ES	FF	VALENCE	DELTA	FORCE	CONSTANT	
2020	I	J	K	CLASS	ANGLE	ANGLE	ΙJ	JК	ENERGY
2021									
2022	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2023	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
2024	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2025	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2026	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
2027	5	1	12	0	109.442	1.280	-0.018	0.380	
2028	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2029	5			0		1.280			-0.121
2030				0		0.606	0.115	0.115	-0.033
2031				0			0.176		
2032	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2033	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2034		TOTA	AL STR	RETCH BEN	DING ENER	GY = -0.695	593 kcal/mol		
2035									
2036	ТО	R S	I O N	A L					
2037									
2038		I TYPI					FORCE CONS		
2039	I	J	K	L	CLASS	ANGLE	V1 V2	V3 ENEI	RGY
2040		1	1					0 214	
2041	5		1				284 -1.386		
2042	5 5	1	1	12 5	0 -100 $0 140$		-0.602 -1.386		
2043	5			5	0 140		284 –1.386 284 –1.386		
2044	5	1	1	12	0 20				0.886
2045	5	1		5		.000 0.2			
2040	12	1	1	5		.000 0.6		0.314	-0.005
2048	12	1		12		.000 0.0			
2049	12	1			0 20				
2050						1.18015 kca		0.000	
2051		1011		U			, 1		
2052	O U	T - 0) F -	PLAN	E BEN	IDING			
1002	5 0	- (-	11 11		1, 0			

```
2053
                        OOP
2054 ATOM TYPES
                  FF
                              FORCE
    I J K L CLASS ANGLE CONSTANT ENERGY
2055
2056
2057
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
2058
2059 VAN DER WAALS
2060
2061
    ATOM TYPES
             Rij R*IJ EPSILON ENERGY
   I J
2062
2063
    _____
    5 5
2064
             2.831
                    2.970
                          0.022 -0.019
2065 5 5
             2.232
                    2.970
                          0.022
                                 0.328
2066 5 12
             3.129
                    3.713
                          0.053
                                 0.104
                          0.022
    5 5
             2.638
                    2.970
2067
                                  0.001
   5 5
             2.831
                    2.970
                          0.022 -0.019
2068
   5 12
             2.547
                    3.713
                          0.053
2069
                                 2.298
2070 12 5
             2.547
                          0.053
                    3.713
                                  2.298
2071 12 5
             3.129
                    3.713
                          0.053
                                  0.104
2072
    12 12
             3.975
                    4.089
                          0.276 -0.269
2073
      TOTAL VAN DER WAALS ENERGY = 4.82482 kcal/mol
2074
2075 ELECTROSTATIC INTERACTIONS
2076
2077
   ATOM TYPES
2078
    I J
             Rij Qi Qj ENERGY
2079
    ______
            4.025
                         -0.290
                  -0.290
    12 12
2080
      TOTAL ELECTROSTATIC ENERGY = 5.20367 kcal/mol
2.081
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
                                   DELTA ENERGY
2091
           LENGTH
                  LENGTH
2092
   ______
2093
    h1 c3 1.000
                 1.093 1406.346 -0.093
                                        12.163
2094 h1 c3
          1.000
                 1.093
                        1406.346
                                 -0.093
                                        12.163
   c3 c3
          1.540
                 1.535
                        1269.019
                                 0.005
2095
                                         0.032
                                -0.093 12.163
                        1406.346
2096 c3 h1
         1.000
                 1.093
          1.670
                 1.786
                        1168.117
                                        15.718
2097 c3 cl
                                 -0.116
                 1.786
2098 c3 cl
          1.670
                        1168.117
                                 -0.116
                                        15.718
   c3 h1 1.000 1.093 1406.346
                                 -0.093 12.163
2099
    TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
2100
2101
```

ANGLE	BENDI	N G							
ATOM TYPES	VALE	NCE :	IDEAL	F	ORCE				
	K ANG						DELT	'A 1	ENERGY
c3 c3 h1	109.500	110.070		194.10	0	-0.010		0.019	
h1 c3 h1	109.442	109.550		164.03	19	-0.002		0.001	
h1 c3 cl	109.442								
c3 c3 h1	109.500								
c3 c3 cl	109.500					-0.014			
h1 c3 cl	109.442								
c3 c3 h1	109.500					-0.010 0.061			
h1 c3 cl h1 c3 h1	109.442 109.442			164.03		-0.002			
c3 c3 cl	109.442								
	109.500								
	109.442								
	ANGLE BEND								
T O R S I	ONAL								
ATOM T	YPES	FORCE			TORSI	ON			
I J	K L	CONSTAN	Т	S	ANGI	LE n		ENERGY	
	1 0 651								
	1 0.651								
	 0.000 0.651 								
	1 0.651								
	1 0.000								
	1 0.651								
	1 0.000								
cl c3 c3 c	1 0.000	(0 :	140.000	3	0.	000		
cl c3 c3 h	1 0.000		0	20.000	3	0.	000		
TOTAL	TORSIONAL	ENERGY =	3	.908 kJ	/mol				
I M P R O	PER TO	R S I O	N A I	L					
	YPES							EMEDGY	
I J	K L	CONSTAN	Л,	S	ANGI	ır n		ENERGY	
тотът.	IMPROPER-TO	ORSTONAT	ENERG	 3Y =	0.000) k.T/mo	 1		
TOTAL	THI NOT EK-10	ONDIONAL	THER	J1 —	0.000	, 10,1110	_		
V A N D	ER WAA	L S							
J									
ATOM TYPES									
I J	Rij	kij		ENERGY					
h1 h1	2.831 -	0.032							
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
2155 cl h1
            2.547
                    2.064
            3.129 -0.106
2156 cl h1
2157 cl cl
            3.975 -0.548
       TOTAL VAN DER WAALS ENERGY = 3.480 kJ/mol
2158
2159
2160 ELECTROSTATIC INTERACTIONS
2161
2162 ATOM TYPES
2163 I J
             Rij 332.17*QiQj ENERGY
    _____
2164
2165 h1 h1
           2.831 1.352 0.478
2166 h1 h1
            2.232
                    1.352
                            0.606
2167 h1 cl
            3.129 -3.809 -1.217
2168 h1 h1
                            0.513
            2.638
                    1.352
            2.831
                    1.352
                            0.478
2169 h1 h1
2170 h1 cl
            2.547 -3.809 -1.495
2171 cl h1
            2.547 -3.809 -1.495
            3.129
2172 cl h1
                    -3.809
                           -1.217
2173 cl cl 3.975 10.728 2.699
      TOTAL ELECTROSTATIC ENERGY = -0.652 kJ/mol
2174
2175
2176 TOTAL ENERGY = 89.796 \text{ kJ/mol}
2177
2178 A T O M T Y P E S
2179
2180 IDX TYPE RING
2181 | 1 1 NO
2182 2 1 NO
2183 | 3 5 NO
2184 4 5 NO
2185 5 12 NO
2186 6 5 NO
2187 7 5 NO
2188 8 12 NO
2189
2190 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
2207 3 0.000000
2208 4 0.000000
2209 5 -0.290000
2210 | 6 0.000000
2211 7 0.000000
2212 8 -0.290000
2213
2214
     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
     6 h1 NO
2231
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...
    SETTING UP TORSION CALCULATIONS...
2251
2252
    SETTING UP IMPROPER TORSION CALCULATIONS...
2253
    SETTING UP VAN DER WAALS CALCULATIONS...
2254
    SETTING UP ELECTROSTATIC CALCULATIONS...
2255
2256
    ENERGY
2257
2258
    BOND STRETCHING
2259
2260
2261 ATOM TYPES FF BOND
                         IDEAL
                                  FORCE
2262
    I J CLASS LENGTH
                         LENGTH
                                                    ENERGY
                                 CONSTANT
                                           DELTA
2263
             0
2264
    5
        1
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                     3.578
    5
2265
        1
             0
                  1.000
                          1.093
                                   4.766
                                            -0.093
                                                    3.578
    12
                          1.773
                                   2.974
2266
        1
             0
                  1.670
                                           -0.103
                                                    2.795
                  1.540
    1
                          1.508
                                   4.258
                                            0.032
2267
        1
             0
                                                    0.294
2268
    1 5
             0
                  1.000
                          1.093
                                   4.766
                                            -0.093
                                                    3.578
2269
    1 12
             0
                  1.670
                          1.773
                                   2.974
                                                    2.795
                                           -0.103
    1 5
                  1.000
                          1.093
                                   4.766
                                           -0.093
2270
              0
                                                    3.578
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
2271
2272
2273
    ANGLE BENDING
2274
    ATOM TYPES
                FF VALENCE IDEAL
                                     FORCE
2275
     I J K
               CLASS ANGLE
2276
                              ANGLE
                                     CONSTANT
                                               DELTA
                                                        ENERGY
2277
2278
    1
        1 5
                0 109.500 110.549
                                       0.636
                                               -1.049
                                                        0.015
                   109.442 108.836
2279
     5
        1
           5
                 0
                                       0.516
                                               0.606
                                                        0.004
        1 12
                0 109.442 108.162
                                               1.280
2280
    5
                                       0.698
                                                       0.025
2281
    1
        1 5
                0 109.500 110.549
                                       0.636
                                               -1.049
                                                       0.015
2282
     1
        1 12
                0 109.500 108.679
                                        1.056
                                               0.821
                                                        0.016
                0 109.442 108.162
                                               1.280
    5
        1 12
                                       0.698
                                                        0.025
2283
                0 109.442 108.162
                                       0.698
2284
    5
        1 12
                                                1.280
                                                       0.025
2285
           5
                0 109.500 110.549
                                       0.636
                                               -1.049
                                                        0.015
    1
        1
                 0 109.442 108.836
    5
        1 5
                                       0.516
                                               0.606
2286
                                                        0.004
                0 109.500 108.679
2287
    1
        1 12
                                       1.056
                                               0.821
                                                       0.016
                                               1.280
2288
    5
        1 12
                    109.442 108.162
                                       0.698
                                                       0.025
                0
                   109.500 110.549 0.636
        1 5
                                               -1.049
2289
                0
                                                        0.015
       TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
2290
2291
2292
    STRETCH BENDING
2293
2294
    ATOM TYPES
                FF VALENCE
                              DELTA
                                       FORCE CONSTANT
                                       IJ JK
2295
    I J K
               CLASS ANGLE
                              ANGLE
                                                      ENERGY
2296
    1 1 5 0 109.500 -1.049 0.227 0.070
```

2298	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
2299	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2300	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2301	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
2302	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2303	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2304	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2305	5	1	5	0	109.442	0.606	0.115	0.115	-0.033
2306	1	1	12	0	109.500	0.821	0.176	0.386	-0.070
2307	5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
2308	1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
2309		TOTA	AL STI	RETCH BE	ENDING ENERGY	Y = -0.6959	3 kcal/mol		
2310									
2311	то	R S I	I O N	A L					
2312									
2313	ATOM	TYPE	ES		FF TO	RSION	FORCE CONS	TANT	
2314	I	J	K	L	CLASS A	NGLE	V1 V2	V3 ENE	RGY
2315									
2316	5	1	1	5	0 40.	000 0.28	4 -1.386	0.314	-0.243
2317					0 -80.				
2318	5			5		000 0.28			
2319	5			5					
2320	5			12					0.449
2321	5			5		000 0.28			
2322	12	1		5		000 0.67			
2323	12				0 160.				
2324					0 40.				0.449
2325					ENERGY = -0				
2326									
2327	ΟU	Т – () F -	PLAN	IE BENI	DING			
2328									
2329	ATOM	TYPE	ES		FF (OOP FOR	CE		
2330					CLASS A			ERGY	
2331									
2332		TOTA	AL OU'	Γ-OF-PL <i>E</i>	ANE BENDING	ENERGY = 0	.00000 kcal	/mol	
2333									
2334	V A	N I	ER	WAA	A L S				
2335									
2336	ATOM	TYPE	ES						
2337	I	J		Rij	R*IJ	EPSILON	ENERGY		
2338									
		5		2.885	2.970	0.022	-0.021		
					2.970				
					3.713				
2342					2.970				
2343					2.970				
2344					3.713				
2345					3.713				
2346					3.713				
2340	12	J		2.900	3./13	0.000	0.331		

				9 0.276			
	TOTA	L VAN DER W	IAALS ENER	GY = 3.6366	3 kcal/mol		
EL	ЕСТ	ROSTA	TICI	NTERAC	TIONS		
	I TYPE						
Ι	J	Rij	Qi	Qj	ENERGY	Y	
						-	
12	12	4.132	-0.290	-0.290	5.069		
	TOTA	L ELECTROSI	ATIC ENER	GY = 5.0691	15 kcal/mol		
TOTA	L ENE	ERGY = 27.86	335 kcal/1	mol			
E N	E R G	Y					
ВО	N D	STRET	CHING				
				FORCE			
					NT DELTA		
					-0.093		
					-0.093		
					-0.116		
					0.005		
					-0.093		
					-0.116		
					-0.093	12.163	
	TOTA	L BOND STRE	TCHING EN	ERGY = 80.	122 kJ/mol		
			TNC				
	G L E	BEND	I N G				
A N				TDE'AT.	iODCF		
A N ATOM	I TYPE	SS VAI	ENCE	IDEAL I		ኮ ድፒ-ጥል	FNERGY
A N ATOM I	I TYPE J	S VAI	ENCE	ANGLE CO	FORCE DNSTANT	DELTA	ENERGY
A N ATOM I	I TYPE J	S VAI K AN	ENCE	ANGLE CO	ONSTANT		
A N ATOM I	J :3 h1	K AN	JENCE JUSTINE	ANGLE CO 	ONSTANT 	0 0.01	 L9
A N ATOM I c3 c h1 c	1 TYPE J :3 h1 :3 h1	K AN	JENCE : : : : : : : : : : : : : : : : : : :	ANGLE CO 	ONSTANT 	0 0.00	 19)1
A N ATOM I c3 c h1 c h1 c	I TYPE J 3 h1 3 h1 3 c1	K AN 109.500 109.442 109.442	LENCE JUNE 110.070 109.550 105.930	ANGLE CO 	ONSTANT 00 -0.010 39 -0.002 05 0.063	0 0.03 2 0.00 1 0.68	
A N ATOM I c3 c h1 c h1 c c3 c	J TYPE J 3 h1 3 h1 3 c1 3 h1	K AN 109.500 109.442 109.500	JENCE JONE 110.070 109.550 105.930 110.070	194.10 164.03 183.00 194.10	ONSTANT 00 -0.010 39 -0.002 05 0.062 00 -0.010	0 0.03 2 0.00 1 0.68 0 0.03	 19 01 88 19
A N ATOM I c3 c h1 c h1 c c3 c c3 c	J 3 h1 3 h1 3 c1 3 h1	K AN 109.500 109.442 109.500 109.500	LENCE 110.070 109.550 105.930 110.070 110.330	194.10 164.03 183.00 194.10 260.41	ONSTANT 00 -0.010 39 -0.002 05 0.063 00 -0.010 19 -0.014	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05	
A N ATOM I c3 c h1 c c3 c h1 c c3 c	J 3 h1 3 h1 3 c1 3 c1	109.500 109.442 109.500 109.442 109.500 109.442	DENCE 110.070 109.550 105.930 110.330 105.930	194.10 164.03 183.00 194.10 260.41	ONSTANT 00	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05 1 0.68	
A N ATOM I c3 c h1 c h1 c c3 c h1 c h1 c	J 3 h1 3 h1 3 c1 3 c1 3 c1 3 c1	109.500 109.442 109.500 109.442 109.500 109.500 109.442	LENCE 110.070 109.550 105.930 110.330 105.930 105.930	194.10 164.03 183.00 194.10 260.41 183.00	ONSTANT 00	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05 1 0.68	1.9 0.1 3.8 3.9 5.5 3.8
A N ATOM I C3 C h1 C c3 C h1 C c3 C c3 C c3 C	1 TYPE J 3 h1 3 h1 3 c1 3 c1 3 c1 3 c1 3 c1 3 c1	K AN 109.500 109.442 109.500 109.442 109.442 109.442 109.442 109.500	LENCE 110.070 109.550 105.930 110.070 105.930 105.930 105.930	194.10 164.03 183.00 194.10 260.41 183.00 183.00	ONSTANT 00	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05 1 0.68 0 0.03	19 01 38 19 55 38 88
A N ATOM I c3 c h1 c c3 c h1 c c3 c h1 c h1 c c1 c	J 3 h1 3 h1 3 c1	109.500 109.442 109.500 109.442 109.500 109.442 109.442 109.442	110.070 109.550 105.930 110.070 110.330 105.930 105.930 105.930	194.10 164.03 183.00 194.10 260.41 183.00 183.00 194.10 164.03	ONSTANT 00	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05 1 0.68 1 0.68 0 0.03	19 01 38 19 55 38 38
A N ATOM I C3 C h1 C c3 C h1 C c3 C h1 C c3 C h1 C c3 C	1 TYPE J 3 h1 3 h1 3 c1 3 c1	K AN 109.500 109.442 109.500 109.442 109.500 109.442 109.442 109.442 109.500 109.442	LENCE 110.070 109.550 105.930 110.070 110.330 105.930 105.930 110.070 109.550 110.330	194.10 164.03 183.00 194.10 260.41 183.00 183.00 194.10 164.03 260.41	ONSTANT 00	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05 1 0.68 1 0.68 0 0.03 2 0.00 4 0.05	19 01 38 19 55 38 88 19
A N ATOM I c3 c h1 c c3 c h1 c c3 c h1 c c3 c h1 c h1 c c3 c h1 c h1 c	J 3 h1 3 h1 3 c1 3 c1 3 h1 3 c1 3 c1 3 c1 3 c1 3 c1 3 c1	109.500 109.442 109.500 109.442 109.500 109.442 109.500 109.442 109.500 109.442	110.070 109.550 105.930 110.070 110.330 105.930 110.070 109.550 110.330 105.930	194.10 164.03 183.00 194.10 260.41 183.00 194.10 164.03 260.41	ONSTANT 00	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05 1 0.68 0 0.03 2 0.00 4 0.05	19 01 38 19 55 38 38 19 01 55
A N ATOM I c3 c h1 c c3 c h1 c c3 c h1 c c3 c h1 c h1 c c3 c h1 c h1 c	1 TYPE J 3 h1 3 h1 3 c1 3 h1 3 h1	K AN 109.500 109.442 109.500 109.442 109.500 109.442 109.500 109.442 109.500 109.442 109.500	LENCE 110.070 109.550 105.930 110.070 105.930 105.930 105.930 110.070 109.550 110.330 105.930 110.070	194.10 164.03 183.00 194.10 260.41 183.00 194.10 164.03 260.41	ONSTANT 00	0 0.03 2 0.00 1 0.68 0 0.03 4 0.05 1 0.68 0 0.03 2 0.00 4 0.05	19 01 38 19 55 38 38 19 01 55

```
2396 TORSIONAL
2397
2398 ----ATOM TYPES----
                   FORCE
                                TORSTON
   I J K L CONSTANT
2399
                                ANGLE n ENERGY
                           S
    _____
2400
2401 h1 c3 c3 h1
              0.651
                      0
                           40.000 3
                                      0.326
2402 h1 c3 c3 cl
              0.000
                       0 -80.000 3
                                      0.000
2403 h1 c3 c3 h1
              0.651
                       0 160.000 3
                                      0.326
2404 h1 c3 c3 h1 0.651
                       0 160.000 3
                                      0.326
2405 h1 c3 c3 cl
              0.000
                       0
                          40.000 3
                                      0.000
2406 h1 c3 c3 h1
                       0 -80.000 3
              0.651
                                      0.326
              0.000
                       0 -80.000 3
2407 cl c3 c3 h1
                                      0.000
                       0 160.000 3
2408 cl c3 c3 cl
              0.000
                                      0.000
              0.000
                       0
                                      0.000
2409 cl c3 c3 h1
                           40.000 3
     TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
2410
2.411
2412 IMPROPER TORSIONAL
2413
2414 ----ATOM TYPES---- FORCE IMPROPER_TORSION
2415
    I J K L CONSTANT S ANGLE N ENERGY
2416
    _____
2417
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2418
2419 VAN DER WAALS
2420
2421 ATOM TYPES
    I J Rij kij ENERGY
2422
2423
         2.885 -0.031
2424 h1 h1
2425 h1 h1
           2.300
                 0.109
2426 h1 cl
          2.960
                 0.012
2427 h1 h1
          2.518 -0.013
2428 h1 h1
          2.885 -0.031
                 1.083
2429 h1 cl
           2.647
          2.647
                 1.083
2430 cl h1
2431 cl h1
          2.960
                 0.012
2432 cl cl
           4.082
                 -0.522
    TOTAL VAN DER WAALS ENERGY = 1.704 kJ/mol
2433
2434
2435 ELECTROSTATIC INTERACTIONS
2436
2437 ATOM TYPES
    I J
           Rij 332.17*QiQj ENERGY
2438
2439
2440 h1 h1
          2.885
                 1.352
                        0.469
2441 h1 h1
          2.300
                 1.352
                        0.588
          2.960 -3.809 -1.287
2442 h1 cl
          2.518
                 1.352
2443 h1 h1
                        0.537
         2.885 1.352
2444 h1 h1
                        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 \text{ kJ/mol}
2452
2453 ATOM TYPES
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
2481 2 0.290000
2482 3 0.000000
2483 4 0.000000
2484 5 -0.290000
     6 0.000000
2485
2486 7 0.000000
     8 -0.290000
2487
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
2498 A T O M T Y P E S
2499
2500 IDX TYPE RING
2501 1 c3 NO
2502 2 c3 NO
2503 | 3 h1 NO
2504 4 h1 NO
    5 cl NO
2505
2506 6 h1 NO
2507 7 h1 NO
2508
    8 cl NO
2509
2510 C H A R G E S
2511
2512 IDX CHARGE
2513 | 1 0.036009
2514 2 0.036009
2515 3 0.044101
2516 4 0.044101
2517 5 -0.124211
2518 | 6 0.044101
2519 7 0.044101
2520 8 -0.124211
2521
2522 SETTING UP CALCULATIONS
2523
2524
    SETTING UP BOND CALCULATIONS...
2525 | SETTING UP ANGLE CALCULATIONS...
2526 SETTING UP TORSION CALCULATIONS...
2527
     SETTING UP IMPROPER TORSION CALCULATIONS...
2528
    SETTING UP VAN DER WAALS CALCULATIONS...
2529
    SETTING UP ELECTROSTATIC CALCULATIONS...
2530
2531 ENERGY
2532
2533
2534 BOND STRETCHING
2535
2536 ATOM TYPES FF BOND IDEAL
                                        FORCE
     I J CLASS LENGTH
                                       CONSTANT
                                                   DELTA ENERGY
2537
                              LENGTH
2538
2539
     5 1
               0
                     1.000
                               1.093
                                          4.766
                                                   -0.093
                                                             3.578
               0
                                         2.974
                     1.670
                              1.773
2540 12 1
                                                   -0.103
                                                             2.795
2541 5 1 0 1.000
2542 1 1 0 1.540
                              1.093
                                         4.766
                                                  -0.093
                                                             3.578
                              1.508
                                         4.258
                                                   0.032
                                                            0.294
```

1	_	0	1.0	000	1.093			
					1.773		-0.103	
					1.093			3.578
	TOTA	L BOND	STRETCH	HING ENER	AGY = 20.1962	29 kcal/mol		
3 37		ъ. п	N D T 1					
A N	GLE	ВЕ	NDI	N G				
ΔͲ∩Ν	י ייעסד	q	ਬਬ	WAT.ENCE	: IDEAL	FORCE		
					ANGLE		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	12	0	109.442	108.162	0.698	1.280	0.025
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
1	1	12	0	109.500	108.679	1.056	0.821	0.016
5	1	12	0	109.442	108.162	0.698	1.280	0.025
				109.442	108.162	0.698	1.280	0.025
		12		109.500	108.679	1.056	0.821	0.016
		12			108.162			
					110.549			
				109.442	108.836	0.516	0.606	
1	1	5			110.549			
					= 0.20058			
S T	RET	СН	BENI) I N G				
ATOM	1 TYPE	S	FF	VALENCE	DELTA			
ATOM I	I TYPE	S K	FF CLASS	VALENCE ANGLE	ANGLE	ΙJ	JК	
ATOM I	I TYPE	S K	FF CLASS	VALENCE ANGLE		I J	J K	
ATOM I	I TYPE	S K	FF CLASS	VALENCE ANGLE 	ANGLE	I J 0.227	J К 	-0.002
ATOM I 1	1 TYPE J 	S K 5	FF CLASS	VALENCE ANGLE 109.500 109.442	ANGLE 	0.227 0.115	J К 	-0.002
ATOM I 1 5	I TYPE J 1 1	S K 5 5	FF CLASS 0	VALENCE ANGLE 109.500 109.442	ANGLE -1.049 0.606 1.280	I J 0.227 0.115	J K 0.070 0.115 0.380	-0.002 -0.033
ATOM I 1 5 5	I TYPE J 1 1	S K 5 5 12	FF CLASS 0 0 0	VALENCE ANGLE 109.500 109.442 109.442	ANGLE -1.049 0.606 1.280	0.227 0.115 -0.018 0.227	J K 0.070 0.115 0.380	-0.002 -0.033 -0.121 -0.002
ATOM I 1 5 5	1 TYPE J 1 1 1	S K 5 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 0.821	0.227 0.115 -0.018 0.227 0.176	J K 0.070 0.115 0.380 0.070	-0.002 -0.033 -0.121 -0.002
I 1 5 5 1	1 TYPE J 1 1 1 1	S K 5 12 5 12	FF CLASS 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500	ANGLE -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	-0.002 -0.033 -0.121 -0.002 -0.070
ATOM 1 5 5 1 1 5	1 TYPE J 1 1 1 1 1 1	S K 5 5 12 5 12	FF CLASS 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442	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	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121
ATOM I 1 5 5 1 1 5	1 TYPE J 1 1 1 1 1 1	S K 5 5 12 5 12 12	FF CLASS 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.500	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 0.176	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
ATOM I 1 5 1 1 5 1 5	1 TYPE J 1 1 1 1 1 1 1 1	S K 5 5 12 5 12 12 12 12	FF CLASS 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.500	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.821 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121 -0.070
ATOM I 1 5 5 1 5 5 1 5 5	1 TYPE J 1 1 1 1 1 1 1 1	S K 5 5 12 5 12 12 12 12 12	FF CLASS 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500 109.442 109.500 109.442 109.500	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.821 1.280	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.380 0.380 0.380	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.070
ATOM I 1 5 1 1 5 1 5 1 5	1 TYPE J 1 1 1 1 1 1 1 1	S K 5 5 12 5 12 12 12 12 12 5 5 5	FF CLASS 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	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 1.280 0.821 1.280	0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227 0.115	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.380 0.380 0.115	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.070 -0.121 -0.002 -0.033
ATOM I 1 5 1 5 1 5 1 5 1 5 1 5	1 TYPE J 1 1 1 1 1 1 1 1 1 1 1 1	S K 5 12 5 12 12 12 12 15 5 5 5 5	FF CLASS 0 0 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.500 109.442 109.500 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.821 1.280 -1.049 0.606	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227 0.115 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.380 0.380 0.115	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.070 -0.121 -0.002 -0.033
ATOM I 1 5 1 5 1 5 1 5 1 5 1 5	1 TYPE J 1 1 1 1 1 1 1 1 1 1 1 1	S K 5 12 5 12 12 12 12 15 5 5 5 5	FF CLASS 0 0 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.500 109.442 109.500 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 1.280 0.821 1.280 -1.049 0.606 -1.049	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227 0.115 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.380 0.380 0.115	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.070 -0.121 -0.002 -0.033
ATOM I 1 5 1 5 1 5 1 5 1	1 TYPE J 1 1 1 1 1 1 1 TOTA	S K 5 12 5 12 12 12 12 15 5 5 5 5	FF CLASS 0 0 0 0 0 0 0 0 0 0 0 0 rch beni	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.500 109.442 109.500 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 1.280 0.821 1.280 -1.049 0.606 -1.049	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227 0.115 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.380 0.380 0.115	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.070 -0.121 -0.002 -0.033
ATOM I 1 5 1 5 1 5 1 5 1 5 1	1 TYPE J 1 1 1 1 1 1 1 TOTA	S K 5 5 12 5 12 12 12 12 12 12 1	FF CLASS 0 0 0 0 0 0 0 0 0 0 0 TCH BENI	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.442 109.500 109.442 109.500 109.442 109.500	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.821 1.280 -1.049 0.606 -1.049	I J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227 0.115 0.227 0.115 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.380 0.385 0.380 0.070 0.115 0.070	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.070 -0.121 -0.002 -0.033
ATOM I 1 5 1 5 1 5 1 5 1 ATOM	1 TYPE J 1 1 1 1 1 1 1 TOTA R S I	S K 5 12 5 12 12 12 12 12 12 10 N S N S	FF CLASS 0 0 0 0 0 0 0 0 0 0 0 TCH BENI	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.500 109.442 109.500 109.442 109.500 109.442 109.500 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.821 1.280 -1.049 0.606 -1.049 0.606 -1.049	I J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227 0.115 0.227 0.115 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.380 0.385 0.380 0.070 0.115 0.070	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.002 -0.033 -0.002
ATOM I 1 5 1 5 1 5 1 T O ATOM I	I TYPE J 1 1 1 1 1 1 1 TOTA R S I	S K 5 5 12 5 12 12 12 12 12 12 1	FF CLASS 0 0 0 0 0 0 0 0 0 0 0 TCH BENI	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.500 109.442 109.500 109.442 109.500 The state of the st	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280 0.821 1.280 -1.049 0.606 -1.049	0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.176 -0.018 0.227 0.115 0.227 0.115 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.380 0.386 0.380 0.070 0.115 0.070	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.070 -0.121 -0.002 -0.033 -0.002

```
2592 5 1 1 5 0 60.000 0.284 -1.386 0.314 -0.827
2593
                   0 -180.000
                                           0.314
    5
       1
           1
              5
                              0.284 -1.386
                                                   0.000
2594
   5
       1
           1 12
                   0
                       60.000 0.678 -0.602
                                           0.398
                                                   0.057
2595 5
       1
           1 5
                   0 -180.000 0.284 -1.386
                                           0.314
                                                   0.000
           1
2596
    5
       1
              5
                   0 -60.000
                              0.284 - 1.386
                                           0.314
                                                  -0.826
       1
          1 12
                   0 180.000 0.000 0.000 0.893
                                                   0.000
2597 12
2598
    12
       1
           1 5
                   0 -60.000 0.678 -0.602
                                           0.398
                                                   0.057
    12
2599
       1
           1
              5
                   0
                       60.000 0.678 -0.602 0.398
                                                  0.057
     TOTAL TORSIONAL ENERGY = -1.42500 kcal/mol
2600
2601
2602 OUT-OF-PLANE BENDING
2603
                   FF
2604 ATOM TYPES
                         OOP
                               FORCE
2605
    I J K L CLASS ANGLE CONSTANT
                                       ENERGY
2606
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
2607
2608
2609
   VAN DER WAALS
2610
2611 ATOM TYPES
             Rij R*IJ EPSILON ENERGY
2612
    I J
2613
    ______
2614
    5 5
             2.903
                    2.970
                           0.022 -0.021
    5 5
                           0.022
                                  0.107
2615
             2.400
                    2.970
    5 12
             2.792
                    3.713
                           0.053
                                  0.792
2616
2617
    5 5
             2.400
                    2.970
                           0.022
                                  0.107
   5 5
                    2.970
2618
             2.903
                           0.022 -0.021
2619
    5 12
             2.792
                     3.713
                           0.053
                                   0.792
2620 12 5
             2.792
                    3.713
                           0.053
                                  0.792
2621 12 5
             2.792
                    3.713
                           0.053
                                  0.792
2622
    12 12
              4.118
                     4.089
                           0.276
                                  -0.275
      TOTAL VAN DER WAALS ENERGY = 3.06216 kcal/mol
2623
2624
2625 ELECTROSTATIC INTERACTIONS
2626
2627 ATOM TYPES
2628
    I J
             Rij Qi Qj ENERGY
2629
2630 12 12
                  -0.290
                         -0.290
            4.168
      TOTAL ELECTROSTATIC ENERGY = 5.02482 kcal/mol
2631
2632
2633 TOTAL ENERGY = 26.36292 kcal/mol
2634
2635
   ENERGY
2636
2637
2638 BOND STRETCHING
2639
2640 ATOM TYPES BOND IDEAL FORCE
```

1 2						LENGTH								
						 1.093								
						1.786								
5						1.093								
6						1.535								
7	c 3	h1		1.000)	1.093	1406	.346	_	0.093	. 1	12.163	3	
8	с3	cl		1.670)	1.786	1168	3.117	_	0.116	. 1	15.718	3	
9	с3	h1		1.000)	1.093	1406	3.346	_	0.093	1	12.163	3	
		T	OTA	AL BOND	STRET	CHING EN	NERGY =	80.	122	kJ/mo	1			
	A N	1 G	L E	В В Е	N D I	N G								
3														
	ATC	r MC	YPE	ES	VALE	NCE	IDEAL	E	FORCE					
						LE								
						110.070								
						109.550								
						105.930								
	c 3					110.070								
		c3				110.330		260.41						
	h1					105.930								
	h1					105.930								
		c3				110.330								
5	h1					105.930		183.00						
5	c3					110.070					010			
						109.550								
						110.070 ING ENEF						0.	019	
		1	OIF	IL ANGL	IE BEND	ING ENER	KGI –	2.90	00 KU	/ IIIO I				
	т () R	SI	ONA	. T.									
			_	. 0 .,										
		AT	MO	TYPES-		FORCE			TOR	SION				
						CONSTAN					n	ENEF	RGY	
	h1	с3	с3	cl	0.000		0 -	-60.000) 3		0.000)		
	h1	с3	с3	h1	0.651		0 -1	80.000) 3		0.000)		
	h1	с3	с3	cl	0.000		0	60.000) 3		0.000)		
	h1	с3	с3	h1	0.651		0 -1	80.000) 3		0.000)		
	h1	c3	c3	h1	0.651		0 -	-60.000) 3		0.000)		
2	cl	c3	c3	cl	0.000		0 1	80.000) 3		0.000)		
3	cl	c3	с3	h1	0.000		0 -	-60.000) 3		0.000)		
	cl										0.000)		
		Г	OTA	AL TORS	SIONAL	ENERGY =	= 0.	000 k	J/mol					
	IM	1 P	R C	PER	R T O	RSIC) N A I							
		_												
		AT	MO	TYPES-		FORCE	II	IPROPEF	R_TOR	SION				

```
2690 I J K L CONSTANT S ANGLE n ENERGY
2691
     TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
2692
2693
2694 VAN DER WAALS
2695
2696 ATOM TYPES
            Rij kij ENERGY
2697
    I J
    _____
2698
2699 h1 h1
           2.903 -0.031
2700 h1 h1
           2.400
                   0.030
           2.792
                   0.356
2701 h1 cl
2702 h1 h1
           2.400
                   0.030
2703 h1 h1
           2.903 -0.031
           2.792
                   0.356
2704 h1 cl
2705 cl h1
           2.792
                   0.356
2706 cl h1
           2.792
                   0.356
           4.118 -0.510
2707 cl cl
     TOTAL VAN DER WAALS ENERGY = 0.910 kJ/mol
2708
2709
2710 ELECTROSTATIC INTERACTIONS
2711
2712 ATOM TYPES
    I J
            Rij 332.17*QiQj ENERGY
2713
2714
2715 h1 h1 2.903 1.352
                          0.466
2716 h1 h1
           2.400
                   1.352
                          0.563
           2.792 -3.809 -1.364
2717 h1 cl
2718 h1 h1
           2.400
                   1.352
                          0.563
2719 h1 h1
           2.903
                   1.352
                          0.466
2720 h1 cl
           2.792
                  -3.809 -1.364
           2.792 -3.809 -1.364
2721 cl h1
2722 cl h1
           2.792
                  -3.809 -1.364
2723 cl cl
            4.118
                  10.728
                          2.605
    TOTAL ELECTROSTATIC ENERGY = -0.794 kJ/mol
2724
2725
2726 TOTAL ENERGY = 83.176 kJ/mol
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
     1 0.000000
2743
2744 2 0.000000
2745 3 0.000000
2746 4 0.000000
2747 5 0.000000
2748 6 0.000000
2749 7 0.000000
     8 0.000000
2750
2751
2752 PARTIAL CHARGES
2753
2754 IDX CHARGE
2755 1 0.290000
2756 2 0.290000
2757 3 0.000000
2758 4 0.000000
2759 5 -0.290000
2760 6 0.000000
2761 7 0.000000
2762 8 -0.290000
2763
2764 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
     ATOM TYPES
2773
2774
2775 IDX TYPE RING
     1 c3 NO
2776
2777
     2 c3 NO
     3 h1 NO
2778
2779
     4 h1 NO
2780 5 cl NO
2781
     6 hl NO
2782
     7 h1 NO
2783 8 cl NO
2784
2785 C H A R G E S
2786
2787
     IDX CHARGE
```

```
2788 1 0.036009
2789 2 0.036009
2790 3 0.044101
2791 4 0.044101
2792
    5 -0.124211
    6 0.044101
2793
2794 7 0.044101
2.795
    8 - 0.124211
2796
    SETTING UP CALCULATIONS
2797
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...
    SETTING UP ELECTROSTATIC CALCULATIONS...
2804
2805
2806 ENERGY
2807
2808
2809 BOND STRETCHING
2810
2811 ATOM TYPES FF BOND IDEAL FORCE
    I J CLASS LENGTH
                                            DELTA
2812
                         LENGTH
                                  CONSTANT
                                                    ENERGY
2813
2814 12 1
            0
                  1.670
                          1.773
                                    2.974
                                            -0.103
                                                     2.795
2815
    5
        1
             0
                  1.000
                          1.093
                                    4.766
                                            -0.093
                                                     3.578
    5
        1
             0
                  1.000
                          1.093
                                    4.766
                                           -0.093
2816
                                                    3.578
2.817
    1
        1
             0
                  1.540
                          1.508
                                    4.258
                                            0.032
                                                    0.294
2818
    1
        5
             0
                  1.000
                           1.093
                                    4.766
                                            -0.093
                                                     3.578
                                    2.974
2819
    1 12
             0
                  1.670
                          1.773
                                            -0.103
                                                    2.795
2820
    1 5
             0
                  1.000
                          1.093
                                    4.766
                                           -0.093
                                                    3.578
2821
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
2822
2823 ANGLE BENDING
2824
    ATOM TYPES FF VALENCE IDEAL FORCE
2825
2826
    I J K
                CLASS ANGLE
                              ANGLE
                                     CONSTANT
                                               DELTA
                                                        ENERGY
2827
    ______
                 0 109.500 110.549
2828
     1
        1
           5
                                        0.636
                                                -1.049
                                                         0.015
2829
    5
           5
                 0
                    109.442
                            108.836
                                       0.516
                                                0.606
                                                        0.004
        1
    5
        1 12
                                        0.698
                                                1.280
2830
                 0 109.442 108.162
                                                         0.025
                   109.500 110.549
        1 5
                 0
                                                -1.049
                                                         0.015
2831
     1
                                        0.636
                 0 109.500
2832
    1
        1 12
                            108.679
                                        1.056
                                                0.821
                                                         0.016
    5
2833
        1 12
                 0
                    109.442 108.162
                                        0.698
                                                1.280
                                                         0.025
        1 12
2834
    5
                 0 109.442 108.162
                                        0.698
                                                1.280
                                                         0.025
        1 12
                 0 109.500 108.679
    1
2835
                                        1.056
                                               0.821
                                                        0.016
                0 109.442 108.162
2836
    5 1 12
                                         0.698
                                                1.280
                                                         0.025
```

1			_					
_			0		110.549		-1.049	
5	1	_	0		108.836		0.606	
1					110.549		-1.049	0.01
	TOTA	AL ANG	SLE BENDII	NG ENERGY =	= 0.20058 kg	cal/mol		
G	D = 0		D D N 1	D T N G				
ST.	REI	Г С Н	BENI	DING				
7 mor	my D.	7.C		WAT ENGE	DELEA	EODGE /	CONCEANE	
					DELTA ANGLE			ENEDCI
			CLASS		ANGLE			
1	1	5	0		-1.049			
5	1	5	0		0.606			
5	1	12	0		1.280			
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
5	1	12	0		1.280			
1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5	1	12	0		1.280			
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
5			0		0.606			
			0		-1.049			
					Y = -0.69593			
го	RS]	I O N						
ATOM	TYPE	ES			RSION I			GY
ATOM	TYPE	ES			NGLE		V3 ENER	.GY
ATOM	TYPE	ES K			NGLE	V1 V2 V	V3 ENER	GY 0.449
ATOM I 	TYPE J	ES K	L (CLASS AN	NGLE 000 0.678	V1 V2 V 	V3 ENER	
ATOM I 5	TYPE J 1 1	ES K 1 1	L (0 -40.0 0 80.0	NGLE 	-0.602 -1.386	V3 ENER 0.398	0.449 -1.099
ATOM I 5 5	TYPE J 1 1 1	ES K 1 1	L (0 -40.0 0 80.0	NGLE 	V1 V2 V 	0.398 0.314	0.449 -1.099
ATOM I 5 5 5	TYPE J 1 1 1	ES K 1 1 1	L (0 -40.0 0 80.0 0 -160.0 0 80.0	NGLE 	-0.602 -1.386 -1.386 -0.602	0.398 0.314 0.314 0.398	0.449 -1.099 -0.075
ATOM I 5 5 5 5	J 1 1 1 1	K	L () 12 5 5 12 5 12 5	0 -40.0 0 80.0 0 -160.0 0 80.0	NGLE	V1 V2 V -0.602 -1.386 -1.386 -0.602 -1.386	0.398 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086
ATOM I 5 5 5 5 5	TYPE J 1 1 1 1	ES K 1 1 1 1 1 1 1 1 1	L () 12 5 5 12 5 12 5	0 -40.0 0 80.0 0 -160.0 0 80.0 0 -160.0 0 -40.0	NGLE 000 0.678 000 0.284 000 0.678 000 0.678 000 0.284 000 0.284	V1 V2 V -0.602 -1.386 -1.386 -0.602 -1.386	0.398 0.314 0.314 0.398 0.314 0.314	0.449 -1.099 -0.075 -0.086 -0.075 -0.243
ATOM I 5 5 5 5 5 12	TYPE J 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1 1 1 1 1	L (1) 12 5 5 12 5 12 5 12	0 -40.0 0 80.0 0 -160.0 0 80.0 0 -160.0 0 -40.0	NGLE 000 0.678 000 0.284 000 0.284 000 0.678 000 0.284 000 0.284	-0.602 -1.386 -1.386 -0.602 -1.386 -1.386 0.000	0.398 0.314 0.314 0.398 0.314 0.314 0.314	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223
ATOM I 5 5 5 5 12	TYPE J 1 1 1 1 1 1 1	K K 1 1 1 1 1 1 1 1 1 1 1 1 1	L 0 12 5 5 12 5 12 5 12 5 5	CLASS AND	NGLE	V1 V2 V1	0.398 0.314 0.314 0.398 0.314 0.314 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
ATOM I 5 5 5 5 12	TYPE J 1 1 1 1 1 1 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1 1 1	L (1) 12 5 5 12 5 12 5 5 12 5 5	CLASS AN 0 -40.0 0 80.0 0 -160.0 0 -160.0 0 -160.0 0 -160.0 0 -40.0 0 -160.0 0 80.0	NGLE	V1 V2 V1	0.398 0.314 0.314 0.398 0.314 0.314 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223
ATOM I 5 5 5 5 12 12	TYPE J 1 1 1 1 1 1 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1 1 1	L (1) 12 5 5 12 5 12 5 5 12 5 5	CLASS AN 0 -40.0 0 80.0 0 -160.0 0 -160.0 0 -160.0 0 -160.0 0 -40.0 0 -160.0 0 80.0	NGLE 000 0.678 000 0.284 000 0.678 000 0.284 000 0.284 000 0.284 000 0.284 000 0.678	V1 V2 V1	0.398 0.314 0.314 0.398 0.314 0.314 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
ATOM I 5 5 5 5 12 12	1 1 1 1 1 1 TOTA	ES K 1 1 1 1 1 1 1 1 1 1 The state of the s	L () 12 5 12 5 12 5 12 5 12 5 8SIONAL EI	CLASS AN 0 -40.0 0 80.0 0 -160.0 0 -160.0 0 -160.0 0 -160.0 0 -40.0 0 -160.0 0 80.0	NGLE 000 0.678 000 0.284 000 0.678 000 0.284 000 0.284 000 0.284 000 0.284 000 0.678 000 0.678 000 0.678	V1 V2 V1	0.398 0.314 0.314 0.398 0.314 0.314 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223
ATOM I 5 5 5 5 12 12	1 1 1 1 1 1 TOTA	ES K 1 1 1 1 1 1 1 1 1 1 The state of the s	L () 12 5 12 5 12 5 12 5 12 5 8SIONAL EI	CLASS AND	NGLE 000 0.678 000 0.284 000 0.678 000 0.284 000 0.284 000 0.284 000 0.284 000 0.678 000 0.678 000 0.678	V1 V2 V1	0.398 0.314 0.314 0.398 0.314 0.314 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223
ATOM I 5 5 5 5 12 12 12	TYPE J 1 1 1 1 1 1 TOTA	ES K 1 1 1 1 1 1 1 CONTROL TOP	L () 12 5 12 5 12 5 12 5 12 5 RSIONAL E	CLASS AND	NGLE 000 0.678 000 0.284 000 0.678 000 0.284 000 0.284 000 0.284 000 0.284 000 0.678 000 0.678 000 0.678	V1 V2 V1	0.398 0.314 0.314 0.398 0.314 0.314 0.314 0.314 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
ATOM I 5 5 5 5 12 12 12	TYPE J 1 1 1 1 1 1 TOTA TYPE	ES K 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 RSIONAL EI	CLASS AN 0 -40.0 0 80.0 0 -160.0 0 -160.0 0 -40.0 0 -160.0 0 -40.0 0 -40.0 E B E N I	NGLE 000 0.678 000 0.284 000 0.678 000 0.284 000 0.284 000 0.284 000 0.284 000 0.678 000 0.678 000 0.678 000 0.678	V1 V2 V1 V1 V2 V1	0.398 0.314 0.314 0.398 0.314 0.314 0.314 0.893 0.398 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
ATOM I 5 5 5 5 12 12 12 12 ATOM I	TYPE J 1 1 1 1 1 TOTA TYPE J	ES K 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	L (CLASS AND	NGLE	V1 V2 V1	0.398 0.314 0.314 0.314 0.314 0.314 0.893 0.398 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223
ATOM I 5 5 5 5 12 12 12 12 ATOM I	TYPE J 1 1 1 1 1 1 TOTE TYPE J	ES K 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	L (CLASS AND	NGLE 000 0.678 000 0.284 000 0.678 000 0.284 000 0.284 000 0.284 000 0.678 000 0.678 000 0.678 000 0.678 000 0.678 000 0.678	V1 V2 V1 V1 V2 V1	0.398 0.314 0.314 0.314 0.314 0.314 0.314 0.893 0.398 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223 0.449
ATOM I 5 5 5 5 12 12 12 12 ATOM I	TYPE J 1 1 1 1 1 1 TOTE TYPE J	ES K 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	L (CLASS AND	NGLE 000 0.678 000 0.284 000 0.678 000 0.284 000 0.284 000 0.284 000 0.284 000 0.678 000 0.678 000 0.678 000 0.678 000 0.678 000 0.678	V1 V2 V1 V1 V2 V1	0.398 0.314 0.314 0.314 0.314 0.314 0.314 0.893 0.398 0.398	0.449 -1.099 -0.075 -0.086 -0.075 -0.243 0.223

ATOM							
			R*IJ	EPSILON	ENERGY		
5	5	2.885	2.970	0.022	-0.021		
5	5	2.518	2.970	0.022	0.036		
5	12	2.647	3.713	0.053	1.520		
5	5	2.300	2.970	0.022	0.215		
5	5	2.885	2.970	0.022	-0.021		
		2.960			0.331		
		2.960			0.331		
				0.053			
				0.276			
				Y = 3.63663			
ELI	ЕСТ	ROSTA	TICI	NTERAC	TIONS		
ATOM	TYPES						
I	J	Rij	Qi	Qj	ENERG	Y	
						-	
12	12	4.132	-0.290	-0.290	5.069		
	TOTAL	ELECTROST	ATIC ENERG	Y = 5.06915	kcal/mol		
			22E 1-021/m	ol			
TOTA	L ENER	GY = 27.86	333 KCaI/III	0±			
TOTA	L ENER	GY = 27.86	333 KCal/III	01			
	L ENER		333 KCaI/III	01			
			333 KCal/III				
			333 RCa1/III				
E N I	E R G						
E N I	ERG	Y S T R E T	CHING				
E N I	E R G N D TYPES	Y S T R E T · BOND	C H I N G IDEAL	FORCE			
E N I B O I ATOM	E R G N D TYPES J	Y S T R E T BOND LENGTH	C H I N G IDEAL LENGTH	FORCE CONSTANT			
E N I B O I ATOM I	E R G N D TYPES J	Y S T R E T BOND LENGTH	C H I N G IDEAL LENGTH	FORCE CONSTANT			
ENI BOI ATOM I cl ci	E R G TYPES J	S T R E T BOND LENGTH 1.670	C H I N G IDEAL LENGTH 1.786	FORCE CONSTANT 1168.117	-0.116	15.718	
E N I B O I ATOM I cl c: h1 c:	ERG ND TYPES J	S T R E T 6 BOND LENGTH 1.670 1.000	C H I N G IDEAL LENGTH 1.786 1.093	FORCE CONSTANT 1168.117 1406.346	-0.116 -0.093	15.718 12.163	
E N I B O I ATOM I cl c: h1 c: h1 c:	E R G TYPES J 3 3	BOND LENGTH 1.670 1.000	C H I N G IDEAL LENGTH 1.786 1.093 1.093	FORCE CONSTANT 1168.117 1406.346 1406.346	-0.116 -0.093 -0.093	15.718 12.163 12.163	
E N I B O I ATOM I cl c: h1 c: c3 c:	ERG ND TYPES J 3 3 3 3	BOND LENGTH 1.670 1.000 1.000	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019	-0.116 -0.093 -0.093 0.005	15.718 12.163 12.163 0.032	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h:	E R G TYPES J 3 3 3 1	BOND LENGTH 1.670 1.000 1.000 1.540 1.000	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093	FORCE CONSTANT 	-0.116 -0.093 -0.093 0.005 -0.093	15.718 12.163 12.163 0.032 12.163	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 c: c3 c:	ERG TYPES J 3 3 3 1	BOND LENGTH 1.670 1.000 1.540 1.000 1.670	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117	-0.116 -0.093 -0.093 0.005 -0.093 -0.116	15.718 12.163 12.163 0.032 12.163 15.718	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h: c3 c: c3 h:	ERG TYPES J 3 3 3 1 1	BOND LENGTH 	C H I N G IDEAL LENGTH 1.786 1.093 1.535 1.093 1.786 1.093	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093	15.718 12.163 12.163 0.032 12.163 15.718	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h: c3 c: c3 h:	ERG TYPES J 3 3 3 1 1	BOND LENGTH 	C H I N G IDEAL LENGTH 1.786 1.093 1.535 1.093 1.786 1.093	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093	15.718 12.163 12.163 0.032 12.163 15.718	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h: c3 c: c3 h:	E R G TYPES J 3 3 3 1 1 1 TOTAL	BOND LENGTH 	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786 1.093 TCHING ENE	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093	15.718 12.163 12.163 0.032 12.163 15.718	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h: c3 c: c3 h:	E R G TYPES J 3 3 3 1 1 1 TOTAL	BOND LENGTH 	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786 1.093 TCHING ENE	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093	15.718 12.163 12.163 0.032 12.163 15.718	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h: c3 c: c3 h:	ERG TYPES J 3 3 3 1 1 TOTAL GLE	BOND LENGTH 1.670 1.000 1.000 1.540 1.000 1.670 1.000 BOND STRE	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786 1.093 TCHING ENE	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 RGY = 80.1	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093 22 kJ/mol	15.718 12.163 12.163 0.032 12.163 15.718	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h: c3 c: d3 h: A N C	E R G TYPES J 3 3 3 1 1 1 TOTAL G L E TYPES	BOND LENGTH 1.670 1.000 1.000 1.540 1.000 1.670 1.000 BOND STRE	C H I N G IDEAL LENGTH 1.786 1.093 1.535 1.093 1.786 1.093 TCHING ENE I N G ENCE I	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 RGY = 80.1	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093 22 kJ/mol	15.718 12.163 12.163 0.032 12.163 15.718 12.163	
E N I B O I ATOM I cl c: h1 c: c3 c: c3 h: c3 c: c3 h:	E R G TYPES J 3 3 3 1 1 TOTAL G L E TYPES J	S T R E T BOND LENGTH 1.670 1.000 1.000 1.540 1.000 1.670 1.000 BOND STRE B E N D VAL: K AN	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786 1.093 TCHING ENE I N G ENCE I GLE A	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 RGY = 80.1	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093 22 kJ/mol	15.718 12.163 12.163 0.032 12.163 15.718 12.163	ENERGY
E N I B O I ATOM I cl cd h1 cd h1 cd c3 cd c3 h2 c3 h2 A N O ATOM I	E R G TYPES J TOTAL TYPES J TOTAL TYPES J	S T R E T BOND LENGTH 1.670 1.000 1.000 1.540 1.000 1.670 1.000 BOND STRE B E N D VAL K ANG	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786 1.093 TCHING ENE I N G ENCE I GLE A	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 RGY = 80.1	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093 22 kJ/mol	15.718 12.163 12.163 0.032 12.163 15.718 12.163	ENERGY
E N I B O I ATOM I cl c3 h1 c3 c3 c3 c3 h2 A N C ATOM I c3 c3	E R G TYPES J TOTAL TYPES J TOTAL TYPES J TYPES J TYPES J	S T R E T BOND LENGTH 1.670 1.000 1.540 1.000 1.670 1.000 BOND STRE B E N D VAL K AN 109.500	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786 1.093 TCHING ENE I N G ENCE I GLE A 110.070	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 RGY = 80.1 DEAL FO NGLE CON 194.100	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093 22 kJ/mol	15.718 12.163 12.163 0.032 12.163 15.718 12.163	ENERGY
E N I B O I ATOM I cl c: h1 c: h1 c: c3 c: c3 h: c3 c: c3 h: c3 c: h1 c:	ERG TYPES J TOTAL TYPES J TOTAL TYPES J TYPES	S T R E T BOND LENGTH 1.670 1.000 1.000 1.540 1.000 1.670 1.000 BOND STRE B E N D VAL K ANG 109.500 109.442	C H I N G IDEAL LENGTH 1.786 1.093 1.093 1.535 1.093 1.786 1.093 TCHING ENE I N G ENCE I GLE A 110.070 109.550	FORCE CONSTANT 1168.117 1406.346 1406.346 1269.019 1406.346 1168.117 1406.346 RGY = 80.1	-0.116 -0.093 -0.093 0.005 -0.093 -0.116 -0.093 22 kJ/mol	15.718 12.163 12.163 0.032 12.163 15.718 12.163	ENERGY

h1 c3 c1 109.442 105.930 183.005 0.061 0.688 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY h1 c3 c3 c1 0.000 0 -40.000 3 0.326 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -40.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 c1 c3 c3 h1 0.000 1 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 c1 c3 c3 h1 0.000 1 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
h1 c3 c1 109.442 105.930 183.005 0.061 0.688 h1 c3 c1 109.442 105.930 183.005 0.061 0.688 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055 h1 c3 c1 109.442 105.930 183.005 0.061 0.688 c3 c3 h1 109.500 110.070 194.100 -0.010 0.015 h1 c3 h1 109.442 109.550 164.039 -0.002 0.003 c3 c3 h1 109.500 110.070 194.100 -0.010 0.015 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY h1 c3 c3 c1 0.000 0 -40.000 3 0.326 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -40.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.001 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 0 -40.000 0 -40.000 0 -40.000 0 -40.000 0 -40.000 0 -40.000 0 -40.000 0 -40.000 0 -40.000 0
h1 c3 c1 109.442 105.930 183.005 0.061 0.688 c3 c3 c1 109.500 110.330 260.419 -0.014 0.055 h1 c3 c1 109.442 105.930 183.005 0.061 0.688 c3 c3 h1 109.500 110.070 194.100 -0.010 0.015 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001 c3 c3 h1 109.500 110.070 194.100 -0.010 0.015 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE n ENERGY h1 c3 c3 c1 0.000 0 -40.000 3 0.326 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 c1 0.000 0 80.000 3 0.326 h1 c3 c3 c1 0.000 0 80.000 3 0.326 h1 c3 c3 c1 0.000 0 80.000 3 0.326 h1 c3 c3 c1 0.000 0 80.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.326 c1 c3 c3 c1 0.000 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.000 c1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 c1 0.000 0 80.000 3 0.000 c1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 c1 0.000 0 80.000 0 80.000 c1 c3 c3 c1 0.000 0 80.000 0 80.000 c1 c3 c3 c1 0.000 0 80.000 0 80.000 c1 c3 c3 c1 0.000 0 80.000 c1 c3 c3 c1 0.000 0 80.000 c
C3 C3 C1 109.500 110.330 260.419 -0.014 0.055 h1 C3 C1 109.442 105.930 183.005 0.061 0.688 C3 C3 h1 109.500 110.070 194.100 -0.010 0.019 h1 C3 h1 109.442 109.550 164.039 -0.002 0.001 C3 C3 h1 109.500 110.070 194.100 -0.010 0.019 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY
h1 c3 c1 109.442 105.930 183.005 0.061 0.688 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 h1 c3 h1 109.442 109.550 164.039 -0.002 0.001 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY
C3 C3 h1 109.500 110.070 194.100 -0.010 0.019 h1 C3 h1 109.442 109.550 164.039 -0.002 0.001 C3 C3 h1 109.500 110.070 194.100 -0.010 0.019 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
h1 c3 h1 109.442 109.550 164.039 -0.002 0.001 c3 c3 h1 109.500 110.070 194.100 -0.010 0.019 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY h1 c3 c3 c1 0.000 0 -40.000 3 0.000 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 c1 0.000 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 1 -30.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
C3 C3 h1 109.500 110.070 194.100 -0.010 0.019 TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY
TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol T O R S I O N A L ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY h1 c3 c3 c1 0.000 0 -40.000 3 0.326 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 c1 0.000 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
TORSIONAL ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY
ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY h1 c3 c3 c1 0.000 0 -40.000 3 0.000 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
ATOM TYPES FORCE TORSION I J K L CONSTANT S ANGLE N ENERGY h1 c3 c3 c1 0.000 0 -40.000 3 0.000 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
I
I J K L CONSTANT S ANGLE N ENERGY
h1 c3 c3 c1 0.000 0 -40.000 3 0.000 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
h1 c3 c3 c1 0.000 0 -40.000 3 0.000 h1 c3 c3 h1 0.651 0 80.000 3 0.326 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 c1 0.000 0 80.000 3 0.000 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE NERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
h1 c3 c3 h1
h1 c3 c3 h1
h1 c3 c3 c1 0.000 0 80.000 3 0.000 h1 c3 c3 h1 0.651 0 -160.000 3 0.326 h1 c3 c3 h1 0.651 0 -40.000 3 0.326 c1 c3 c3 c1 0.000 0 -160.000 3 0.000 c1 c3 c3 h1 0.000 0 -40.000 3 0.000 c1 c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
h1 c3 c3 h1
h1 c3 c3 h1
Cl c3 c3 cl 0.000 0 -160.000 3 0.000 cl c3 c3 h1 0.000 0 -40.000 3 0.000 cl c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
Cl c3 c3 h1 0.000 0 -40.000 3 0.000 cl c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
cl c3 c3 h1 0.000 0 80.000 3 0.000 TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT s ANGLE n ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY h1 h1 2.885 -0.031
TOTAL TORSIONAL ENERGY = 1.303 kJ/mol I M P R O P E R T O R S I O N A L ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE n ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
<pre>IMPROPER TORSIONALATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT s ANGLE n ENERGY</pre>
ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY h1 h1 2.885 -0.031
ATOM TYPES FORCE IMPROPER_TORSION I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY h1 h1 2.885 -0.031
I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol VAN DER WAALS ATOM TYPES I J Rij kij ENERGY h1 h1 2.885 -0.031
I J K L CONSTANT S ANGLE N ENERGY TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol VAN DER WAALS ATOM TYPES I J Rij kij ENERGY h1 h1 2.885 -0.031
TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY h1 h1 2.885 -0.031
V A N D E R W A A L S ATOM TYPES I J Rij kij ENERGY
ATOM TYPES I J Rij kij ENERGYh1 h1 2.885 -0.031
ATOM TYPES I J Rij kij ENERGYh1 h1 2.885 -0.031
I J Rij kij ENERGY h1 h1 2.885 -0.031
I J Rij kij ENERGY h1 h1 2.885 -0.031
h1 h1 2.885 -0.031
h1 h1 2.885 -0.031
h1 h1 2.518 -0.013
h1 cl 2.647 1.083
h1 h1 2.300 0.109
h1 h1 2.885 -0.031
h1 cl 2.960 0.012
cl h1 2.960 0.012
cl h1 2.960 0.012 cl h1 2.647 1.083
cl h1 2.960 0.012

```
2984
2985 ELECTROSTATIC INTERACTIONS
2986
2987 ATOM TYPES
2988
    I J
               Rij 332.17*QiQj ENERGY
2989
    _____
2990 h1 h1
            2.885 1.352
                            0.469
2991 h1 h1
            2.518
                    1.352
                            0.537
            2.647 -3.809 -1.439
2992 h1 cl
2993 h1 h1
            2.300
                    1.352
                            0.588
2994 h1 h1
            2.885
                    1.352
                            0.469
            2.960 -3.809 -1.287
2995 h1 cl
2996 cl h1
            2.960 -3.809 -1.287
2997 cl h1
            2.647
                   -3.809 -1.439
2998 cl cl
            4.082 10.728 2.628
2999
     TOTAL ELECTROSTATIC ENERGY = -0.761 kJ/mol
3000
3001 TOTAL ENERGY = 85.306 \text{ kJ/mol}
3002
3003 ATOM TYPES
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
```

```
3033 4 0.000000
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...
     SETTING UP TORSION CALCULATIONS...
3043
3044
     SETTING UP OOP CALCULATIONS...
3045 SETTING UP VAN DER WAALS CALCULATIONS...
     SETTING UP ELECTROSTATIC CALCULATIONS...
3046
3047
3048 ATOM TYPES
3049
3050 IDX TYPE RING
3051 1 c3 NO
3052 2 c3 NO
3053
     3 h1 NO
3054 4 h1 NO
3055 5 cl NO
     6 hl NO
3056
     7 h1 NO
3057
3058 8 cl NO
3059
3060
     CHARGES
3061
3062 IDX CHARGE
3063
     1 0.036009
3064 2 0.036009
3065 3 0.044101
3066
     4 0.044101
3067
     5 -0.124211
3068 6 0.044101
3069 7 0.044101
     8 -0.124211
3070
3071
     SETTING UP CALCULATIONS
3072
3073
3074 SETTING UP BOND CALCULATIONS...
     SETTING UP ANGLE CALCULATIONS...
3075
3076
     SETTING UP TORSION CALCULATIONS...
3077
     SETTING UP IMPROPER TORSION CALCULATIONS...
     SETTING UP VAN DER WAALS CALCULATIONS...
3078
     SETTING UP ELECTROSTATIC CALCULATIONS...
3079
3080
3081
     ENERGY
```

3082									
3083									
3084	ВО	N D	S T R E	T C F	HING				
3085									
3086	ATOM	TYPES	FF	BONI) II	DEAL	FORCE		
3087	I	J	CLASS	LENG	GTH L	ENGTH	CONSTANT	DELTA	ENERGY
3088									
3089	12	1	0	1.6	570	1.773	2.974	-0.103	2.795
3090	5	1	0	1.0	000	1.093	4.766	-0.093	3.578
3091	1	1	0	1.5	540	1.508	4.258	0.032	0.294
3092	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
3093	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
3094	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
3095	1	12	0	1.6	570	1.773	2.974	-0.103	2.795
3096		TOTAL	BOND S	TRETCE	HING ENER	GY = 20.19	629 kcal/mol		
3097									
3098	AN	GLE	B E N	DII	1 G				
3099									
							FORCE		
3101	I	J	K	CLASS	ANGLE	ANGLE	CONSTAN	T DELTA	ENERGY
3102									
3103							0.63		
3104							0.51	6 0.606	
3105					109.442	108.162	0.69		0.025
3106			5		109.500	110.549	0.63	6 -1.049	0.015
3107			12		109.500	108.679	1.05	6 0.821	0.016
3108			12		109.442		0.69	8 1.280	0.025
					109.500		1.05		
					109.442		0.69		
							0.69		
3112							0.63		
3113					109.500		0.63		
3114	5						0.51	6 0.606	0.004
3115		TOTAL	ANGLE	BENDI	NG ENERGY	= 0.2005	8 kcal/mol		
3116									
3117	ST	RET	С Н В	ENI	DING				
3118	7 EOM	mu DE C			173 T DNOD	DDI	FORG		
3119							FORC		ENEDGY
3120							IJ		
3121 3122							0.227		
3123	5						0.227		
3124	5		12				-0.018		
3125	1		5	0			0.227		
3126	1		12				0.227		
3127	5		12	0			-0.018		
3128	1		12				0.176		
3129	5		12	0		1.280		0.380	
3130	5		12	0		1.280		0.380	
0100	J	_		Ü	107.112	1.200	0.010	0.500	V • T L T

_		5	0		-1.0				
5					0.60				5 -0.033
	101A.	r SIKI	EICH BEI	NDING END	ERGY = -0.0	09393	KCa1/IIIO1		
ΤО	RSI	ONZ	Δ Т.						
		0 1, 1							
ATOM	4 TYPE	S		FF	TORSION	F	ORCE CONS	STANT	
I					ANGLE				ENERGY
12	1	1	5	0 -2	20.000	0.678	-0.602	0.398	0.886
12	1	1	5	0 10	0.000	0.678	-0.602	0.398	-0.005
12	1	1	12	0 -14	10.000	0.000	0.000	0.893	0.670
5	1	1	5	0 10	0.000	0.284	-1.386	0.314	-0.991
5	1	1	5	0 -14	0.000	0.284	-1.386	0.314	-0.304
5	1	1	12	0 -2	20.000	0.678	-0.602	0.398	0.886
5	1	1	5	0 -14	10.000	0.284	-1.386	0.314	-0.304
5	1	1	5	0 -2	20.000	0.284	-1.386	0.314	0.349
5	1	1	12	0 10	00.000	0.678	-0.602	0.398	-0.005
	TOTA	L TOR	SIONAL E	ENERGY =	1.18015	kcal/m	ol		
O U	T - O	F - 1	PLAN	E B E	NDING				
ATOM	1 TYPE:	S		FF	OOD				
_									
I					ANGLE (IERGY	
	J	K 	L 	CLASS	ANGLE (CONSTA	NT EI		
	J	K 	L 	CLASS		CONSTA	NT EI		
	J TOTA:	K L OUT-	L -OF-PLAN	CLASS	ANGLE (CONSTA	NT EI		
	J TOTA:	K L OUT-	L 	CLASS	ANGLE (CONSTA	NT EI		
 V A	J TOTA: N D	K L OUT- E R	L -OF-PLAN	CLASS	ANGLE (CONSTA	NT EI		
V A	J TOTA: N D	K L OUT- E R	L -OF-PLAN W A A	CLASS NE BENDIN	ANGLE (CONSTA = 0.0	NT EN		
V A ATOM	J TOTA: N D TYPE:	K L OUT- E R	L -OF-PLAN W A A Rij	CLASS NE BENDIN L S R*IJ	ANGLE (CONSTA 0.0	NT EN		
V A ATOM I	J TOTA: N D TYPE: J	K L OUT- E R	L -OF-PLAN W A A Rij	CLASS NE BENDIN L S R*IJ	ANGLE (CONSTA = 0.0	NT EN		
V A ATOM I 5	J TOTA: N D TYPE: J 5	K L OUT- E R S	L OF-PLAN W A A Rij 	CLASS NE BENDIN L S R*IJ 2.970	ANGLE (CONSTA = 0.0 N E 2 -	NT EN		
V A ATOM I 5 5	J TOTA: N D TYPE: J 5 5	K L OUT- E R S	L -OF-PLAN W A A Rij 2.831 2.638	CLASS NE BENDIN L S R*IJ 2.970	EPSILOI O 0.022	CONSTA = 0.0 N E 2 - 2	NT EN		
V A ATOM 5 5 5	J TOTA N D TYPE J 5 5 12	K L OUT- E R S	L 	CLASS NE BENDIN L S R*IJ 2.970 2.970 3.713	EPSILOI 0 0.02: 0 0.05:	CONSTA = 0.0 N E 2 - 2 3	NT EN		
UV A ATOM I 5 5 5	TOTA: N D TYPE: J 5 5 12	K L OUT- E R S	L -OF-PLAN W A A Rij 2.831 2.638 2.547 2.232	CLASS NE BENDIN L S R*IJ 2.970 2.970 3.713 2.970	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02:	CONSTA = 0.0 N E 2 - 2 3 2	NERGY 0.019 0.001 2.298 0.328		
V A ATOM 5 5 5 5	J TOTA: N D TYPE: J 5 5 12 5 5	K L OUT- E R S	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 2.970	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.02:	CONSTA = 0.0 N E 2 - 2 3 2 2 -	NERGY 0.019 0.001 2.298 0.328 0.019		
V A ATOM I 5 5 5 5 5	J TOTA: N D TYPE: J 5 5 12 5 12	K L OUT- E R S	L -OF-PLAN W A A Rij -2.831 2.638 2.547 2.232 2.831 3.129	CLASS NE BENDIN L S R*IJ 2.970 2.970 3.713 2.970 3.713	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.05:	CONSTA = 0.0 N E 2 - 2 3 2 2 3	NERGY 0.019 0.001 2.298 0.328 0.019 0.104		
V A ATOM I 5 5 5 5 12	J TOTA N D TYPE J 5 5 12 5 12 5	K L OUT- E R S	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831 3.129 3.129	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 3.713 3.713	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05:	N E	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104		
V A ATOM I 5 5 5 5 12 12	J TOTA: N D TYPE: J 5 5 12 5 12 5 5 5 5	K L OUT- E R S	L -OF-PLAN W A A Rij -2.831 2.638 2.547 2.232 2.831 3.129 3.129 2.547	CLASS NE BENDIN L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05: 0 0.05:	CONSTA = 0.0 N E 2 - 2 3 2 2 3 3 3 3	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104 2.298		
V A ATOM 1 5 5 5 5 12 12	J TOTA: N D TYPE: J 5 5 12 5 12 5 12 5 12	K L OUT- E R	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831 3.129 3.129 3.129 3.975	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 3.713 4.089	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05:	ONSTA = 0.0 N E 2 - 2 3 2 2 3 3 3 6 -	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104 2.298 0.269		
V A ATOM 1 5 5 5 5 12 12	J TOTA: N D TYPE: J 5 5 12 5 12 5 12 5 12	K L OUT- E R	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831 3.129 3.129 3.129 3.975	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 3.713 4.089	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05: 0 0.05:	ONSTA = 0.0 N E 2 - 2 3 2 2 3 3 3 6 -	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104 2.298 0.269		
V A ATOM I 5 5 5 12 12 12	J TOTA: N D TYPE: J 5 5 12 5 12 5 12 5 12 7 TOTA:	K L OUT- E R S	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831 3.129 3.129 3.129 2.547 3.975 DER WAA	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 3.713 3.713 4.089 ALS ENERG	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05:	CONSTA = 0.0 N E 2 - 2 3 2 - 3 3 3 6 - 482 kc	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104 2.298 0.269 al/mol		
V A ATOM I 5 5 5 12 12 12	J TOTA: N D TYPE: J 5 5 12 5 12 5 12 5 12 7 TOTA:	K L OUT- E R S	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831 3.129 3.129 3.129 2.547 3.975 DER WAA	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 3.713 3.713 4.089 ALS ENERG	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05:	CONSTA = 0.0 N E 2 - 2 3 2 - 3 3 3 6 - 482 kc	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104 2.298 0.269 al/mol		
V A ATOM I 5 5 5 12 12 12	J TOTA: N D TYPE: J 5 5 12 5 12 5 12 5 12 TOTA:	K L OUT- E R S	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831 3.129 3.129 3.129 2.547 3.975 DER WAA	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 3.713 3.713 4.089 ALS ENERG	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05:	CONSTA = 0.0 N E 2 - 2 3 2 - 3 3 3 6 - 482 kc	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104 2.298 0.269 al/mol		
V A ATOM I 5 5 5 12 12 12 12	J TOTA: N D TYPE: J 5 5 12 5 12 5 12 5 12 6 TOTA:	K L OUT- E R S S S S	LOF-PLAN W A A Rij 2.831 2.638 2.547 2.232 2.831 3.129 3.129 2.547 3.975 DER WAA	CLASS NE BENDIN L S R*IJ 2.970 3.713 2.970 3.713 3.713 4.089 ALS ENERG	EPSILOI 0 0.02: 0 0.02: 0 0.02: 0 0.02: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05: 0 0.05:	CONSTA = 0.0 N E 2 - 2 3 2 2 - 3 3 3 6 - 482 kc C T I	NERGY 0.019 0.001 2.298 0.328 0.019 0.104 0.104 2.298 0.269 al/mol		

```
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
                   LENGTH CONSTANT DELTA ENERGY
           LENGTH
3191
    I J
3192 -----
                         1168.117
3193 | cl c3
          1.670
                 1.786
                                 -0.116
                                         15.718
                        1406.346 -0.093
    h1 c3
          1.000
                 1.093
                                         12.163
3194
                 1.535
                         1269.019
                                  0.005
                                          0.032
3195 c3 c3
          1.540
                                         12.163
3196 c3 h1
          1.000
                  1.093
                         1406.346
                                 -0.093
3197 c3 h1
          1.000
                 1.093
                         1406.346
                                 -0.093
                                         12.163
          1.000
                  1.093
                         1406.346
                                         12.163
3198 c3 h1
                                  -0.093
3199
    c3 cl 1.670 1.786
                        1168.117 -0.116 15.718
    TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
3200
3201
3202 ANGLE BENDING
3203
                       IDEAL
3204
    ATOM TYPES
               VALENCE
                               FORCE
3205
    I J K
               ANGLE
                       ANGLE
                              CONSTANT
                                       DELTA ENERGY
3206
    ______
                                    -0.010
3207
    c3 c3 h1 109.500
                   110.070
                            194.100
                                             0.019
3208 h1 c3 h1 109.442 109.550
                           164.039
                                    -0.002
                                            0.001
3209 h1 c3 cl 109.442 105.930
                           183.005
                                    0.061
                                            0.688
3210 c3 c3 h1 109.500
                  110.070
                            194.100
                                    -0.010
                                            0.019
3211 c3 c3 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
          109.500
                           260.419
3213 c3 c3 c1
                  110.330
                                    -0.014
                                            0.055
3214 h1 c3 cl 109.442 105.930
                           183.005
                                    0.061
                                            0.688
3215 h1 c3 cl 109.442
                  105.930
                           183.005
                                    0.061
                                            0.688
3216 c3 c3 h1 109.500
                  110.070
                            194.100
                                    -0.010
                                            0.019
3217 c3 c3 h1 109.500 110.070
                           194.100
                                    -0.010
                                            0.019
3218 h1 c3 h1 109.442
                  109.550
                           164.039
                                    -0.002
                                            0.001
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
3219
3220
3221 TORSIONAL
3222
    ----ATOM TYPES---- FORCE
                                TORSION
3223
    I J K
                  CONSTANT
                                 ANGLE n
3224
              T.
                                          ENERGY
                           S
3225
    ______
                                      0.000
3226 cl c3 c3 h1 0.000
                     0 -20.000 3
                       0 100.000 3
3227 cl c3 c3 h1
              0.000
                                      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 -140.000 3
               0.651
                                        0.977
3231 h1 c3 c3 cl
               0.000
                        0
                            -20.000 3
                                        0.000
3232 h1 c3 c3 h1
               0.651
                        0 -140.000 3
                                        0.977
               0.651
                        0
3233 h1 c3 c3 h1
                            -20.000 3
                                        0.977
3234 h1 c3 c3 cl 0.000 0
                            100.000 3
                                        0.000
     TOTAL TORSIONAL ENERGY = 3.908 kJ/mol
3235
3236
3237 IMPROPER TORSIONAL
3238
3239
    ----ATOM TYPES---- FORCE IMPROPER TORSION
    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
    I J Rij kij
                            ENERGY
3247
3248
    h1 h1
3249
           2.831 -0.032
           2.638
3250 h1 h1
                  -0.029
3251 h1 cl
           2.547
                  2.064
3252 h1 h1
           2.232
                  0.205
           2.831
3253 h1 h1
                  -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
    TOTAL VAN DER WAALS ENERGY = 3.480 kJ/mol
3258
3259
3260 ELECTROSTATIC INTERACTIONS
3261
3262 ATOM TYPES
    I J
             Rij 332.17*QiQj ENERGY
3263
3264
3265 h1 h1
          2.831
                  1.352
                         0.478
           2.638
                  1.352
3266 h1 h1
                         0.513
3267 h1 cl
           2.547 -3.809 -1.495
3268 h1 h1
           2.232
                         0.606
                  1.352
    h1 h1
           2.831
                  1.352
3269
                         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
     TOTAL ELECTROSTATIC ENERGY = -0.652 kJ/mol
3274
3275
3276 TOTAL ENERGY = 89.796 kJ/mol
3277
```

```
3278 ATOM TYPES
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
3320 4 h1 NO
3321
     5 cl NO
3322 6 h1 NO
3323 7 h1 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
                                CONSTANT
                                         DELTA
3356
                        LENGTH
                                                 ENERGY
3357
                                  2.974
    12 1 0
                 1.670
3358
                         1.773
                                         -0.103
                                                  2.795
3359
    5
       1
            0
                 1.000
                         1.093
                                  4.766
                                         -0.093
                                                 3.578
3360
    1
       1
            0
                 1.540
                         1.508
                                  4.258
                                         0.032
                                                 0.294
    1 5
                 1.000
                         1.093
3361
            0
                                  4.766
                                         -0.093
                                                 3.578
3362 1 5
            0
                 1.000
                         1.093
                                  4.766
                                         -0.093
                                                 3.578
3363
    1 5
            0
                 1.000
                         1.093
                                  4.766
                                         -0.093
                                                 3.578
                         1.773 2.974 -0.103 2.795
    1 12
           0
                 1.670
3364
      TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
3365
3366
3367 ANGLE BENDING
3368
                FF VALENCE
                            IDEAL
                                   FORCE
3369
    ATOM TYPES
                            ANGLE CONSTANT DELTA ENERGY
    I J K
               CLASS ANGLE
3370
3371
    ______
3372
    1
       1 5
                0 109.500 110.549
                                     0.636
                                             -1.049
                                                     0.015
                0 109.442 108.836
       1 5
    5
                                             0.606
3373
                                     0.516
                                                     0.004
               0 109.442 108.162
                                             1.280
    5 1 12
                                     0.698
                                                     0.025
3374
              0 109.500 110.549
3375
    1 1 5
                                   0.636
                                            -1.049
                                                     0.015
```

1								
	1	12	0	109.500	108.679	1.056	0.821	0.01
5	1	12	0	109.442	108.162	0.698	1.280	0.02
1	1	12	0	109.500	108.679	1.056	0.821	0.01
5	1	12	0	109.442	108.162	0.698	1.280	0.02
5	1	12	0	109.442	108.162	0.698	1.280	0.02
1	1	5	0	109.500	110.549	0.636	-1.049	0.01
1	1	5	0	109.500	110.549	0.636	-1.049	0.01
5	1	5	0	109.442	108.836	0.516	0.606	0.00
	TOTA	AL ANG	GLE BENDI	NG ENERGY	= 0.20058]	ccal/mol		
ST	REI	г с н	B E N	D I N G				
ATOM	TYPE	ES	FF	VALENCE	DELTA	FORCE	CONSTANT	
I	J	K	CLASS	ANGLE	ANGLE	ΙJ	JК	ENERGY
				109.500	-1.049	0.227	0.070	-0.002
5	1	5	0	109.442	0.606	0.115	0.115	-0.033
	1			109.442	1.280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
5	1	5	0	109.442	0.606	0.115	0.115	-0.033
	TOTA	AL STE	RETCH BEN	DING ENERG	SY = -0.69593	3 kcal/mol		
	R S I	O N	A L					
ТО								
T O	I TYPE	ES			ORSION			
T O ATOM	I TYPE	ES			ORSION NGLE			RGY
T O ATOM I	I TYPE J	ES K	L	CLASS A	NGLE	V1 V2	V3 ENER	
T O ATOM I 12	I TYPE J 	ES K 	L 5	CLASS A	NGLE 000 0.678	V1 V2 3 -0.602	V3 ENER	1.076
T O ATOM I 12 12	J J 1 1	ES K 1 1	L 5 5	CLASS A 0	NGLE 000 0.678	V1 V2 	V3 ENER 0.398 0.398	1.076 0.116
T O ATOM I 12 12 12	J J 1 1 1	ES K 1 1 1	L 5 5 12	0 0. 0 120. 0 -120.	NGLE 000 0.678 000 0.678 000 0.000	V1 V2 	V3 ENER 0.398 0.398 0.893	1.076 0.116 0.893
T O ATOM I 12 12 12 5	J TYPE J 1 1 1 1	ES K 1 1 1 1 1	L 5 5 12 5	CLASS A 0 0. 0 120. 0 -120. 0 120.	NGLE 000 0.678 000 0.678 000 0.000 000 0.284	V1 V2 	0.398 0.398 0.398 0.893 0.314	1.076 0.116 0.893 -0.654
T O ATOM I 12 12 12 5 5	J TYPE J 1 1 1 1 1	K	L 5 5 12 5	CLASS A 0 0. 0 120. 0 -120. 0 120. 0 120.	NGLE 000 0.678 000 0.678 000 0.000 000 0.284	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386	V3 ENER 0.398 0.398 0.893 0.314 0.314	1.076 0.116 0.893 -0.654 -0.655
T O ATOM I 12 12 12 5 5 5	J TYPE J 1 1 1 1 1 1	K K 1 1 1 1 1 1 1 1 1	L 5 5 12 5 5 12	CLASS P. 0 0. 0 120. 0 120. 0 120. 0 -120. 0 -0.	000 0.678 000 0.678 000 0.000 000 0.284 000 0.284 000 0.678	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602	0.398 0.398 0.398 0.893 0.314 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076
T O ATOM I 12 12 12 5 5 5 5	J 1 1 1 1 1 1 1 1	K	L 5 5 12 5 12 5 12 5	CLASS 0 0 120 0 -120 0 120 0 -120 0 -120 0 0 -120	NGLE 000 0.678 000 0.678 000 0.000 000 0.284 000 0.284 000 0.284	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386	V3 ENER 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655
T O ATOM I 12 12 12 5 5 5 5	J 1 1 1 1 1 1 1 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1 1 1 1 1 1 1 1	L 5 5 12 5 5 12 5	CLASS 0 0 120 0 -120 0 120 0 -120 0 -120 0 0 -120 0 0 0 0 0 0 0 0 0 0 0 0	000 0.678 000 0.678 000 0.000 000 0.284 000 0.284 000 0.284 000 0.284	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386 4 -1.386	0.398 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655 0.598
T O ATOM I 12 12 12 5 5 5 5 5	I TYPE J 1 1 1 1 1 1 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1 1 1	L 5 5 12 5 12 5 12 5 12	CLASS A 0 0. 0 120. 0 -120. 0 -120. 0 -120. 0 -120. 0 0 -120. 0 120.	NGLE 000 0.678 000 0.678 000 0.000 000 0.284 000 0.678 000 0.284 000 0.284 000 0.678	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386 4 -1.386 5 -0.602	0.398 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655 0.598
T O ATOM I 12 12 12 5 5 5 5	I TYPE J 1 1 1 1 1 1 1 1 1 1 1 1	ES K 1 1 1 1 1 1 1 1 1	L 5 5 12 5 12 5 12 5 12	CLASS A 0 0. 0 120. 0 -120. 0 -120. 0 -120. 0 -120. 0 0 -120. 0 120.	000 0.678 000 0.678 000 0.000 000 0.284 000 0.284 000 0.284 000 0.284	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386 4 -1.386 5 -0.602	0.398 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655 0.598
T O ATOM I 12 12 12 5 5 5 5 5	TYPE J 1 1 1 1 1 1 TOTA	ES K 1 1 1 1 1 1 1 1 1 1 THE STATE OF	L 5 5 12 5 12 5 12 5 12 5 RSIONAL E	CLASS A 0 0. 0 120. 0 -120. 0 -120. 0 -120. 0 0 -120. 0 120. SNERGY = 1	000 0.678 000 0.678 000 0.000 000 0.284 000 0.678 000 0.284 000 0.284 000 0.678 000 0.284	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386 4 -1.386 5 -0.602	0.398 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655 0.598
T O ATOM I 12 12 12 5 5 5 5 5	TYPE J 1 1 1 1 1 1 TOTA	ES K 1 1 1 1 1 1 1 1 1 1 THE STATE OF	L 5 5 12 5 12 5 12 5 12 5 RSIONAL E	CLASS A 0 0. 0 120. 0 -120. 0 -120. 0 -120. 0 -120. 0 0 -120. 0 120.	000 0.678 000 0.678 000 0.000 000 0.284 000 0.678 000 0.284 000 0.284 000 0.678 000 0.284	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386 4 -1.386 5 -0.602	0.398 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655 0.598
T O ATOM I 12 12 12 5 5 5 5 0 U	1 TYPE J 1 1 1 1 1 TOTA	ES K 1 1 1 1 1 1 1 OF -	L 5 5 12 5 12 5 12 5 12 7 RSIONAL E	CLASS A 0 0. 0 120. 0 -120. 0 -120. 0 -120. 0 -120. 0 0. 120. ENERGY = 1	NGLE 000 0.678 000 0.678 000 0.000 000 0.284 000 0.678 000 0.284 000 0.678 000 0.284 000 0.678 .91150 kcal	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386 4 -1.386 4 -1.386 7 -0.602 7 mol	0.398 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655 0.598
T O ATOM I 12 12 12 5 5 5 5 0 U ATOM	I TYPE J 1 1 1 1 1 1 TOTA	ES K 1 1 1 1 1 1 1 1 1 CONTRACTOR	L 5 5 12 5 12 5 12 5 12 8 PLAN	CLASS A 0 0. 0 120. 0 -120. 0 -120. 0 -120. 0 -120. 0 0. 120. ENERGY = 1	000 0.678 000 0.678 000 0.000 000 0.284 000 0.284 000 0.284 000 0.284 000 0.284 000 0.284 000 0.284 000 0.284 000 0.284	V1 V2 3 -0.602 3 -0.602 0 0.000 4 -1.386 4 -1.386 3 -0.602 4 -1.386 3 -0.602 /mol	0.398 0.398 0.398 0.893 0.314 0.314 0.398 0.314	1.076 0.116 0.893 -0.654 -0.655 1.076 -0.655 0.598

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

3474 3475	I	J	K	ANGI	LE A	NGLE	CON	STANT	DEL'	ГА	ENERGY
		3 h1	109.	 500	110.070		194.100		0.010	0.019	
3477					109.550						
3478		3 cl			105.930				0.061		
3479		3 h1			110.070		194.100		0.010		
3480	c3 c	3 cl	109.	500	110.330	2	260.419	-0	0.014	0.055	
3481	h1 c	3 cl	109.	442	105.930	1	183.005	C	0.061	0.688	
3482	c3 c	3 cl	109.	500	110.330	2	260.419	-0	0.014	0.055	
3483	h1 c	3 cl	109.	442	105.930	1	183.005	C	0.061	0.688	
3484	h1 c	3 cl	109.	442	105.930	1	183.005	C	0.061	0.688	
3485	c3 c	3 h1	109.	500	110.070	1	194.100	– C	0.010	0.019	
3486	c3 c	3 h1	109.	500	110.070	1	194.100	-0	0.010	0.019	
3487	h1 c	3 h1	109.	442	109.550	1	164.039	-0	0.002	0.001	
3488		TOT	AL ANGL	E BENDI	ING ENERG	У =	2.938	kJ/mol	L		
3489											
3490	ТО	R S	I O N A	L							
3491											
3492		MOTA	TYPES-		FORCE			TORSION	1		
3493	I	J	K	L	CONSTANT	\$	5	ANGLE	n	ENERGY	
3494											
3495					0						
3496					0						
3497					0						
3498			h1								
3499					0						
3500					0						
					0						
					0						
3503 3504					0 ENERGY =				0.000		
3504		101.	AL IORS	TONAL I	INEKGI -	9.2	210 KJ/	шот			
3506	тм	D R	OPER	т О	RSIO	NIZAT.					
3507	1 M	F IX	OFER	1 0	K D I O	илп					
3508		АТОМ	TYPES-		FORCE	ТМТ	PROPER	TORSTON	1		
					CONSTANT					ENERGY	
3510											
		TOT	AL IMPR	OPER-TO	ORSIONAL	ENERGY	Y =	0.000 k	J/mol		
3512											
	V A	N :	DER	W A A	L S						
3514											
3515	ATOM	TYP	ES								
3516	I	J		Rij	kij	I	ENERGY				
3518	h1 h	1	2.74	6 –0	0.033						
3519	h1 h	1	2.74	6 –(0.033						
3520	h1 c	:1	2.51	2 2	2.571						
3521	h1 h	1	2.20	8 (.251						
3522	h1 h	1	2.74	6 –0	0.033						

```
3523 h1 cl 3.280 -0.134
3524 cl h1
            3.280
                   -0.134
3525 cl h1
            2.512
                    2.571
3526 cl cl
            3.806 -0.542
3527
      TOTAL VAN DER WAALS ENERGY = 4.485 kJ/mol
3528
3529 ELECTROSTATIC INTERACTIONS
3530
3531 ATOM TYPES
3532 I J
             Rij 332.17*QiQj ENERGY
3533
    _____
            2.746 1.352 0.493
3534 h1 h1
3535 h1 h1
            2.746
                    1.352
                            0.493
3536 h1 cl
            2.512 -3.809 -1.516
            2.208
3537 h1 h1
                    1.352
                            0.613
3538 h1 h1
            2.746
                    1.352
                            0.493
3539 h1 cl
            3.280 -3.809
                           -1.161
3540 cl h1
            3.280 -3.809 -1.161
            2.512
3541 cl h1
                   -3.809
                           -1.516
3542 cl cl 3.806 10.728 2.819
3543
      TOTAL ELECTROSTATIC ENERGY = -0.446 kJ/mol
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
     4 0.000000
3577
3578 5 -0.290000
3579 6 0.000000
3580 7 0.000000
3581 8 -0.290000
3582
3583 ATOM TYPES
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
     8 cl NO
3593
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
     8 -0.124211
3605
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
     6 0.044101
3615
3616 7 0.044101
     8 -0.124211
3617
3618
3619 ENERGY
3620
```

3621									
3622	BON	1 D	STRE	ТСЕ	HING				
3623									
3624						IDEAL			
3625								DELTA	
3626 3627								-0.103	
3628	5	1	0	1.0	000	1.093	4.766	-0.093	3.578
3629	1	1	0	1.5	540	1.508	4.258	0.032	0.294
3630	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
3631	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
632	1	5	0	1.0	000	1.093	4.766	-0.093	3.578
33	1	12	0	1.6	570	1.773	2.974	-0.103	2.795
34		TOTAL	BOND S	TRETCE	HING ENE	RGY = 20.1	9629 kcal/mc	ol	
35									
36	A N G	G L E	B E N	DII	N G				
37									
38	ATOM	TYPES		FF	VALENC	E IDEA	L FORCE		
39	I	J	K	CLASS	ANGLE	ANGL	E CONSTA	NT DELTA	ENERGY
40									
41								-1.049	
12								0.606	
3			12					1.280	
4			5					-1.049	
5			12			108.67		0.821	
6			12			108.16		1.280	
7			12			108.67		0.821	
			12					1.280	
								1.280	
	1	1	5	0	109.500			-1.049	
	1	1				110.54		-1.049	
	5		5					0.606	0.004
		TOTAL	ANGLE	RENDI	NG ENERG	y = 0.200	58 kcal/mol		
4	С П Т		<i>a</i>) T N G				
5	STF	K E T	Сн в	ENI	DING				
6	л ПОМ	шилыс		चच	777 T ENI	- DET M	A FOR	OCE CONCEANE	
7								J K	FNFDCV
9									
50	1							0.070	
61	5		5	0			6 0.115		
52	5		12	0	109.442		0 -0.018		
63	1		5	0	109.500				
64	1		12	0	109.500				
55	5		12	0	109.442				-0.121
6	1		12	0	109.500				-0.070
7	5		12	0	109.442				-0.121
3	5		12	0		1.28			-0.121
9	1	1	5	0	109.500				-0.002
	-	_	_			1.01	J . L L /	0.070	0.002

5	1		0						
			0					0.070	-0.002 -0.033
	ТОТА			DING ENER					
	10111		1011 2211		.01		noul, mol		
ΤО	RST	ONA	T.						
		0 21 21	_						
ATOM	I TYPE	S		FF T	ORSION	F	ORCE CONS	TANT	
I								V3 E	NERGY
12	1	1	5	0 20	.000	0.678	-0.602	0.398	0.886
12	1	1	5	0 140	.000	0.678	-0.602	0.398	0.129
12	1	1	12	0 -100	.000	0.000	0.000	0.893	0.670
5	1	1	5	0 140	.000	0.284	-1.386	0.314	-0.304
5	1	1	5	0 -100	.000	0.284	-1.386	0.314	-0.991
5	1	1	12	0 20	.000	0.678	-0.602	0.398	0.886
5	1	1	5	0 -100	.000	0.284	-1.386	0.314	-0.991
5	1	1	5	0 20	.000	0.284	-1.386	0.314	0.349
5	1	1	12	0 140	.000	0.678	-0.602	0.398	0.129
	TOTA	L TORS	IONAL E	NERGY =	0.76131	kcal/m	ol		
O U	Т - О	F - P	L A N	E BEN	D I N G				
ΔΤΩМ						TODGE			
111 01.	TYPE	S		FF	OOP	FORCE			
I 	J TOTA	K L OUT-0	L OF-PLAN	CLASS E E BENDING	ANGLE	CONSTAI	NT EN		
I 	J TOTA	K L OUT-0	L 	CLASS E E BENDING	ANGLE	CONSTAI	NT EN		
I 	J TOTA	K L OUT-(E R	L OF-PLAN	CLASS E E BENDING	ANGLE	CONSTAI	NT EN		
I V A ATOM	J TOTA N D	K L OUT-(L OF-PLAN W A A	CLASS E E BENDING	ANGLE E ENERGY	CONSTAI = 0.00	NT EN		
I V A ATOM I	J TOTA N D TYPE J	K L OUT-(L OF-PLAN W A A	CLASS E BENDING L S R*IJ	ANGLE ENERGY EPSILO	CONSTAI	NT EN		
I V A ATOM I 5	J TOTA N D TYPE J 5	K LOUT-G ER S	L OF-PLAN W A A Rij 2.638	CLASS E BENDING L S R*IJ 2.970	EPSILO	CONSTAI = 0.00	NT EN 0000 kcal NERGY 0.001		
I V A ATOM I 5 5	J TOTA N D TYPE J 5 5	K COUT-C E R S	L OF-PLAN W A A Rij 2.638 2.831	CLASS E BENDING L S R*IJ 2.970 2.970	EPSILO 0.02	CONSTAI = 0.00	NT EN 00000 kcal NERGY 0.001		
I V A ATOM I 5 5 5	J TOTA N D TYPE J 5 5 12	K L OUT-G E R S	L OF-PLAN W A A Rij 2.638 2.831 2.547	CLASS E BENDING L S R*IJ 2.970 2.970 3.713	EPSILO 0.02 0.02 0.05	CONSTAI = 0.00	NT EN 00000 kcal NERGY 0.001 0.019 2.298		
I V A ATOM I 5 5 5 5 5	J TOTA N D TYPE J 5 5 12 5	K COUT-C E R S	L DF-PLAN W A A Rij 2.638 2.831 2.547 2.232	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970	EPSILO 0.02 0.02 0.05 0.02	N E1 2 (2 3 2	NERGY 0.001 0.019 2.298 0.328		
I V A ATOM I 5 5 5 5 5 5	J TOTA N D TYPE J 5 5 12 5 5	K L OUT-C E R S	L DF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 2.970	EPSILO 0.02 0.02 0.05 0.02	N E1 2 (2 3 : 2 2 (2	NERGY 0.001 0.019 2.298 0.328 0.001		
I V A ATOM I 5 5 5 5 5 5 5 5	J TOTA N D TYPE J 5 5 12 5 12	K COUT-C E R S	L DF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970	EPSILO	N E1 2 (2 3 2 2 (3 3 -(4)	NERGY 0.001 0.019 2.298 0.328		
I VV A ATOM 5 5 5 5 5 5	J TOTA N D TYPE J 5 5 12 5 12 5 12 5	K L OUT-(E R S	L DF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 2.970 3.713 3.713	EPSILO	N E1 2 (2 3 : 2 2 3 - (3 3 - (3) 3 - (3)	NERGY 0.001 0.019 2.298 0.328 0.001 0.028		
I V A ATOM I 5 5 5 5 5 5	J TOTA N D TYPE J 5 5 12 5 12 5 5 12 5	K COUT-C E R S	L DF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713 3.713	EPSILO	N EI 2 (2 3 3 -(3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298		
I V A ATOM I 5 5 5 5 5 5	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12	K L OUT-(E R S	L OF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547 3.587	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713 4.089	EPSILO	N E1 2 (2 3 : 2 3 - (3 3 - (3 3 - (4) 3 - (4) 6 (6)	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298 0.100		
I V A ATOM I 5 5 5 5 5 12 12	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12	K L OUT-(E R S	L OF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547 3.587	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713 3.713	EPSILO	N E1 2 (2 3 : 2 3 - (3 3 - (3 3 - (4) 3 - (4) 6 (6)	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298 0.100		
I V A ATOM I 5 5 5 5 5 12 12	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12	K L OUT-(E R S	L OF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547 3.587	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713 4.089	EPSILO	N E1 2 (2 3 : 2 3 - (3 3 - (3 3 - (4) 3 - (4) 6 (6)	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298 0.100		
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 5 12 TOTA	K L OUT-(E R S S L VAN 1	L OF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547 3.587 DER WAA	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713 4.089	EPSILO	CONSTAI 0.00 N El 2 -(3 -(3 -(3 -(3 -(4 -(4 -(4 -(4 -(4 -(4 -(4 -(4	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298 0.100 al/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 5 12 TOTA	K L OUT-(E R S S L VAN 1	L OF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547 3.587 DER WAA	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713 4.089 LS ENERGY	EPSILO	CONSTAI 0.00 N El 2 -(3 -(3 -(3 -(3 -(4 -(4 -(4 -(4 -(4 -(4 -(4 -(4	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298 0.100 al/mol		
I V A ATOM I 5 5 5 5 12 12 12 12 12	J TOTA N D TYPE J 5 5 12 5 12 5 12 TOTA E C T	K L OUT-C E R S S L VAN 1	L DF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547 3.587 DER WAA T A T	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 4.089 LS ENERGY I C I N	EPSILO	CONSTAI = 0.00 N EI 2 (2 -) 3 : 2 (3 -) 3 -) 6 (916 kc) C T I	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298 0.100 al/mol		
I V A ATOM I 5 5 5 5 12 12 12 12 12	J TOTA N D TYPE J 5 5 12 5 12 5 12 TOTA E C T	K L OUT-C E R S S L VAN 1	L DF-PLAN W A A Rij 2.638 2.831 2.547 2.232 2.638 3.399 3.399 2.547 3.587 DER WAA T A T	CLASS E BENDING L S R*IJ 2.970 2.970 3.713 2.970 3.713 3.713 3.713 4.089 LS ENERGY	EPSILO	CONSTAI = 0.00 N EI 2 (2 -) 3 : 2 (3 -) 3 -) 6 (916 kc) C T I	NERGY 0.001 0.019 2.298 0.328 0.001 0.028 0.028 2.298 0.100 al/mol		

```
3719 TOTAL ELECTROSTATIC ENERGY = 5.75922 kcal/mol
3720
    TOTAL ENERGY = 31.17064 kcal/mol
3721
3722
3723 ENERGY
3724
3725
3726 BOND STRETCHING
3727
                            FORCE
3728 ATOM TYPES BOND
                   IDEAL
3729
    I J
           LENGTH
                   LENGTH
                           CONSTANT
                                     DELTA ENERGY
3730
                         1168.117
                                   -0.116
3731 cl c3
           1.670
                  1.786
                                           15.718
3732 h1 c3
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
                         1269.019
3733 c3 c3
          1.540
                  1.535
                                   0.005
                                          0.032
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
3734 c3 h1
3735 c3 h1
          1.000
                  1.093
                         1406.346
                                  -0.093
                                          12.163
          1.000
3736 c3 h1
                  1.093
                         1406.346
                                  -0.093
                                          12.163
3737 c3 cl
          1.670
                  1.786
                         1168.117
                                          15.718
                                  -0.116
     TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
3738
3739
3740 ANGLE BENDING
3741
3742 ATOM TYPES VALENCE IDEAL FORCE
    I J K
               ANGLE
                       ANGLE
3743
                               CONSTANT
                                         DELTA ENERGY
3744
    ______
3745 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                             0.019
3746 h1 c3 h1 109.442
                   109.550
                            164.039
                                     -0.002
                                             0.001
3747 h1 c3 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
                            194.100 -0.010
3748 c3 c3 h1 109.500 110.070
                                             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
3752 h1 c3 cl 109.442
                   105.930
                            183.005
                                     0.061
                                             0.688
3753 h1 c3 cl 109.442 105.930
                            183.005
                                     0.061
                                             0.688
3754 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                             0.019
3755 c3 c3 h1 109.500
                   110.070
                            194.100
                                     -0.010
                                             0.019
    h1 c3 h1 109.442 109.550 164.039 -0.002 0.001
3756
     TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
3757
3758
3759
    TORSIONAL
3760
3761
    ----ATOM TYPES----
                   FORCE
                                 TORSION
    I J K L
                  CONSTANT
3762
                                 ANGLE n ENERGY
                            S
3763 | -----
3764 cl c3 c3 h1
              0.000
                       0
                            20.000 3
                                       0.000
                       0 140.000 3
3765 cl c3 c3 h1
              0.000
                                       0.000
                       0 -100.000 3
3766 cl c3 c3 cl
              0.000
                                       0.000
3767 h1 c3 c3 h1 0.651 0 140.000 3
                                      0.977
```

```
3768 h1 c3 c3 h1 0.651 0 -100.000 3 0.977
                             20.000 3
3769 h1 c3 c3 cl
               0.000
                        0
                                        0.000
3770 h1 c3 c3 h1
               0.651
                        0 -100.000 3
                                        0.977
                            20.000 3
3771 h1 c3 c3 h1
               0.651
                        0
                                        0.977
    h1 c3 c3 cl
                      0 140.000 3
3772
               0.000
                                        0.000
3773
     TOTAL TORSIONAL ENERGY = 3.908 kJ/mol
3774
3775 IMPROPER TORSIONAL
3776
3777 ----ATOM TYPES---- FORCE IMPROPER_TORSION
    I J K L CONSTANT
3778
                            s ANGLE n ENERGY
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
                  2.064
3789 h1 cl
3790 h1 h1
           2.232
                  0.205
3791 h1 h1
           2.638 -0.029
           3.399
3792 h1 cl
                  -0.133
3793 cl h1
           3.399 -0.133
                  2.064
3794 cl h1
           2.547
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
3801
            Rij 332.17*QiQj ENERGY
3802
3803 h1 h1 2.638
                  1.352
                         0.513
3804 h1 h1
           2.831
                  1.352
                          0.478
           2.547 -3.809 -1.495
3805 h1 cl
3806 h1 h1
           2.232
                  1.352
                          0.606
3807 h1 h1
           2.638
                  1.352
                          0.513
           3.399 -3.809 -1.121
3808 h1 cl
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
3812
3813
3814 TOTAL ENERGY = 90.486 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...
3855 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
     SETTING UP TORSION CALCULATIONS...
3856
3857
     SETTING UP OOP CALCULATIONS...
3858
     SETTING UP VAN DER WAALS CALCULATIONS...
3859
     SETTING UP ELECTROSTATIC CALCULATIONS...
3860
3861 ATOM TYPES
3862
3863 IDX TYPE RING
3864 1 c3 NO
3865
     2 c3 NO
```

```
3866 3 h1 NO
3867 4 h1 NO
3868 5 cl NO
3869
    6 hl NO
3870 7 h1 NO
    8 cl NO
3871
3872
3873 C H A R G E S
3874
3875 IDX CHARGE
3876 1 0.036009
3877
    2 0.036009
3878 3 0.044101
3879 4 0.044101
    5 -0.124211
3880
3881 6 0.044101
3882 7 0.044101
3883 8 -0.124211
3884
3885 SETTING UP CALCULATIONS
3886
3887 SETTING UP BOND CALCULATIONS...
    SETTING UP ANGLE CALCULATIONS...
3888
3889
    SETTING UP TORSION CALCULATIONS...
3890
    SETTING UP IMPROPER TORSION CALCULATIONS...
3891
    SETTING UP VAN DER WAALS CALCULATIONS...
3892
    SETTING UP ELECTROSTATIC CALCULATIONS...
3893
3894 ENERGY
3895
3896
3897 BOND STRETCHING
3898
3899 ATOM TYPES FF BOND IDEAL
                                    FORCE
    I J CLASS LENGTH
                           LENGTH
                                   CONSTANT
3900
                                              DELTA ENERGY
3901
3902
    12 1 0
                   1.670
                            1.773
                                      2.974
                                               -0.103
                                                       2.795
                   1.000
    5 1
             0
                            1.093
                                      4.766
                                              -0.093
                                                       3.578
3903
        1
             0
                   1.000
                                      4.766
                                              -0.093
3904
    5
                            1.093
                                                       3.578
3905
        1
                                      4.258
    1
             0
                   1.540
                            1.508
                                               0.032
                                                       0.294
    1 5
3906
              0
                   1.000
                            1.093
                                      4.766
                                               -0.093
                                                        3.578
3907
    1 12
             0
                   1.670
                            1.773
                                      2.974
                                              -0.103
                                                       2.795
3908
    1 5
                   1.000
                            1.093
                                      4.766
                                              -0.093
                                                       3.578
              0
3909
        TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
3910
3911 ANGLE BENDING
3912
3913 ATOM TYPES
                 FF VALENCE
                                IDEAL
                                        FORCE
    I J K CLASS ANGLE ANGLE CONSTANT DELTA ENERGY
3914
```

915														
916	1	1	5	0	109.5	500	110.54	19		0.636		-1.049	9	0.015
7	5	1	5	0		142	108.83					0.606		0.004
	5	1	12	0		109.442		52	0.6			1.280		0.025
	1	1	5	0	109.5		110.54	19		0.636		-1.049	9	0.015
	1	1	12	0	109.5	500	108.67	79		1.056		0.82	1	0.016
	5	1	12	0	109.4	142	108.16	52		0.698		1.280)	0.025
	5	1	12	0	109.4	142	108.16	52		0.698		1.280)	0.025
	1	1	12	0	109.5	500	108.67			1.056		0.82	1	0.016
	5	1	12	0	109.4	142	108.16	52		0.698		1.280	0	0.025
	1	1	5	0	109.5	500	110.54	19		0.636		-1.049	9	0.015
	5	1	5	0	109.4	142	108.83	36		0.516		0.606	5	0.004
	1	1	5	0	109.5	500	110.54	19		0.636		-1.049	9	0.015
		TOTA	L ANG	LE BENDI	NG ENE	ERGY =	0.200)58 k	cal/m	ol				
	ST	REI	СН	BEN	DIN	G								
	ATOM	TYPE	S	FF	VALE	VALENCE		DELTA		FORCE		CONSTANT		
	I	J	K	CLASS	ANG	GLE	ANGI	ĹΕ		IJ		J K	El	NERGY
	1	1	5	0	109.5	500	-1.04	19	0.	227	0	.070	-0	.002
	5	1	5	0	109.4	142	0.60)6	0.115			.115	-0	.033
	5	1	12	0	109.4	142	1.28	30	-0.	018	0	.380	-0	.121
	1	1	5	0	109.5	500	-1.04	19	0.	227	0	.070	-0	.002
	1	1	12	0	109.5	500	0.82					.386	-0	.070
	5	1	12	0	109.4	142	1.28	30		018		.380		.121
	5	1	12	0		142		30		018		.380		.121
	1	1	12	0	109.5			21		176		.386		.070
	5	1	12	0	109.4	142	1.28	30	-0.	018	0	.380	-0	.121
		1		0		500			0.			.070		.002
				0										.033
	1			0							0	.070	-0	.002
		TOTA	L STF	RETCH BEN	DING E	ENERGY	= -0.6	59593	kcal	/mol				
	m 0													
	то.	R S I	O N	АЬ										
	лπОм	mv D E	· C		rr	π∩ъс	Z T O NI		FODCE	COME	ייי א איייי			
	ATOM TYPES I J K													
				12									0.4	449
				5										
				5								314		
	5			12						.602			0.	050
	5			5			00 (.386		314		
	5	1	1	5						.386		314		
				12								893		
				5									0.0	
	12	1	1	5	0	40.00	00 (.678	-0	.602	0.	398	0.	449
		TOTA	L TOF	RSIONAL E	NERGY	= -1.2	29534 }	cal/	mol					

```
3964
3965
    OUT-OF-PLANE BENDING
3966
3967 ATOM TYPES
                   FF
                         OOP
                              FORCE
                  CLASS ANGLE CONSTANT
3968
    I J K
              L
                                       ENERGY
3969
3970
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
3971
    VAN DER WAALS
3972
3973
3974
    ATOM TYPES
           Rij R*IJ EPSILON ENERGY
3975
    I J
3976
    _____
             2.518
3977
    5 5
                    2.970
                           0.022
                                  0.036
    5 5
                    2.970
                           0.022
3978
             2.885
                                  -0.021
3979 5 12
             2.647
                    3.713
                           0.053
                                  1.520
3980 5 5
             2.300
                    2.970
                           0.022
                                  0.215
    5 5
             2.518
                           0.022
3981
                    2.970
                                  0.036
   5 12
             3.474
                    3.713
                           0.053 -0.041
3982
3983 12 5
             3.474
                    3.713
                           0.053 -0.041
3984 12 5
             2.647
                    3.713
                           0.053
                                  1.520
3985 12 12
                           0.276
                                  1.129
             3.338
                    4.089
      TOTAL VAN DER WAALS ENERGY = 4.35500 kcal/mol
3986
3987
3988
    ELECTROSTATIC INTERACTIONS
3989
3990 ATOM TYPES
    I J Rij Qi Qj ENERGY
3991
3992
    12 12 3.388
3993
                   -0.290 \quad -0.290
                                 6.182
3994
      TOTAL ELECTROSTATIC ENERGY = 6.18170 kcal/mol
3995
3996 | TOTAL ENERGY = 28.94230 kcal/mol
3997
3998
    ENERGY
3999
4000
4001 BOND STRETCHING
4002
4003
   ATOM TYPES BOND
                   IDEAL
                           FORCE
           LENGTH
                          CONSTANT DELTA ENERGY
4004
    I J
                   LENGTH
4005
   ______
4006 cl c3
          1.670
                 1.786
                         1168.117
                                  -0.116
                                         15.718
                         1406.346
   h1 c3
          1.000
                 1.093
                                  -0.093
                                         12.163
4007
4008 h1 c3
          1.000
                 1.093
                         1406.346
                                 -0.093
                                         12.163
4009 c3 c3
          1.540
                  1.535
                                  0.005
                         1269.019
                                          0.032
4010 c3 h1
                                 -0.093 12.163
          1.000
                 1.093
                         1406.346
4011 c3 cl
          1.670
                 1.786
                         1168.117
                                         15.718
                                 -0.116
4012 c3 h1
          1.000 1.093
                         1406.346
                                 -0.093
                                         12.163
```

```
4013 TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
4014
4015 ANGLE BENDING
4016
4017 ATOM TYPES
                                FORCE
               VALENCE
                        IDEAL
    I J K
               ANGLE ANGLE CONSTANT DELTA ENERGY
4018
4019
    c3 c3 h1 109.500
                   110.070
4020
                             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
                                      0.061
                            183.005
                                              0.688
    c3 c3 h1 109.500 110.070
4023
                             194.100
                                     -0.010
                                              0.019
    c3 c3 cl 109.500 110.330
                            260.419
                                     -0.014
4024
                                              0.055
                                              0.688
4025 h1 c3 cl 109.442 105.930
                             183.005
                                      0.061
4026 h1 c3 cl 109.442 105.930
                             183.005
                                      0.061
                                              0.688
                            260.419 -0.014
           109.500 110.330
4027 c3 c3 c1
                                              0.055
4028 h1 c3 cl 109.442 105.930
                             183.005
                                      0.061
                                              0.688
4029 c3 c3 h1 109.500 110.070
                             194.100
                                     -0.010
                                              0.019
                            164.039 -0.002
                                              0.001
4030 h1 c3 h1 109.442 109.550
4031 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                              0.019
      TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
4032
4033
4034 T O R S I O N A L
4035
4036 ----ATOM TYPES---- FORCE
                                  TORSION
    I J K L CONSTANT
                                 ANGLE n
4037
                            S
                                            ENERGY
4038
4039 h1 c3 c3 cl
              0.000
                      0
                            40.000 3
                                        0.000
                        0 -80.000 3
4040 h1 c3 c3 h1
               0.651
                                        0.326
4041 h1 c3 c3 h1 0.651
                        0 160.000 3
                                        0.326
4042 h1 c3 c3 cl
              0.000
                        0 160.000 3
                                        0.000
                        0
4043 h1 c3 c3 h1
               0.651
                            40.000 3
                                        0.326
4044 h1 c3 c3 h1 0.651
                        0 -80.000 3
                                        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
    cl c3 c3 h1 0.000 0
                            40.000 3
4047
                                        0.000
     TOTAL TORSIONAL ENERGY = 1.303 kJ/mol
4048
4049
4050 IMPROPER TORSIONAL
4051
    ----ATOM TYPES---- FORCE IMPROPER TORSION
4052
                  CONSTANT S ANGLE n ENERGY
4053
    I J K L
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
```

```
4062 h1 h1 2.518 -0.013
4063 h1 h1
            2.885
                   -0.031
4064 h1 cl
            2.647
                    1.083
4065 h1 h1
            2.300
                    0.109
4066 h1 h1
            2.518
                   -0.013
4067 h1 cl
            3.474 -0.129
4068 cl h1
            3.474
                   -0.129
4069
    cl h1
            2.647
                    1.083
    cl cl
            3.338 0.738
4070
     TOTAL VAN DER WAALS ENERGY = 2.701 kJ/mol
4071
4072
4073
    ELECTROSTATIC INTERACTIONS
4074
4075 ATOM TYPES
4076
    I J
             Rij 332.17*QiQj ENERGY
4077
    _____
4078 h1 h1 2.518
                    1.352
                           0.537
    h1 h1
            2.885
                    1.352
                           0.469
4079
            2.647 -3.809 -1.439
4080 h1 cl
4081 h1 h1
            2.300
                    1.352
                           0.588
4082 h1 h1
            2.518
                    1.352
                            0.537
4083 h1 cl
            3.474
                   -3.809 -1.097
4084 cl h1
            3.474 -3.809 -1.097
4085 cl h1
            2.647 -3.809 -1.439
                            3.214
4086
    cl cl
            3.338
                   10.728
     TOTAL ELECTROSTATIC ENERGY = 0.273 kJ/mol
4087
4088
4089
    TOTAL ENERGY = 87.337 \text{ kJ/mol}
4090
4091 ATOM TYPES
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...
4133 SETTING UP VAN DER WAALS CALCULATIONS...
4134 SETTING UP ELECTROSTATIC CALCULATIONS...
4135
4136 A T O M T Y P E S
4137
4138 IDX TYPE RING
4139 1 c3 NO
4140 2 c3 NO
4141 3 h1 NO
4142 4 h1 NO
4143 5 cl NO
     6 h1 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
4153 3 0.044101
4154
     4 0.044101
4155 5 -0.124211
4156 | 6 0.044101
4157 7 0.044101
4158 8 -0.124211
4159
```

```
4160 SETTING UP CALCULATIONS
4161
4162
    SETTING UP BOND CALCULATIONS...
4163
    SETTING UP ANGLE CALCULATIONS...
4164
    SETTING UP TORSION CALCULATIONS...
4165
    SETTING UP IMPROPER TORSION CALCULATIONS...
4166
    SETTING UP VAN DER WAALS CALCULATIONS...
     SETTING UP ELECTROSTATIC CALCULATIONS...
4167
4168
    ENERGY
4169
4170
4171
4172
    BOND STRETCHING
4173
    ATOM TYPES FF
4174
                    BOND
                            IDEAL
                                      FORCE
     I J
                                     CONSTANT
                                                 DELTA
4175
             CLASS LENGTH
                            LENGTH
                                                          ENERGY
4176
4177
     5
         1
               0
                    1.000
                             1.093
                                        4.766
                                                 -0.093
                                                           3.578
    12
         1
               0
                    1.670
                             1.773
                                        2.974
                                                 -0.103
                                                           2.795
4178
4179
     5
         1
               0
                    1.000
                             1.093
                                        4.766
                                                 -0.093
                                                           3.578
4180
         1
               0
                    1.540
                             1.508
                                        4.258
                                                 0.032
                                                           0.294
     1
        5
               0
                                        4.766
4181
     1
                    1.000
                             1.093
                                                 -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
4184
         TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
4185
4186
    ANGLE BENDING
4187
                                 IDEAL
    ATOM TYPES
                  FF VALENCE
                                         FORCE
4188
4189
     I J K
                  CLASS ANGLE
                                 ANGLE
                                         CONSTANT
                                                     DELTA
                                                               ENERGY
4190
         1
             5
                  0 109.500 110.549
                                            0.636
                                                     -1.049
                                                               0.015
4191
     1
4192
     5
         1
             5
                   0
                      109.442
                               108.836
                                            0.516
                                                     0.606
                                                               0.004
4193
     5
         1
            12
                   0
                      109.442
                               108.162
                                            0.698
                                                     1.280
                                                               0.025
         1 5
                   0
                      109.500 110.549
                                             0.636
                                                     -1.049
                                                               0.015
4194
     1
                      109.500
                               108.679
                                             1.056
                                                     0.821
                                                               0.016
4195
     1
         1
             12
                   0
4196
     5
         1 12
                   0
                      109.442
                               108.162
                                             0.698
                                                      1.280
                                                               0.025
         1 12
                      109.442 108.162
4197
     5
                   0
                                             0.698
                                                     1.280
                                                               0.025
4198
     1
         1 12
                   0
                      109.500
                               108.679
                                             1.056
                                                     0.821
                                                               0.016
4199
     5
         1 12
                   0
                      109.442
                               108.162
                                             0.698
                                                     1.280
                                                               0.025
                              110.549
4200
     1
         1 5
                   0
                       109.500
                                             0.636
                                                     -1.049
                                                               0.015
4201
     5
         1
             5
                   0
                      109.442
                                                     0.606
                                                               0.004
                               108.836
                                             0.516
              5
                       109.500
42.02
     1
         1
                   0
                               110.549
                                             0.636
                                                     -1.049
                                                               0.015
         TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol
4203
4204
4205
    STRETCH BENDING
4206
4207
    ATOM TYPES
                  FF
                                            FORCE CONSTANT
                        VALENCE
                                  DELTA
                                             IJ JK
4208
     I J K
                                  ANGLE
                 CLASS ANGLE
                                                             ENERGY
```

1	1	5	0			0.227		-0.002
5	1	5	0	109.442	0.606	0.115	0.115	-0.033
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
1	1	5	0	109.500	-1.049	0.227	0.070	-0.002
1	1	12	0	109.500	0.821	0.176	0.386	-0.070
5	1	12	0	109.442	1.280	-0.018	0.380	-0.121
5	1	12	0	109.442	1.280	-0.018		
1		12	0			0.176		
5		12	0		1.280	-0.018	0.380	-0.121
			0			0.227		
						0.115		
1							0.070	-0.002
	TOTA	L STF	RETCH BE	NDING ENER	GY = -0.695	93 kcal/mol		
ТО	RSI	O N	A L					
		. ~						
	I TYPE					FORCE CON		an av
							V3 ENI	
							0.398	
					.000 0.0		0.398	
	1				.000 0.2		0.314	
5					.000 0.2		0.398	
5				0 60				
5			5		.000 0.2		0.314	
			12			00 0.000		0.000
							0.398	
	1					78 -0.602		0.057
					2.36550 kca			
O U	T - 0) F -	PLAN	E BEN	DING			
ATOM	I TYPE	S		FF	OOP FO	RCE		
I	J	K	L	CLASS	ANGLE CON	STANT E	NERGY	
	TOTA	L OUI	-OF-PLA	NE BENDING	ENERGY =	0.00000 kca	l/mol	
V A	N D	ER	WAA	LS				
	I TYPE							
					EPSILON	ENERGY		
				2 070		0.105		
					0.022			
					0.022			
	12				0.053			
					0.022			
					0.022			
5	12		3.499	3./13	0.053	-0.044		

```
4258 12 5 3.499 3.713 0.053 -0.044
4259
    12
              2.792
                      3.713
                             0.053
                                    0.792
4260 12 12
              3.087
                     4.089
                            0.276
                                    3.947
4261
       TOTAL VAN DER WAALS ENERGY = 5.74158 kcal/mol
4262
4263 ELECTROSTATIC INTERACTIONS
4264
4265 ATOM TYPES
    I J Rij Qi Qj ENERGY
4266
4267
    12 12 3.137 -0.290 -0.290 6.678
4268
     TOTAL ELECTROSTATIC ENERGY = 6.67788 kcal/mol
4269
4270
4271 TOTAL ENERGY = 29.75490 kcal/mol
4272
4273 E N E R G Y
4274
4275
4276 BOND STRETCHING
4277
4278 ATOM TYPES BOND IDEAL FORCE
    I J LENGTH
                                      DELTA
                    LENGTH
                            CONSTANT
                                              ENERGY
4279
4280
4281 h1 c3
          1.000
                  1.093
                          1406.346
                                   -0.093
                                           12.163
                  1.786
                          1168.117
                                           15.718
4282 cl c3
           1.670
                                    -0.116
4283 h1 c3
          1.000
                  1.093
                          1406.346
                                   -0.093
                                           12.163
4284 c3 c3
          1.540
                  1.535
                          1269.019
                                    0.005
                                            0.032
4285 c3 h1
           1.000
                   1.093
                          1406.346
                                    -0.093
                                           12.163
          1.670
                  1.786
                          1168.117
                                   -0.116
                                           15.718
4286 c3 cl
4287 c3 h1
          1.000
                   1.093
                          1406.346
                                    -0.093
                                           12,163
4288
      TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
4289
4290 ANGLE BENDING
4291
    ATOM TYPES VALENCE IDEAL FORCE
4292
                                         DELTA ENERGY
    I J K
                                CONSTANT
4293
                ANGLE
                        ANGLE
4294
    ______
    c3 c3 h1 109.500 110.070
                             194.100
                                      -0.010
                                              0.019
4295
4296 h1 c3 h1 109.442
                   109.550
                             164.039
                                      -0.002
                                              0.001
4297
    h1 c3 cl 109.442 105.930
                             183.005
                                      0.061
                                              0.688
    c3 c3 h1 109.500 110.070
                             194.100
                                      -0.010
4298
                                              0.019
4299 c3 c3 cl 109.500
                   110.330
                             260.419
                                      -0.014
                                              0.055
4300 h1 c3 cl 109.442 105.930
                             183.005
                                      0.061
                                              0.688
4301 h1 c3 cl
           109.442 105.930
                             183.005
                                      0.061
                                              0.688
                   110.330
                                      -0.014
4302 c3 c3 cl 109.500
                             260.419
                                              0.055
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
4311 ----ATOM TYPES----
                                 TORSION
    I J K L CONSTANT s
                                ANGLE n ENERGY
4312
4313
4314 h1 c3 c3 cl
              0.000
                                       0.000
                      0
                            60.000 3
4315 h1 c3 c3 h1 0.651
                      0 -60.000 3
                                       0.000
4316 h1 c3 c3 h1
                       0 -180.000 3
              0.651
                                       0.000
4317 h1 c3 c3 c1
              0.000
                       0 -180.000 3
                                       0.000
4318 h1 c3 c3 h1 0.651
                        0
                            60.000 3
                                       0.000
                       0 -60.000 3
4319 h1 c3 c3 h1
              0.651
                                       0.000
                        0
4320 cl c3 c3 cl
              0.000
                           -60.000 3
                                       0.000
4321 cl c3 c3 h1
              0.000
                        0 180.000 3
                                       0.000
                            60.000 3
4322 cl c3 c3 h1
              0.000
                       0
                                       0.000
      TOTAL TORSIONAL ENERGY = 0.000 kJ/mol
4323
4324
4325 IMPROPER TORSIONAL
4326
4327
    ----ATOM TYPES---- FORCE IMPROPER_TORSION
    I J K L CONSTANT S ANGLE n ENERGY
4328
4329
4330
      TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
4331
4332 VAN DER WAALS
4333
4334 ATOM TYPES
    I J Rij kij ENERGY
4335
4336 -----
          2.400
4337 h1 h1
                  0.030
4338 h1 h1
           2.903 -0.031
4339 h1 cl
           2.792
                  0.356
4340 h1 h1
           2.400
                  0.030
           2.400
                  0.030
4341 h1 h1
4342 h1 cl
           3.499 -0.127
4343 cl h1
           3.499
                  -0.127
4344 cl h1
           2.792
                  0.356
                  4.588
4345 cl cl
           3.087
4346
     TOTAL VAN DER WAALS ENERGY = 5.105 kJ/mol
4347
4348 ELECTROSTATIC INTERACTIONS
4349
4350 ATOM TYPES
    I J
            Rij 332.17*QiQj ENERGY
4351
4352
    ______
4353 h1 h1
           2.400 1.352 0.563
4354 h1 h1
           2.903
                  1.352
                         0.466
4355 h1 cl 2.792 -3.809 -1.364
```

```
4356 h1 h1 2.400 1.352 0.563
4357 h1 h1
             2.400
                      1.352
                              0.563
4358 h1 cl
             3.499 -3.809 -1.089
4359 cl h1
             3.499
                     -3.809 -1.089
    cl h1
                              -1.364
4360
              2.792
                     -3.809
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
4374 6 5 NO
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
    4 0.000000
4396
4397 5 -0.290000
4398 6 0.000000
4399
    7 0.000000
4400 8 -0.290000
4401
4402 SETTING UP CALCULATIONS
4403
4404
    SETTING UP BOND CALCULATIONS...
```

```
4405 SETTING UP ANGLE & STRETCH-BEND CALCULATIONS...
4406
     SETTING UP TORSION CALCULATIONS...
4407
     SETTING UP OOP CALCULATIONS...
4408
     SETTING UP VAN DER WAALS CALCULATIONS...
4409
     SETTING UP ELECTROSTATIC CALCULATIONS...
4410
4411 ATOM TYPES
4412
4413 IDX TYPE RING
4414 1 c3 NO
4415 2 c3 NO
4416 | 3 h1 NO
4417 4 h1 NO
4418 5 cl NO
4419
     6 hl NO
4420 7 h1 NO
4421 8 cl NO
4422
4423 C H A R G E S
4424
4425 IDX CHARGE
4426 1 0.036009
4427 2 0.036009
4428 3 0.044101
4429 4 0.044101
4430 5 -0.124211
4431 6 0.044101
4432 7 0.044101
4433 8 -0.124211
4434
4435
     SETTING UP CALCULATIONS
4436
4437 | SETTING UP BOND CALCULATIONS...
4438
     SETTING UP ANGLE CALCULATIONS...
     SETTING UP TORSION CALCULATIONS...
4439
4440 SETTING UP IMPROPER TORSION CALCULATIONS...
4441
     SETTING UP VAN DER WAALS CALCULATIONS...
4442 SETTING UP ELECTROSTATIC CALCULATIONS...
4443
4444 E N E R G Y
4445
4446
4447 BOND STRETCHING
4448
4449 ATOM TYPES FF BOND
                              IDEAL
                                         FORCE
4450
     I J
              CLASS LENGTH
                              LENGTH
                                        CONSTANT
                                                     DELTA
                                                               ENERGY
4451
         1
              0 1.000 1.093
0 1.000 1.093
                                                    -0.093
     5
                                           4.766
4452
                                                               3.578
                                         4.766
4453
     5 1
                                                    -0.093
                                                              3.578
```

1	12				.773			3.578 2.795
	E					4.766 -0		
					SY = 20.1962		.093	3.5/6
A N	GLI	Е ВІ	ENDII	N G				
ATOM	г түрг	ES	FF	VALENCE	IDEAL	FORCE		
						CONSTANT	DELTA	ENERGY
						0.636		
						0.516		
5	1	12	0	109.442	108.162	0.698	1.280	0.025
			0		110.549		-1.049	0.015
1	1	12	0	109.500	108.679	1.056	0.821	0.016
5	1	12	0	109.442	108.162	0.698	1.280	0.025
5	1	12	0	109.442	108.162	0.698	1.280	0.025
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
5	1	5	0	109.442	108.836	0.516	0.606	0.004
1	1	12	0	109.500	108.679	1.056	0.821	0.016
5	1	12	0	109.442	108.162	0.698	1.280	0.025
1	1	5	0	109.500	110.549	0.636	-1.049	0.015
			B E N I		DELTA	FORCE C	ONSTANT	
		ES	FF		DELTA ANGLE	FORCE C	ONSTANT J K	ENERGY
ATOM	I TYPI J	ES	FF	VALENCE ANGLE	ANGLE	I J	J K	
ATOM I	I TYPI J	ES K	FF CLASS	VALENCE ANGLE	ANGLE	I J 0.227	J K	-0.002
ATOM I 	I ТҮРН Ј 	ES K 5	FF CLASS 0	VALENCE ANGLE	ANGLE 	I J 0.227	J К 	-0.002
ATOM I 1 5	I ТҮРI Ј 1 1	ES K 5 5	FF CLASS 0 0 0	VALENCE ANGLE 109.500	ANGLE1.049 0.606 1.280	I J 0.227 0.115	J K 0.070 0.115	-0.002 -0.033
ATOM I 1 5	J J 1 1	ES K 5 5 12	FF CLASS 0 0 0	VALENCE ANGLE 109.500 109.442 109.442	ANGLE1.049 0.606 1.280	0.227 0.115 -0.018 0.227	J K 0.070 0.115 0.380	-0.002 -0.033 -0.121
ATOM I 1 5 5 1	J J 1 1 1	ES 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	I J 0.227 0.115 -0.018 0.227 0.176	J K 0.070 0.115 0.380 0.070	-0.002 -0.033 -0.121 -0.002
ATOM I 1 5 1 1 1	J	ES K 5 12 5 12	FF CLASS 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500	ANGLE1.049 0.606 1.280 -1.049 0.821	I J 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
ATOM I 1 5 1 1 5 5 1 1 5	J TYPI 1 1 1 1 1 1 1	ES K 5 12 5 12 12	FF CLASS 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442	ANGLE -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
ATOM I 1 5 1 1 5 5 1 1 5 5	J TYPR 1 1 1 1 1 1 1 1 1 1	ES K 5 5 12 5 12 12	FF CLASS 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500 109.442	ANGLE -1.049 0.606 1.280 -1.049 0.821 1.280	I J 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
ATOM I 1 5 1 1 5 1 1 5 1	J TYPE 1 1 1 1 1 1 1 1 1 1 1 1	ES K 5 5 12 5 12 12 12 5	FF CLASS 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442	ANGLE1.049 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	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
ATOM I 1 5 1 1 5 1 1 5 5 1 5 5 1	J TYPR J 1 1 1 1 1 1 1 1 1 1 1 1	ES K 5 5 12 5 12 12 12 5 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	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.500 109.442 109.442 109.442 109.500	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 1.280 -1.049 0.606	I 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	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.121 -0.002 -0.033
ATOM I 1 5 1 1 5 1 1 5 1 1 5 1	J J 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	ES K 5 12 5 12 12 12 12 12	FF CLASS 0 0 0 0 0 0 0 0 0	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.500 109.442 109.500	ANGLE	I 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 -0.02 -0.033 -0.070
ATOM I 1 5 5 1 1 5 1 5 1 5 1 5	J	ES K 5 5 12 5 12 12 12 12 5 12 5 5 5 5 6 6 7 7 8 8 8 8 8 8 8 8 8 8 8	FF CLASS 	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.442 109.500 109.442 109.500	ANGLE	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176 -0.018 0.227	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 -0.002 -0.033 -0.070 -0.121
ATOM I 1 5 5 1 1 5 1 5 1 5 1 5	J	ES K 5 5 12 5 12 12 12 12 5 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 0 0	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.442 109.500 109.442 109.500	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 -1.049 0.606 0.821 1.280 -1.049	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176 -0.018 0.227	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 -0.002 -0.033 -0.070 -0.121
ATOM I 1 5 1 1 5 1 1 5 1 1 5 1	1 TYPE J 1 1 1 1 1 1 1 1 1 TOTA	ES K 5 5 12 5 12 12 12 12 5 12 5 5 5 5 6 6 7 7 8 8 8 8 8 8 8 8 8 8 8	FF CLASS 	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.442 109.500 109.442 109.500	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 -1.049 0.606 0.821 1.280 -1.049	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176 -0.018 0.227	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 -0.002 -0.033 -0.070 -0.121
ATOM I 1 5 1 1 5 1 1 5 1 1 5 1	1 TYPE J 1 1 1 1 1 1 1 1 1 TOTA	ES K 5 5 12 5 12 12 12 12 5 12 5 AL STRE	FF CLASS 	VALENCE ANGLE 109.500 109.442 109.442 109.500 109.442 109.442 109.442 109.500 109.442 109.500	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 -1.049 0.606 0.821 1.280 -1.049	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176 -0.018 0.227	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 -0.002 -0.033 -0.070 -0.121
ATOM I 1 5 1 1 5 1 1 5 1 1 5 1	1 TYPE J 1 1 1 1 1 1 1 1 1 TOTA	ES K 5 12 12 12 12 12 5 12 12 5 12 12	FF CLASS 	VALENCE ANGLE 109.500 109.442 109.500 109.500 109.442 109.442 109.442 109.500 109.442 109.500 109.442 109.500 109.442	ANGLE1.049 0.606 1.280 -1.049 0.821 1.280 -1.049 0.606 0.821 1.280 -1.049	1 J 0.227 0.115 -0.018 0.227 0.176 -0.018 -0.018 0.227 0.115 0.176 -0.018 0.227	J K 0.070 0.115 0.380 0.070 0.386 0.380 0.070 0.115 0.386 0.380 0.070	-0.002 -0.033 -0.121 -0.002 -0.070 -0.121 -0.002 -0.033 -0.070 -0.121

```
4503 -----
4504
              5
                   0
                      -40.000
                              0.284 - 1.386
                                           0.314
                                                   -0.243
       1 1 12
    5
                   0
                       80.000 0.678 -0.602 0.398
                                                  -0.086
4505
4506
   5
       1
           1 5
                   0 -160.000 0.284 -1.386
                                           0.314
                                                   -0.075
           1
4507
    5
        1
              5
                   0
                       80.000
                              0.284
                                    -1.386
                                           0.314
                                                   -1.099
    5
       1
           1 12
                   0 -160.000 0.678 -0.602
                                           0.398
                                                   0.050
4508
4509
    5
       1
           1 5
                   0 \quad -40.000 \quad 0.284 \quad -1.386
                                           0.314
                                                  -0.243
              5
                                                   0.050
4510
   12
       1
           1
                   0 -160.000 0.678 -0.602
                                           0.398
       1
           1 12
                   0 -40.000 0.000 0.000 0.893
                                                   0.223
4511
    12
       1
                       80.000 0.678 -0.602
4512 12
           1
              5
                   0
                                           0.398
                                                  -0.086
      TOTAL TORSIONAL ENERGY = -1.51155 kcal/mol
4513
4514
4515 OUT-OF-PLANE BENDING
4516
                   FF OOP FORCE
4517
    ATOM TYPES
    I J K
                  CLASS ANGLE CONSTANT
                                       ENERGY
4518
              L
4519
      TOTAL OUT-OF-PLANE BENDING ENERGY = 0.00000 kcal/mol
4520
4521
4522 VAN DER WAALS
4523
    ATOM TYPES
4524
             Rij R*IJ EPSILON ENERGY
4525
    I J
4526
    ______
4527
    5
              2.300
                     2.970
                            0.022
                                   0.215
4528
   5 5
             2.885
                     2.970
                           0.022 -0.021
                                   0.331
4529
   5 12
             2.960
                     3.713
                           0.053
    5 5
4530
             2.518
                     2.970
                            0.022
                                   0.036
    5 5
             2.300
                     2.970
                           0.022
                                   0.215
4531
4532
    5 12
             3.474
                     3.713
                           0.053
                                  -0.041
4533
    12 5
              3.474
                     3.713
                            0.053
                                  -0.041
    12 5
              2.960
                     3.713
                           0.053
                                   0.331
4534
4535
    12 12
              2.865
                     4.089
                           0.276
4536
       TOTAL VAN DER WAALS ENERGY = 10.69051 kcal/mol
4537
4538 ELECTROSTATIC INTERACTIONS
4539
4540 ATOM TYPES
             Rij Qi Qj ENERGY
4541
    I J
4542
    12 12 2.915 -0.290 -0.290 7.185
4543
4544
     TOTAL ELECTROSTATIC ENERGY = 7.18544 kcal/mol
4545
4546
    TOTAL ENERGY = 36.06534 kcal/mol
4547
4548 E N E R G Y
4549
4550
4551 BOND STRETCHING
```

ATOM TYPE	S BOND	IDEAL	FORCE			
					TA ENER	
h1 c3	1.000	1.093	1406.346	-0.093	12.163	
h1 c3	1.000	1.093	1406.346	-0.093	12.163	
cl c3	1.670	1.786	1168.117	-0.116	15.718	
c3 c3	1.540	1.535	1269.019	0.005	0.032	
c3 h1	1.000	1.093	1406.346	-0.093	12.163	
c3 cl	1.670	1.786	1168.117	-0.116	15.718	
3 h1	1.000	1.093	1406.346	-0.093	12.163	
TOTA	L BOND STRE	TCHING ENER	agy = 80.1	22 kJ/mol		
ANGLE	BEND	I N G				
том тург	S VAT.	ENCE ID	EAL FO	RCE		
					DELTA	ENERGY
					10 0.01	9
11 c3 h1		109.550		-0.0		
1 c3 cl		105.930		0.0		
3 c3 h1		110.070			10 0.01	
3 c3 c1		110.330		-0.0		
1 c3 cl		105.930		0.0		
1 c3 cl		105.930		0.0		
3 c3 h1		110.070			10 0.01	
1 c3 h1		109.550			02 0.00	
3 c3 cl		110.330		-0.0		
1 c3 cl		105.930		0.0		
					10 0.01	
			= 2.938			
ORSI	ONAL					
ATOM	TYPES	FORCE	1	TORSION		
I J	K L	CONSTANT	S	ANGLE	n ENERGY	
n1 c3 c3	h1 0.65	1 0	-40.000	3	0.326	
			80.000			
11 c3 c3	h1 0.65	1 0	-160.000	3	0.326	
n1 c3 c3	h1 0.65	1 0	80.000	3	0.326	
n1 c3 c3	cl 0.00	0 0	-160.000	3	0.000	
h1 c3 c3	h1 0.65	1 0	-40.000	3	0.326	
cl c3 c3	h1 0.00	0 0	-160.000	3	0.000	
cl c3 c3	cl 0.00	0 0	-40.000	3	0.000	
cl c3 c3	h1 0.00	0 0	80.000	3	0.000	
TOTA	L TORSIONAL	ENERGY =	1.303 kJ/	mol		
MPRO	PER T	ORSION	I A L			

```
4601
4602
    ----ATOM TYPES---- FORCE IMPROPER TORSION
    I J K L CONSTANT S ANGLE n ENERGY
4603
4604
4605
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
4606
4607 VAN DER WAALS
4608
4609 ATOM TYPES
4610 I J Rij kij ENERGY
4611
    _____
4612 h1 h1
            2.300
                   0.109
4613 h1 h1
           2.885
                  -0.031
4614 h1 cl
           2.960
                   0.012
           2.518 -0.013
4615 h1 h1
4616 h1 h1
           2.300
                   0.109
4617 h1 cl
           3.474
                  -0.129
4618 cl h1
           3.474 -0.129
           2.960
                   0.012
4619 cl h1
4620 cl cl 2.865 15.169
4621
     TOTAL VAN DER WAALS ENERGY = 15.111 kJ/mol
4622
4623 ELECTROSTATIC INTERACTIONS
4624
4625 ATOM TYPES
              Rij 332.17*QiQj ENERGY
4626
    I J
4627
    _____
          2.300
4628 h1 h1
                   1.352
                          0.588
4629 h1 h1
           2.885
                  1.352
                          0.469
4630 h1 cl
           2.960 -3.809 -1.287
4631 h1 h1
           2.518
                   1.352
                          0.537
           2.300
                  1.352
4632 h1 h1
                          0.588
4633 h1 cl
           3.474 -3.809 -1.097
4634 cl h1
            3.474
                  -3.809 -1.097
            2.960 -3.809 -1.287
4635 cl h1
            2.865
                  10.728
                          3.745
4636 cl cl
4637
      TOTAL ELECTROSTATIC ENERGY = 1.160 kJ/mol
4638
4639 TOTAL ENERGY = 100.634 kJ/mol
4640
4641 A T O M T Y P E S
4642
4643 IDX TYPE RING
4644 1 1 NO
4645 2 1 NO
4646 3 5 NO
4647 4 5 NO
4648 5 12 NO
4649 6 5 NO
```

```
4650 7 5 NO
4651
     8 12 NO
4652
4653 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
     6 0.000000
4661
4662 7 0.000000
4663 8 0.000000
4664
4665 PARTIAL CHARGES
4666
     IDX CHARGE
4667
4668 1 0.290000
4669 2 0.290000
     3 0.000000
4670
4671 4 0.000000
4672 5 -0.290000
     6 0.000000
4673
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
     A T O M T Y P E S
4686
4687
4688 IDX TYPE RING
     1 c3 NO
4689
4690
     2 c3 NO
4691 3 h1 NO
4692
     4 h1 NO
4693
     5 cl NO
4694 6 h1 NO
4695 7 h1 NO
     8 cl NO
4696
4697
4698 C H A R G E S
```

```
4700 IDX CHARGE
4701 1 0.036009
4702
    2 0.036009
4703
    3 0.044101
    4 0.044101
4704
4705
    5 -0.124211
4706
    6 0.044101
    7 0.044101
4707
    8 -0.124211
4708
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...
4717
    SETTING UP ELECTROSTATIC CALCULATIONS...
4718
4719
    ENERGY
4720
4721
4722
    BOND STRETCHING
4723
    ATOM TYPES FF BOND IDEAL
4724
                                 FORCE
                                 CONSTANT
                                           DELTA
4725
    I J
           CLASS LENGTH
                         LENGTH
                                                   ENERGY
4726
    5 1
            0
                  1.000
                          1.093
4727
                                   4.766
                                           -0.093
                                                    3.578
4728
    5
        1
             0
                  1.000
                          1.093
                                   4.766
                                           -0.093
                                                   3.578
4729
    1
        1
            0
                  1.540
                          1.508
                                   4.258
                                           0.032
                                                    0.294
                  1.000
                          1.093
4730
    1 5
             0
                                   4.766
                                           -0.093
                                                   3.578
4731
    1 12
            0
                  1.670
                          1.773
                                   2.974
                                           -0.103
                                                   2.795
4732
    1 12
             0
                  1.670
                          1.773
                                   2.974
                                           -0.103
                                                    2.795
                          1.093 4.766 -0.093
                   1.000
    1 5
            0
                                                   3.578
4733
       TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol
4734
4735
    ANGLE BENDING
4736
4737
4738
    ATOM TYPES
                FF VALENCE
                             IDEAL
                                     FORCE
                CLASS ANGLE
                              ANGLE CONSTANT DELTA ENERGY
4739
     I J K
4740
    ______
4741
    1
        1 5
                0 109.500 110.549
                                       0.636
                                               -1.049
                                                        0.015
        1 5
                0 109.442 108.836
                                       0.516
                                               0.606
                                                        0.004
4742
    5
                0 109.442 108.162
                                               1.280
4743
    5
        1 12
                                       0.698
                                                       0.025
        1 5
4744
    1
                0 109.500 110.549
                                       0.636
                                               -1.049
                                                        0.015
                0 109.500 108.679
                                       1.056
                                               0.821
4745
    1
        1 12
                                                        0.016
                0 109.442 108.162
                                               1.280
    5
        1 12
                                       0.698
4746
                                                       0.025
                0 109.500 110.549
4747
    1 1 5
                                     0.636
                                              -1.049
                                                        0.015
```

4699

5	_								0 00
	1	12	0	109.442	108.1	L62	0.698	1.280	0.02
5	1	5	0	109.442	108.8	336	0.516	0.606	0.00
1	1	12	0	109.500	108.6	579	1.056	0.821	0.01
1	1	5	0	109.500	110.5	549	0.636	-1.049	0.01
5	1	12	0	109.442	108.1	L62	0.698	1.280	0.02
	TOTA	AL ANO	GLE BENDI	NG ENERG	Y = 0.20	0058 kc	:al/mol		
ST	REI	СН	BEN	DING					
ATOM	TYPE	S	FF	VALENC	E DEI	LTA	FORCE	CONSTANT	
I	J	K	CLASS	ANGLE	ANG	GLE	ΙJ	JК	ENERG
1	1	5	0	109.500	-1.0)49	0.227	0.070	-0.002
5	1	5	0	109.442	0.6	506	0.115	0.115	-0.033
5	1	12					-0.018		
							0.227		-0.002
			0				0.176		
		12					-0.018		
			0				0.227		
5			0				-0.018		
			0				0.115		
							0.176		
	1	Э	0	109.500	-1.(149	0.227	0.070	-0.002
	1	1.2	0	100 442	1 1	0.00	0 010	0 200	0 121
	TOTA		RETCH BEN				-0.018 kcal/mol	0.380	-0.121
то	TOT <i>E</i> R S I TYPE	AL STE	RETCH BEN	DING ENE	RGY = -0. TORSION	.69593 F	corce const	FANT	
то	TOT <i>i</i>	AL STE	RETCH BEN	DING ENE	RGY = -0	.69593 F	kcal/mol	FANT	-0.121
T O I	TOTA R S I TYPE J	L STE	RETCH BEN	DING ENE FF CLASS	TORSION ANGLE	. 69593 F	CORCE CONST	FANT	ERGY
T O I	TOTA R S I TYPE J 1	L STE	RETCH BEN A L L 5	FF CLASS 0 -2	TORSION ANGLE	.69593 F	CORCE CONST	FANT V3 ENF	ERGY 0.349
T O I ATOM I 5	TOTA R S I TYPE J 1 1	AL STE	RETCH BEN A L L 5	FF CLASS 0 -2 0 10	TORSION ANGLE	.69593 F 0.284 0.678	**CORCE CONS*** V1 V2 -1.386 -0.602	FANT V3 ENE 0.314	ERGY 0.349 -0.005
T O 1 ATOM I 5 5	TOTA R S I TYPE J 1 1	AL STE	A L L 5 12 5	FF CLASS0 -2 0 10 0 -14	TORSION ANGLE 0.000 0.000	.69593 F 0.284 0.678 0.284	**CORCE CONS*** V1 V2 -1.386 -0.602	FANT V3 ENF 0.314 0.398 0.314	ERGY 0.349 -0.005 -0.304
T O 1 ATOM I 5 5 5	TOTA R S I TYPE J 1 1 1	I O N SS K 1 1 1	A L L 5 12 5 5	FF CLASS0 10 0 -14 0 10	TORSION ANGLE 0.000 0.000 0.000	.69593 F 0.284 0.678 0.284 0.284	**CORCE CONS** V1 V2 -1.386 -0.602 -1.386 -1.386	FANT V3 ENF 0.314 0.398 0.314 0.314	ERGY 0.349 -0.005 -0.304 -0.991
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	L 5 12 5 12	FF CLASS0 -2 0 10 0 -14 0 10 0 -14	TORSION ANGLE 0.000 0.000 0.000 0.000	.69593 F 0.284 0.678 0.284 0.284	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -1.386 -0.602	V3 ENF 0.314 0.398 0.314 0.314 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129
ATOM I 5 5 5 5 5	TOTA R S I TYPE J 1 1 1 1	I O N SS K 1 1 1 1	L L 5 12 5 12 5 5 5 12 5 5	FF CLASS 0 -2 0 10 0 -14 0 10 0 -14 0 -2	TORSION ANGLE 0.000 0.000 0.000 0.000 0.000	.69593 F 0.284 0.678 0.284 0.284 0.678 0.284	CORCE CONSO V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386	V3 ENF 0.314 0.398 0.314 0.314 0.398 0.314	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349
T O 1 ATOM I 5 5 5 5 5 12	TOTA TYPE J 1 1 1 1 1 1	I O N IS K 1 1 1 1 1	L	FF CLASS0 -2 0 10 0 -14 0 10 0 -14 0 -2 0 -14	TORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000	.69593 F 0.284 0.678 0.284 0.678 0.284 0.678	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602	V3 ENE 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129
T O 1 ATOM I 5 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 12 5 12 5 5 12 5 12 12 12	FF CLASS0 10 0 -14 0 10 0 -14 0 -2 0 -14 0 -2	TORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000	.69593 F 0.284 0.678 0.284 0.678 0.284 0.678 0.000	CORCE CONSO V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000	V3 ENF 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
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 IS K 1 1 1 1 1 1	L L 5 12 5 12 5 12 5 12 5 5 12 5 5 12 5 5 12 5 5 12 5 5 12 5 12 5 5 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 12 5 5 5 12 5 5 5 12 5 5 5 12 5 5 5 5	FF CLASS 0 -2 0 10 0 -14 0 10 0 -14 0 -2 0 -14 0 -2 0 10	TORSION ANGLE 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 0.284 0.678 0.000 0.678	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 ENE 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
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 IS K 1 1 1 1 1 1	L L 5 12 5 12 5 5 12 5 12 12 12	FF CLASS 0 -2 0 10 0 -14 0 10 0 -14 0 -2 0 -14 0 -2 0 10	TORSION ANGLE 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 0.284 0.678 0.000 0.678	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 ENF 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
T O 1 ATOM I 5 5 5 12 12 12	TOTA R S I TYPE J 1 1 1 1 1 TOTA	AL STE	A L L 5 12 5 12 5 12 5 12 5 8 SIONAL E	FF CLASS 0 -2 0 10 0 -14 0 10 0 -14 0 -2 0 -14 0 -2 0 10 NERGY =	TORSION ANGLE 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 0.284 0.678 0.000 0.678 kcal/m	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 ENF 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
T O 1 ATOM I 5 5 5 12 12 12	TOTA R S I TYPE J 1 1 1 1 1 TOTA	AL STE	L L 5 12 5 12 5 12 5 12 5 5 12 5 5 12 5 5 12 5 5 12 5 5 12 5 12 5 5 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 12 5 5 5 12 5 5 5 12 5 5 5 12 5 5 5 5	FF CLASS 0 -2 0 10 0 -14 0 10 0 -14 0 -2 0 -14 0 -2 0 10 NERGY =	TORSION ANGLE 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 0.284 0.678 0.000 0.678 kcal/m	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 ENF 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
T O I ATOM I 5 5 5 12 12 12	TOTA R S I TYPE J 1 1 1 1 1 TOTA TOTA	I O N SS K 1 1 1 1 1 1 1 1 1 1 1 1	L L 5 12 5 12 5 12 5 12 5 PLAN	FF CLASS 0 -2 0 10 0 -14 0 10 0 -14 0 -2 0 -14 0 -2 0 10 NERGY =	TORSION ANGLE 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 0.284 0.678 0.000 0.678 kcal/m	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 -0.602 0.000 -0.602	V3 ENF 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
T O I ATOM I 5 5 5 12 12 12 12 ATOM	TOTA R S I TYPE J 1 1 1 1 TOTA TYPE	I O N ISS K 1 1 1 1 1 1 1 1 1 1 1 I I	RETCH BEN A L L 5 12 5 12 5 12 5 RSIONAL E	FF CLASS 0 -2 0 10 0 -14 0 -14 0 -2 0 -14 0 -2 0 -14 EBE FF	TORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	.69593 FORCE	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 0.000 -0.602	V3 ENE 0.314 0.398 0.314 0.398 0.314 0.398 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
T O I ATOM I 5 5 5 5 12 12 12 12 ATOM	TOTA R S I TYPE J 1 1 1 1 TOTA TYPE	I O N ISS K 1 1 1 1 1 1 1 1 1 1 1 I I	L L 5 12 5 12 5 12 5 12 5 PLAN	FF CLASS 0 -2 0 10 0 -14 0 -14 0 -2 0 -14 0 -2 0 -14 EBE FF	TORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	.69593 FORCE	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 0.000 -0.602	V3 ENF 0.314 0.398 0.314 0.398 0.314 0.398 0.314 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670
T O 1 ATOM I 5 5 5 12 12 12 12	TOTA R S I TYPE J 1 1 1 1 TOTA TYPE J TYPE J	I O N IS K 1 1 1 1 1 1 1 Control I I I I I I I I I I I I I	ETCH BEN A L L 5 12 5 12 5 12 5 RSIONAL E	FF CLASS 0 -2 0 10 0 -14 0 -14 0 -2 0 -14 0 -2 0 -14 EBE FF CLASS	TORSION ANGLE 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	.69593 FORCE CONSTA	CORCE CONST V1 V2 -1.386 -0.602 -1.386 -0.602 -1.386 -0.602 0.000 -0.602	V3 ENE 0.314 0.398 0.314 0.398 0.314 0.398 0.398 0.398	ERGY 0.349 -0.005 -0.304 -0.991 0.129 0.349 0.129 0.670

ATOM TYP						
	Rij					
	2.232					
	2.232					
	3.129		0.053			
	2.638		0.022			
	2.232		0.022			
	3.399					
	3.399		0.053			
	3.129					
	2.711					
TOT	AL VAN DER W	AALS ENERGY	x = 17.78153	kcal/mol		
ELEC	TROSTA	T I C I N	TERACI	TIONS		
ATOM TYP	ES					
I J	Rij	Qi	Qj	ENERGY		
12 12	2.761	-0.290	-0.290	7.587		
тот	AL ELECTROST	ATIC ENERGY	7 = 7.58721	kcal/mol		
101			7.30721	KCGI/ MOI		
101			7.30721	RCQ17 MO1		
	ERGY = 45.38			KGGI/ MOI		
				Kear/ mor		
TOTAL EN	ERGY = 45.38			Ked1/ Mo1		
TOTAL EN	ERGY = 45.38			Ked1/ Mo1		
TOTAL EN	ERGY = 45.38			Ked1/ Mo1		
TOTAL EN E N E R	ERGY = 45.38	946 kcal/mo		KCCI7 MOI		
TOTAL EN E N E R B O N D	ERGY = 45.38 G Y S T R E T	946 kcal/mo	ol	KCCI7 MOI		
TOTAL EN E N E R B O N D ATOM TYP	ERGY = 45.38 G Y S T R E T ES BOND	946 kcal/mc C H I N G IDEAL	FORCE			
TOTAL EN E N E R B O N D ATOM TYP I J	ERGY = 45.38 G Y S T R E T ES BOND LENGTH	946 kcal/mo C H I N G IDEAL LENGTH	FORCE CONSTANT	DELTA		
TOTAL EN E N E R B O N D ATOM TYP I J	ERGY = 45.38 G Y S T R E T ES BOND LENGTH	946 kcal/mc C H I N G IDEAL LENGTH	FORCE CONSTANT	DELTA		
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000	946 kcal/mc C H I N G IDEAL LENGTH	FORCE CONSTANT	DELTA -0.093	12.163	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093	FORCE CONSTANT 1406.346 1406.346	DELTA -0.093 -0.093	12.163 12.163	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535	FORCE CONSTANT 1406.346 1406.346 1269.019	DELTA -0.093 -0.093 0.005	12.163 12.163 0.032	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346	DELTA -0.093 -0.093 0.005 -0.093	12.163 12.163 0.032 12.163	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670	946 kcal/mc 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	DELTA -0.093 -0.093 0.005 -0.093 -0.116	12.163 12.163 0.032 12.163 15.718	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.786	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117	DELTA -0.093 -0.093 0.005 -0.093 -0.116 -0.116	12.163 12.163 0.032 12.163 15.718	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1 c3 h1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670 1.670 1.000	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.786 1.786 1.093	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117	DELTA -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -0.093	12.163 12.163 0.032 12.163 15.718	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1 c3 h1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.786 1.786 1.093	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117	DELTA -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -0.093	12.163 12.163 0.032 12.163 15.718	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1 c3 h1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670 1.000 AL BOND STRE	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.786 1.786 1.786 1.093 TCHING ENEF	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117	DELTA -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -0.093	12.163 12.163 0.032 12.163 15.718	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1 c3 h1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670 1.670 1.000	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.786 1.786 1.786 1.093 TCHING ENEF	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117	DELTA -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -0.093	12.163 12.163 0.032 12.163 15.718	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 c3 h1 c3 c1 c3 c1 c3 c1 c3 h1	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670 1.670 1.000 AL BOND STRE E B E N D	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.786 1.786 1.786 I.N G	FORCE CONSTANT	DELTA -0.093 -0.093 0.005 -0.093 -0.116 -0.116 -0.093	12.163 12.163 0.032 12.163 15.718	
TOTAL EN E N E R B O N D ATOM TYP I J h1 c3 h1 c3 c3 c3 h1 c3 c1 c3 c1 c3 h1 TOT A N G L ATOM TYP	ERGY = 45.38 G Y S T R E T ES BOND LENGTH 1.000 1.000 1.540 1.000 1.670 1.670 1.000 AL BOND STRE	946 kcal/mc C H I N G IDEAL LENGTH 1.093 1.093 1.535 1.093 1.786 1.786 1.786 1.093 TCHING ENEF	FORCE CONSTANT 1406.346 1406.346 1269.019 1406.346 1168.117 1168.117 1406.346 RGY = 80.12	DELTA -0.093 -0.093 -0.093 -0.116 -0.116 -0.093 22 kJ/mol	12.163 12.163 0.032 12.163 15.718 15.718 12.163	

h	1 c3	h1	109	.442	109.550	164.03) -	-0.002	0.001
h:	1 c3	cl	109	.442	105.930	183.00	5	0.061	0.688
C.	3 c3	h1	109	.500	110.070	194.10) –	-0.010	0.019
C.	3 c3	cl	109	.500	110.330	260.41	9 –	-0.014	0.055
h	1 c3	cl	109	.442	105.930	183.00	5	0.061	0.688
C.	3 c3	h1		.500		194.10) –	-0.010	0.019
h:	1 c3	cl	109	.442	105.930	183.00	5	0.061	0.688
h:	1 c3	h1	109	.442	109.550	164.03		-0.002	
C.	3 c3	cl	109	.500	110.330	260.41	9 –	-0.014	0.055
	3 c3					194.10			
						183.00			0.688
		TOTA	AL ANG	LE BENI	DING ENERG	Y = 2.93	8 kJ/mo	ol	
Т	O R	. S :	ION	A L					
					T07.47		monato		
						a			ENEDGY
						s 			
						-20.000			
						100.000			
						-140.000			
						100.000		0.977	
						-140.000			
	1 c3					-20.000		0.977	
	1 c3					-140.000			
						-20.000			
						100.000			
						3.908 kJ			
Ι	M P	R	OPE:	R T (ORSIO	N A L			
	A	MOT	TYPES		FORCE	IMPROPER	_TORSIO	ON	
	I	J	K	L	CONSTANT	S	ANGLE	E n	ENERGY
		TOTA	AL IMP	ROPER-	TORSIONAL :	ENERGY =	0.000	kJ/mol	
V	A N	I	DER	WAA	ALS				
70.1	TION.	шил	E.C.						
	TOM			D/ -	1-2 *	D100.			
						ENERGY			
				 32					
				31 - 29 -					
				29 - 38 -					
				38 - 32					
				99 - 99 -					
				99 - 29 -					
Ċ.	- 111		J.1.	٠.	-0.100				

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4895 cl cl 2.711 33.340
4896
       TOTAL VAN DER WAALS ENERGY = 33.209 kJ/mol
4897
4898 ELECTROSTATIC INTERACTIONS
4899
4900 ATOM TYPES
4901 I J
            Rij 332.17*QiQj ENERGY
4902
    _____
            2.232 1.352
4903 h1 h1
                           0.606
4904 h1 h1
            2.831
                    1.352
                            0.478
4905 h1 cl
            3.129 -3.809 -1.217
            2.638
                   1.352
4906 h1 h1
                            0.513
4907 h1 h1
            2.232
                    1.352
                           0.606
4908 h1 cl
            3.399 -3.809 -1.121
4909 cl h1
            3.399 -3.809 -1.121
                   -3.809 -1.217
4910 cl h1
            3.129
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
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4944 2 0.290000
4945 3 0.000000
4946 4 0.000000
4947 5 -0.290000
4948
     6 0.000000
     7 0.000000
4949
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
4958
     SETTING UP VAN DER WAALS CALCULATIONS...
4959
     SETTING UP ELECTROSTATIC CALCULATIONS...
4960
4961
     ATOM TYPES
4962
4963 IDX TYPE RING
4964
     1 c3 NO
4965 2 c3 NO
     3 h1 NO
4966
     4 h1 NO
4967
     5 cl NO
4968
4969
     6 hl NO
     7 h1 NO
4970
4971
     8 cl NO
4972
4973
     CHARGES
4974
     IDX CHARGE
4975
4976
     1 0.036009
4977
     2 0.036009
4978
     3 0.044101
4979
     4 0.044101
4980 5 -0.124211
     6 0.044101
4981
4982 7 0.044101
     8 -0.124211
4983
4984
4985 SETTING UP CALCULATIONS
4986
4987
     SETTING UP BOND CALCULATIONS...
     SETTING UP ANGLE CALCULATIONS...
4988
     SETTING UP TORSION CALCULATIONS...
4989
     SETTING UP IMPROPER TORSION CALCULATIONS...
4990
     SETTING UP VAN DER WAALS CALCULATIONS...
4991
4992
     SETTING UP ELECTROSTATIC CALCULATIONS...
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4993 4994 ENERGY 4995 4996 BOND STRETCHING 4997 4998 4999 ATOM TYPES FF BOND IDEAL FORCE 5000 CLASS LENGTH LENGTH CONSTANT I J DELTA ENERGY 5001 ______ 0 5002 5 1.000 1.093 4.766 -0.093 3.578 3.578 5003 5 0 1.000 1.093 4.766 -0.093 1 5004 1 1 0 1.540 1.508 4.258 0.032 0.294 5005 1 5 0 1.000 1.093 4.766 -0.093 3.578 5006 1 12 0 1.670 1.773 2.974 2.795 -0.103 5007 1 5 0 1.000 1.093 -0.093 4.766 3.578 1 12 5008 0 1.773 2.974 -0.103 2.795 1.670 TOTAL BOND STRETCHING ENERGY = 20.19629 kcal/mol 5009 5010 ANGLE BENDING 5011 5012 5013 ATOM TYPES FF VALENCE IDEAL FORCE CLASS ANGLE I J K ANGLE CONSTANT DELTA 5014 ENERGY 5015 0.636 5016 1 5 0 109.500 110.549 -1.049 0.015 1 109.442 108.836 5017 5 1 5 0 0.516 0.606 0.004 5018 5 1 12 0 109.442 108.162 0.698 1.280 0.025 1 5 5019 1 0 109.500 110.549 0.636 -1.049 0.015 5020 1 1 12 0 109.500 108.679 1.056 0.821 0.016 109.442 108.162 1.280 5021 5 1 12 0 0.698 0.025 5022 1 1 5 0 109.500 110.549 0.636 -1.0490.015 5023 5 1 5 0 109.442 108.836 0.516 0.606 0.004 0 109.442 108.162 5024 5 1 12 0.698 1.280 0.025 5025 1 1 5 0 109.500 110.549 0.636 -1.049 0.015 108.679 5026 1 1 12 0 109.500 1.056 0.821 0.016 109.442 108.162 1.280 5027 5 1 12 0 0.698 0.025 TOTAL ANGLE BENDING ENERGY = 0.20058 kcal/mol 5028 5029 STRETCH BENDING 5030 5031 5032 FF VALENCE FORCE CONSTANT ATOM TYPES DELTA IJ JK 5033 CLASS ANGLE I J K ANGLE ENERGY 5034 ______ 5035 1 1 5 0 109.500 -1.0490.227 0.070 -0.0025 1 0 109.442 0.606 0.115 5036 5 0.115 -0.033 1.280 5037 5 1 12 0 109.442 -0.018 0.380 -0.121 1 5 5038 1 0 109.500 -1.0490.227 0.070 -0.002 109.500 0.821 0.176 5039 1 1 12 0 0.386 -0.0700 109.442 1.280 5040 5 1 12 -0.018 0.380 -0.1215041 1 5 0 109.500 -1.0490.227 0.070 -0.002

	1	5	^						
5					2 0.60				
					2 1.28				
					0 -1.04				
					0 0.82				
					2 1.28			0.38	0 -0.12
	TOTA	L STR	RETCH BE	ENDING EN	ERGY = -0.6	59593 k	cal/mol		
го:	RSI	ON	AL						
3 mon		ı.a			MODGTON	T0	Dan aou		
					TORSION				ENEDGY
					ANGLE				
									0.598
									-0.655
									0.116
					20.000			0.396	
					0.000				0.598
					20.000				
			12					0.398	
					20.000				0.116
					20.000				
								0.893	0.893
	TOTA	T TOR	RSIONAL	ENERGY =	1.24400	ccal/mo	1		
ט ט י	T - O) F –	PLAN	IE BE	NDTNC				
					N D I N G				
\ TIOM						FORGE			
	TYPE				ООР		m 57	IFDCV	
I	J	K	L	CLASS	OOP ANGLE	CONSTAN	T EN	IERGY	
I 	J	К	L	CLASS	OOP ANGLE (CONSTAN			
I 	J	К	L	CLASS	OOP ANGLE	CONSTAN			
I 	J TOTA	K L OUT	L I-OF-PL	CLASS	OOP ANGLE (CONSTAN			
I 	J TOTA	K L OUT	L	CLASS	OOP ANGLE (CONSTAN			
I 	J TOTA N D	K L OUT	L I-OF-PL	CLASS	OOP ANGLE (CONSTAN			
I V A :	J TOTA N D	K L OUT E R	L '-OF-PLA W A A	CLASS	OOP ANGLE (NG ENERGY =	CONSTAN = 0.00	 000 kcal		
I V A :	J TOTA N D TYPE J	K L OUT E R	L C-OF-PLA W A A	CLASS ANE BENDI A L S R*IJ	OOP ANGLE (NG ENERGY =	CONSTAN = 0.00	 000 kcal ERGY		
I V A :	J TOTA N D TYPE J	K L OUT E R	L C-OF-PLA W A A	CLASS ANE BENDI	OOP ANGLE (CONSTAN = 0.00	 000 kcal ERGY		
I 7 A 1 ATOM I 5	J TOTA N D TYPE J 5	K L OUT E R	L C-OF-PLA W A A Rij	CLASS ANE BENDITAL S R*IJ	OOP ANGLE (NG ENERGY = EPSILON 0 0.022	CONSTAN = 0.00 N EN 2 0	000 kcal ERGY		
I V A : ATOM I 5 5	J TOTA N D TYPE J 5 5	K LOUT ER	L C-OF-PLA W A A Rij 2.208 2.746	CLASS ALS R*IJ 2.97	OOP ANGLE (CONSTAN = 0.00 N EN 2 0 2 -0	ERGY377		
I ATOM I 5 5 5	J TOTA N D TYPE J 5 5 12	K L OUT ER	L C-OF-PLA W A A Rij 2.208 2.746 3.280	CLASSANE BENDITAL S R*IJ 2.97 2.97 3.71	OOP ANGLE (NG ENERGY = EPSILOR 0 0.022 0 0.022 3 0.053	EONSTAN = 0.00 N EN 2 0 2 -0 3 0	ERGY377 .014		
I V A : ATOM I 5 5 5 5	J TOTA N D TYPE J 5 5 12 5	K LOUT ER	L C-OF-PLA W A A Rij 2.208 2.746 3.280 2.746	CLASS	OOP ANGLE (N EN 2 0 0 2 -0 3 0 2 -0	ERGY377 .014 .009		
I V A : ATOM I 5 5 5 5	J TOTA N D TYPE J 5 5 12 5 5	K L OUT ER	L C-OF-PLA W A A Rij 2.208 2.746 3.280 2.746 2.208	CLASS ANE BENDITAL S R*IJ 2.97 2.97 3.71 2.97 2.97	OOP ANGLE (NG ENERGY = EPSILOR 0 0.022 0 0.022 0 0.022 0 0.022 0 0.022	EONSTAN = 0.00 N EN 2 0 2 -0 3 0 2 -0 2 0	ERGY377 .014 .009 .014		
I	J TOTA N D TYPE J 5 5 12 5 12	K LOUT ER	L	CLASS	OOP ANGLE (EONSTAN = 0.00 N EN 2 0 2 -0 3 0 2 -0 2 0 3 0	ERGY377 .014 .009 .014 .377		
I V A : ATOM I 5 5 5 5 5 5	J TOTA N D TYPE J 5 5 12 5 12 5 12 5	K L OUT ER	L C-OF-PLA W A A Rij 2.208 2.746 3.280 2.746 2.208 3.280 3.280 3.280	CLASS ANE BENDITAL S R*IJ 2.97 2.97 2.97 2.97 3.71 2.97 3.71 3.71	OOP ANGLE (NG ENERGY = EPSILON 0 0.022 0 0.022 0 0.022 0 0.022 0 0.023 0 0.053 0 0.053	EONSTAN = 0.00 N EN 2 0 2 -0 3 0 2 -0 2 0 3 0 3 0	ERGY377 .014 .009 .014 .377 .009		
I	J TOTA N D TYPE J 5 5 12 5 12 5 5 12 5	K LOUT ER	L R-OF-PLA W A A Rij 2.208 2.746 3.280 2.746 2.208 3.280 3.280 3.280	CLASS	OOP ANGLE (NG ENERGY = EPSILON 0 0.022 0 0.022 0 0.022 3 0.053 0 0.053 3 0.053 3 0.053	EONSTAN = 0.00 N EN 2 0 3 0 2 -0 3 0 2 0 3 0 3 0	ERGY377 .014 .009 .014 .377 .009 .009		
I V A : ATOM I 5 5 5 5 5 5 12	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12	K L OUT ER	L C-OF-PLA W A A Rij 2.208 2.746 3.280 2.746 2.208 3.280 3.280 3.280 3.280 2.655	CLASS	OOP ANGLE (NG ENERGY = EPSILON 0 0.022 0 0.022 0 0.022 0 0.022 0 0.023 0 0.053 0 0.053 0 0.053	EONSTAN = 0.00 N EN 2 0 2 -0 3 0 2 -0 2 0 3 0 3 0 5 20	ERGY377 .014 .009 .014 .377 .009 .009		
I	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12	K L OUT ER	L C-OF-PLA W A A Rij 2.208 2.746 3.280 2.746 2.208 3.280 3.280 3.280 3.280 2.655	CLASS	OOP ANGLE (NG ENERGY = EPSILON 0 0.022 0 0.022 0 0.022 3 0.053 0 0.053 3 0.053 3 0.053	EONSTAN = 0.00 N EN 2 0 2 -0 3 0 2 -0 2 0 3 0 3 0 5 20	ERGY377 .014 .009 .014 .377 .009 .009		
I 	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12 5 12 TOTA	K L OUT E R	L C-OF-PLA W A A Rij 2.208 2.746 3.280 2.746 2.208 3.280 3.280 3.280 3.280 3.280	CLASS ANE BENDIT A L S R*IJ 2.97 2.97 3.71 2.97 3.71 3.71 4.08 AALS ENERG	OOP ANGLE (NG ENERGY = EPSILON 0 0.022 0 0.022 0 0.022 3 0.053 0 0.053 3 0.053 3 0.053 3 0.053 6 0.276 GY = 21.415	EONSTAN = 0.00 N EN 2 0 2 -0 3 0 2 -0 3 0 3 0 5 20 5 12 kca	ERGY377 .014 .009 .014 .377 .009 .009 .009		
I ATOM I 5 5 5 5 12 12	J TOTA N D TYPE J 5 5 12 5 12 5 12 5 12 5 12 TOTA	K L OUT E R	L C-OF-PLA W A A Rij 2.208 2.746 3.280 2.746 2.208 3.280 3.280 3.280 3.280 3.280	CLASS ANE BENDIT A L S R*IJ 2.97 2.97 3.71 2.97 3.71 3.71 4.08 AALS ENERG	OOP ANGLE (NG ENERGY = EPSILON 0 0.022 0 0.022 0 0.022 0 0.022 0 0.023 0 0.053 0 0.053 0 0.053	EONSTAN = 0.00 N EN 2 0 2 -0 3 0 2 -0 3 0 3 0 5 20 5 12 kca	ERGY377 .014 .009 .014 .377 .009 .009 .009		

```
5091 I J Rij Qi Qj ENERGY
5092
5093
    12 12 2.705 -0.290 -0.290 7.743
5094
      TOTAL ELECTROSTATIC ENERGY = 7.74347 kcal/mol
5095
5096 | TOTAL ENERGY = 50.10353 kcal/mol
5097
5098 E N E R G Y
5099
5100
5101 BOND STRETCHING
5102
5103 ATOM TYPES BOND
                            FORCE
                   IDEAL
5104
    I J
           LENGTH
                   LENGTH
                           CONSTANT
                                     DELTA ENERGY
5105
5106 hl c3
           1.000
                  1.093
                                   -0.093
                          1406.346
                                           12,163
5107 h1 c3
          1.000
                  1.093
                          1406.346
                                   -0.093
                                           12.163
          1.540
                         1269.019
5108 c3 c3
                  1.535
                                    0.005
                                           0.032
5109 c3 h1
          1.000
                  1.093
                          1406.346
                                  -0.093
                                           12.163
5110 c3 cl
          1.670
                  1.786
                          1168.117
                                   -0.116
                                           15.718
5111 c3 h1
          1.000
                  1.093
                         1406.346
                                   -0.093
                                           12.163
5112 c3 cl
                  1.786
          1.670
                          1168.117
                                           15.718
                                   -0.116
      TOTAL BOND STRETCHING ENERGY = 80.122 kJ/mol
5113
5114
5115 ANGLE BENDING
5116
5117 ATOM TYPES VALENCE IDEAL FORCE
    I J K
                ANGLE
5118
                        ANGLE
                               CONSTANT
                                         DELTA
                                                 ENERGY
5119
    ______
5120 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                              0.019
5121 h1 c3 h1 109.442
                   109.550
                             164.039
                                     -0.002
                                              0.001
5122 h1 c3 cl 109.442 105.930
                            183.005
                                      0.061
                                              0.688
5123 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                              0.019
           109.500
                            260.419
5124 c3 c3 c1
                   110.330
                                     -0.014
                                              0.055
5125 h1 c3 cl 109.442 105.930
                            183.005
                                      0.061
                                              0.688
5126 c3 c3 h1 109.500 110.070
                            194.100
                                     -0.010
                                              0.019
5127 h1 c3 h1 109.442
                   109.550
                             164.039
                                     -0.002
                                              0.001
                            183.005
5128 h1 c3 cl 109.442 105.930
                                      0.061
                                              0.688
5129 c3 c3 h1 109.500
                   110.070
                            194.100
                                     -0.010
                                              0.019
5130 c3 c3 cl 109.500 110.330
                            260.419
                                     -0.014
                                              0.055
    h1 c3 cl 109.442 105.930 183.005 0.061 0.688
5131
5132
     TOTAL ANGLE BENDING ENERGY = 2.938 kJ/mol
5133
5134 T O R S I O N A L
5135
5136 ----ATOM TYPES----
                   FORCE
                                 TORSION
    I J K L CONSTANT
5137
                                  ANGLE n ENERGY
                            S
5138
    _____
5139 h1 c3 c3 h1 0.651 0 0.000 3 1.303
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5140 h1 c3 c3 h1 0.651 0 -120.000 3 1.303
5141 h1 c3 c3 cl
              0.000
                        0
                           120.000 3
                                       0.000
5142 h1 c3 c3 h1
              0.651
                        0 120.000 3
                                       1.303
                            0.000 3
5143 h1 c3 c3 h1
              0.651
                        0
                                       1.303
                                       0.000
5144 h1 c3 c3 cl
              0.000
                        0 -120.000 3
5145 cl c3 c3 h1
              0.000
                        0 -120.000 3
                                       0.000
5146 cl c3 c3 h1
               0.000
                        0 120.000 3
                                       0.000
    cl c3 c3 cl
                        0
                            -0.000 3
                                       0.000
5147
               0.000
     TOTAL TORSIONAL ENERGY = 5.210 kJ/mol
5148
5149
5150 IMPROPER TORSIONAL
5151
5152 ----ATOM TYPES---- FORCE IMPROPER_TORSION
5153
    I J K L CONSTANT
                            s ANGLE n ENERGY
5154
       TOTAL IMPROPER-TORSIONAL ENERGY = 0.000 kJ/mol
5155
5156
5157 VAN DER WAALS
5158
5159 ATOM TYPES
5160
    I J
           Rij kij ENERGY
5161 -----
5162 h1 h1
           2.208
                  0.251
5163 h1 h1
           2.746
                  -0.033
           3.280
5164 h1 cl
                  -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
5176
    I J
            Rij 332.17*QiQj ENERGY
5177
    _____
5178 h1 h1 2.208
                  1.352
                         0.613
5179 h1 h1
           2.746
                  1.352
                         0.493
           3.280 -3.809 -1.161
5180 h1 cl
5181 h1 h1
           2.746
                  1.352
                         0.493
5182 h1 h1
           2.208
                  1.352
                         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
    TOTAL ELECTROSTATIC ENERGY = 1.607 kJ/mol
5187
5188
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