分子模拟技术栈

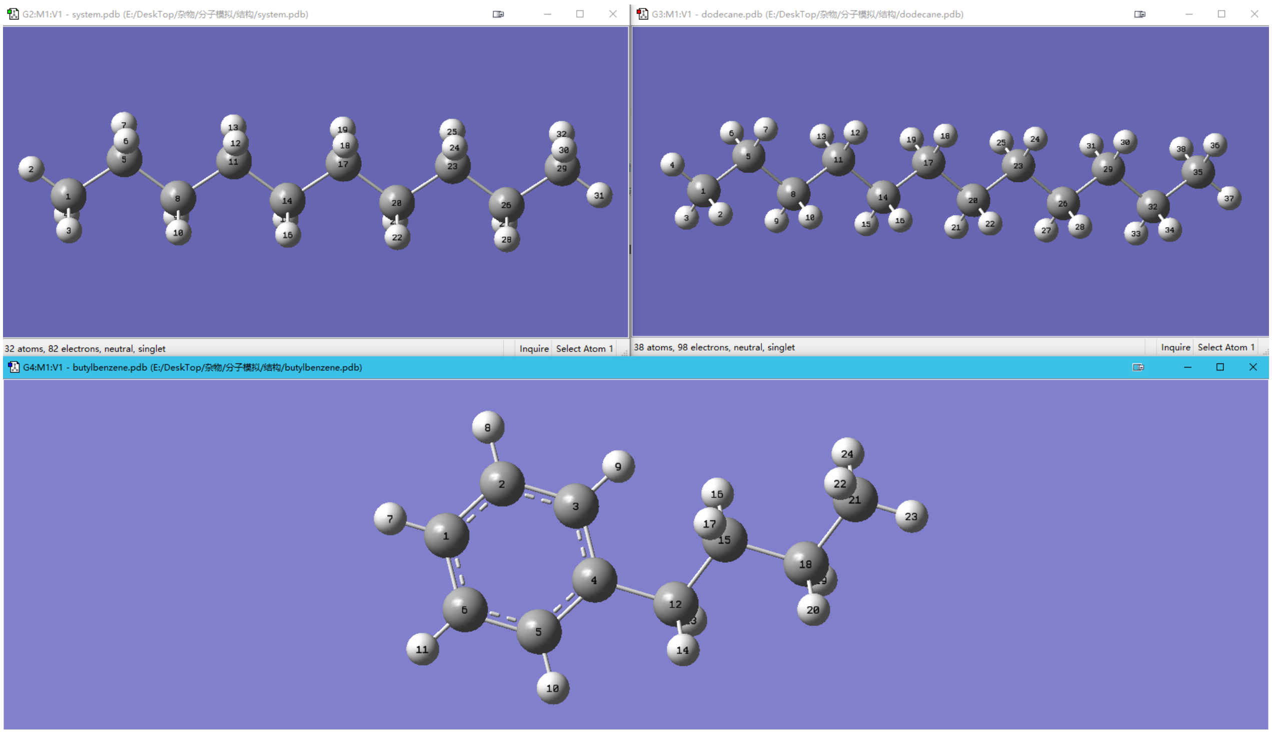
> 学习参考 .."LAMMPS data文件创建工具--moltemplate", Roy Kid

1. gaussview 绘制基本小分子，导出pdb文件
2. packmol 导入上一步的pdb文件，进行空间排布，导出系统的pdb文件
3. moltemplate 导入系统的pdb文件，同时提供力场信息，生成lammps模拟所需的data文件和力场文件
4. lammps 模拟

虽然moltemplate本身就具备建模功能，但是必须显式指定各原子和分子的位置，长链烷烃还比较好算，带支链的环烷烃等就比较复杂了.. 上面的一套流程不需要指定位置，直接建模就可以了.. 之后在moltemplate里给出力场信息.. 也就是说模型的构建和力场基本上是解耦的，这给MD尤其是在lammps中进行MD模拟提供了很大的方便，也可以较简单地切换不同力场进行比较.

622 decane +118 dodecane + 260 butylbenzene 均相体系为例

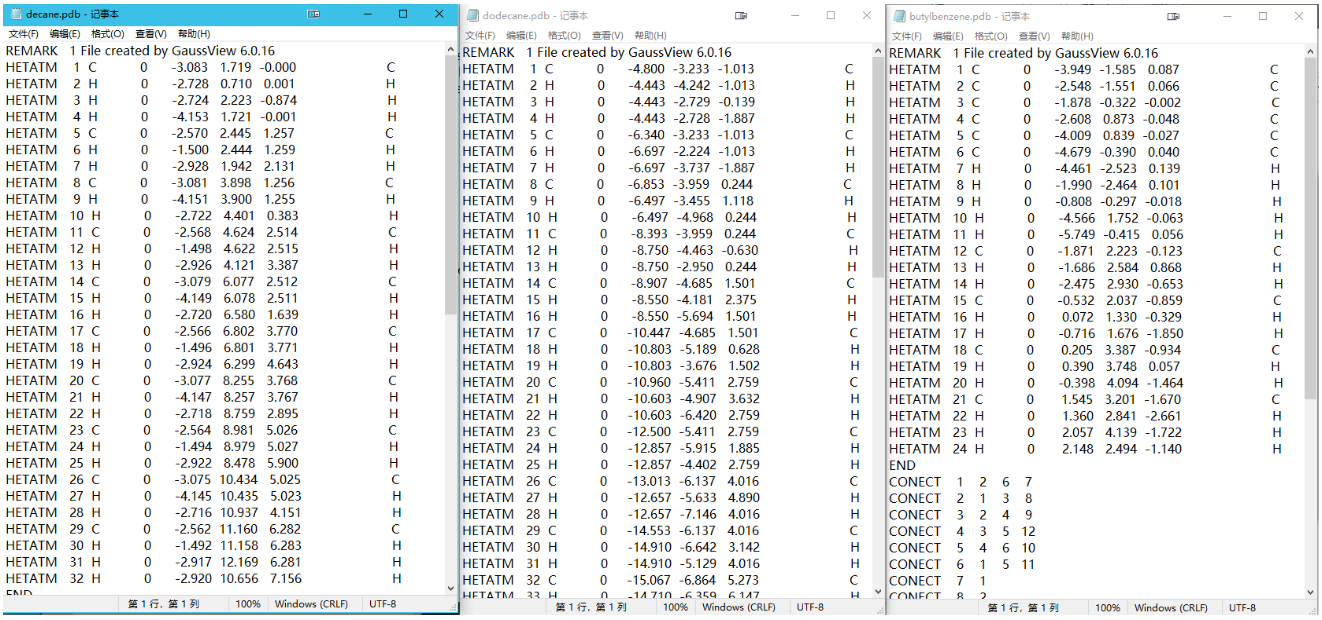
1. gaussview绘制基本单元


G2:M1:V1 - system.pdb (E:/DeskTop/杂物/分子模拟/结构/system.pdb)
G3:M1:V1 - dodecane.pdb (E:/DeskTop/杂物/分子模拟/结构/dodecane.pdb)
Inquire
Select Atom 1
Inquire
Select Atom 1
G4:M1:V1 - butylbenzene.pdb (E:/DeskTop/杂物/分子模拟/结构/butylbenzene.pdb)

32 atoms, 82 electrons, neutral, singlet

38 atoms, 98 electrons, neutral, singlet

- 使用gaussview绘制出小分子，导出pdb文件，如下图所示：


decane.pdb - 记事本
dodecane.pdb - 记事本
butylbenzene.pdb - 记事本
文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)
第 1 行，第 1 列 100% Windows (CRLF) UTF-8

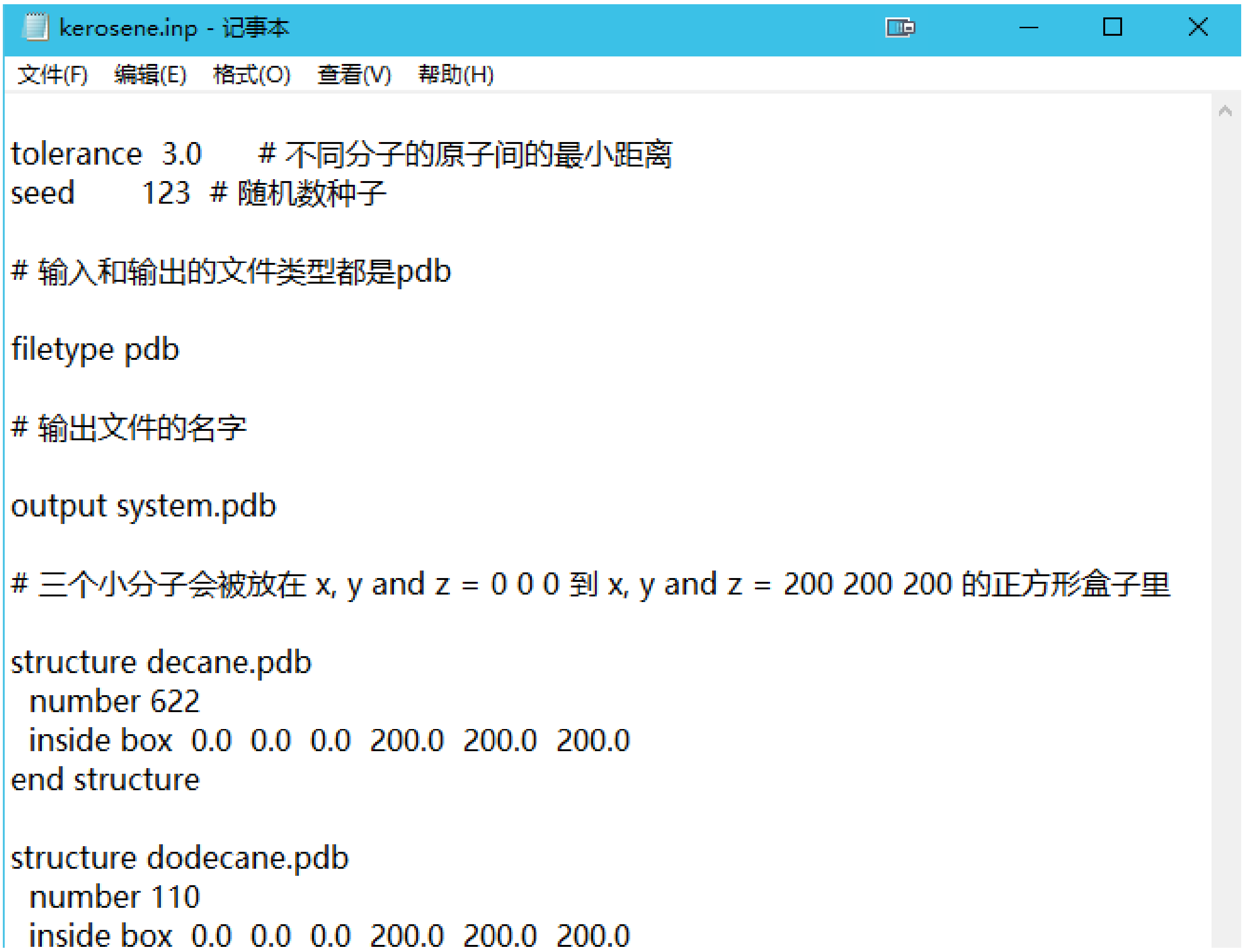
```
REMARK   1 File created by GaussView 6.0.16
HETATM   1  C         0      -3.083   1.719  -0.000                  C
HETATM   2  H         0      -2.728   0.710   0.001                  H
HETATM   3  H         0      -2.724   2.223  -0.874                  H
HETATM   4  H         0      -4.153   1.721  -0.001                  H
HETATM   5  C         0      -2.570   2.445   1.257                  C
HETATM   6  H         0      -1.500   2.444   1.259                  H
HETATM   7  H         0      -2.928   1.942   2.131                  H
HETATM   8  C         0      -3.081   3.898   1.256                  C
HETATM   9  H         0      -4.151   3.900   1.255                  H
HETATM  10  H         0      -2.722   4.401   0.383                  H
HETATM  11  C         0      -2.568   4.624   2.514                  C
HETATM  12  H         0      -1.498   4.622   2.515                  H
HETATM  13  H         0      -2.926   4.121   3.387                  H
HETATM  14  C         0      -3.079   6.077   2.512                  C
HETATM  15  H         0      -4.149   6.078   2.511                  H
HETATM  16  H         0      -2.720   6.580   1.639                  H
HETATM  17  C         0      -2.566   6.802   3.770                  C
HETATM  18  H         0      -1.496   6.801   3.771                  H
HETATM  19  H         0      -2.924   6.299   4.643                  H
HETATM  20  C         0      -3.077   8.255   3.768                  C
HETATM  21  H         0      -4.147   8.257   3.767                  H
HETATM  22  H         0      -2.718   8.759   2.895                  H
HETATM  23  C         0      -2.564   8.981   5.026                  C
HETATM  24  H         0      -1.494   8.979   5.027                  H
HETATM  25  H         0      -2.922   8.478   5.900                  H
HETATM  26  C         0      -3.075  10.434   5.025                  C
HETATM  27  H         0      -4.145  10.435   5.023                  H
HETATM  28  H         0      -2.716  10.937   4.151                  H
HETATM  29  C         0      -2.562  11.160   6.282                  C
HETATM  30  H         0      -1.492  11.158   6.283                  H
HETATM  31  H         0      -2.917  12.169   6.281                  H
HETATM  32  H         0      -2.920  10.656   7.156                  H
END
```

```
REMARK   1 File created by GaussView 6.0.16
HETATM   1  C         0      -4.800  -3.233  -1.013                  C
HETATM   2  H         0      -4.443  -4.242  -1.013                  H
HETATM   3  H         0      -4.443  -2.729  -0.139                  H
HETATM   4  H         0      -4.443  -2.728  -1.887                  H
HETATM   5  C         0      -6.340  -3.233  -1.013                  C
HETATM   6  H         0      -6.697  -2.224  -1.013                  H
HETATM   7  H         0      -6.697  -3.737  -1.887                  H
HETATM   8  C         0      -6.853  -3.959   0.244                  C
HETATM   9  H         0      -6.497  -3.455   1.118                  H
HETATM  10  H         0      -6.497  -4.968   0.244                  H
HETATM  11  C         0      -8.393  -3.959   0.244                  C
HETATM  12  H         0      -8.750  -4.463  -0.630                  H
HETATM  13  H         0      -8.750  -2.950   0.244                  H
HETATM  14  C         0      -8.907  -4.685   1.501                  C
HETATM  15  H         0      -8.550  -4.181   2.375                  H
HETATM  16  H         0      -8.550  -5.694   1.501                  H
HETATM  17  C         0     -10.447  -4.685   1.501                  C
HETATM  18  H         0     -10.803  -5.189   0.628                  H
HETATM  19  H         0     -10.803  -3.676   1.502                  H
HETATM  20  C         0     -10.960  -5.411   2.759                  C
HETATM  21  H         0     -10.603  -4.907   3.632                  H
HETATM  22  H         0     -10.603  -6.420   2.759                  H
HETATM  23  C         0     -12.500  -5.411   2.759                  C
HETATM  24  H         0     -12.857  -5.915   1.885                  H
HETATM  25  H         0     -12.857  -4.402   2.759                  H
HETATM  26  C         0     -13.013  -6.137   4.016                  C
HETATM  27  H         0     -12.657  -5.633   4.890                  H
HETATM  28  H         0     -12.657  -7.146   4.016                  H
HETATM  29  C         0     -14.553  -6.137   4.016                  C
HETATM  30  H         0     -14.910  -6.642   3.142                  H
HETATM  31  H         0     -14.910  -5.129   4.016                  H
HETATM  32  C         0     -15.067  -6.864   5.273                  C
HETATM  33  H         0     -14.710  -6.359   6.147                  H
```

```
REMARK   1 File created by GaussView 6.0.16
HETATM   1  C         0      -3.949  -1.585   0.087                  C
HETATM   2  C         0      -2.548  -1.551   0.066                  C
HETATM   3  C         0      -1.878  -0.322  -0.002                  C
HETATM   4  C         0      -2.608   0.873  -0.048                  C
HETATM   5  C         0      -4.009   0.839  -0.027                  C
HETATM   6  C         0      -4.679  -0.390   0.040                  C
HETATM   7  H         0      -4.461  -2.523   0.139                  H
HETATM   8  H         0      -1.990  -2.464   0.101                  H
HETATM   9  H         0      -0.808  -0.297  -0.018                  H
HETATM  10  H         0      -4.566   1.752  -0.063                  H
HETATM  11  H         0      -5.749  -0.415   0.056                  H
HETATM  12  C         0      -1.871   2.223  -0.123                  C
HETATM  13  H         0      -1.686   2.584   0.868                  H
HETATM  14  H         0      -2.475   2.930  -0.653                  H
HETATM  15  C         0      -0.532   2.037  -0.859                  C
HETATM  16  H         0       0.072   1.330  -0.329                  H
HETATM  17  H         0      -0.716   1.676  -1.850                  H
HETATM  18  C         0       0.205   3.387  -0.934                  C
HETATM  19  H         0       0.390   3.748   0.057                  H
HETATM  20  H         0      -0.398   4.094  -1.464                  H
HETATM  21  C         0       1.545   3.201  -1.670                  C
HETATM  22  H         0       1.360   2.841  -2.661                  H
HETATM  23  H         0       2.057   4.139  -1.722                  H
HETATM  24  H         0       2.148   2.494  -1.140                  H
END
CONECT    1    2    6    7
CONECT    2    1    3    8
CONECT    3    2    4    9
CONECT    4    3    5   12
CONECT    5    4    6   10
CONECT    6    1    5   11
CONECT    7    1
CONECT    8    2
```

- 这里元素种类，名称等均不重要，唯一有用的就是各个原子的顺序，比如decane.pdb中定义原子的顺序和图中label的顺序是一样的，先是定义了CH3中的四个原子，然后是剩下链中的八个原子，最后是链尾端的CH3，每一个基团定义原子的顺序都是从C到H. Moltemplate中定义分子和系统信息时原子的顺序必须和pdb中的顺序完全一致，否则就会出现问题.

2. 用packmol进行空间排布



```
tolerance  3.0      # 不同分子的原子间的最小距离
seed       123  # 随机数种子

# 输入和输出的文件类型都是pdb

filetype pdb

# 输出文件的名字

output system.pdb

# 三个小分子会被放在 x, y and z = 0 0 0 到 x, y and z = 200 200 200 的正方形盒子里

structure decane.pdb
  number 622
  inside box  0.0  0.0  0.0  200.0  200.0  200.0
end structure

structure dodecane.pdb
  number 110
  inside box  0.0  0.0  0.0  200.0  200.0  200.0
```

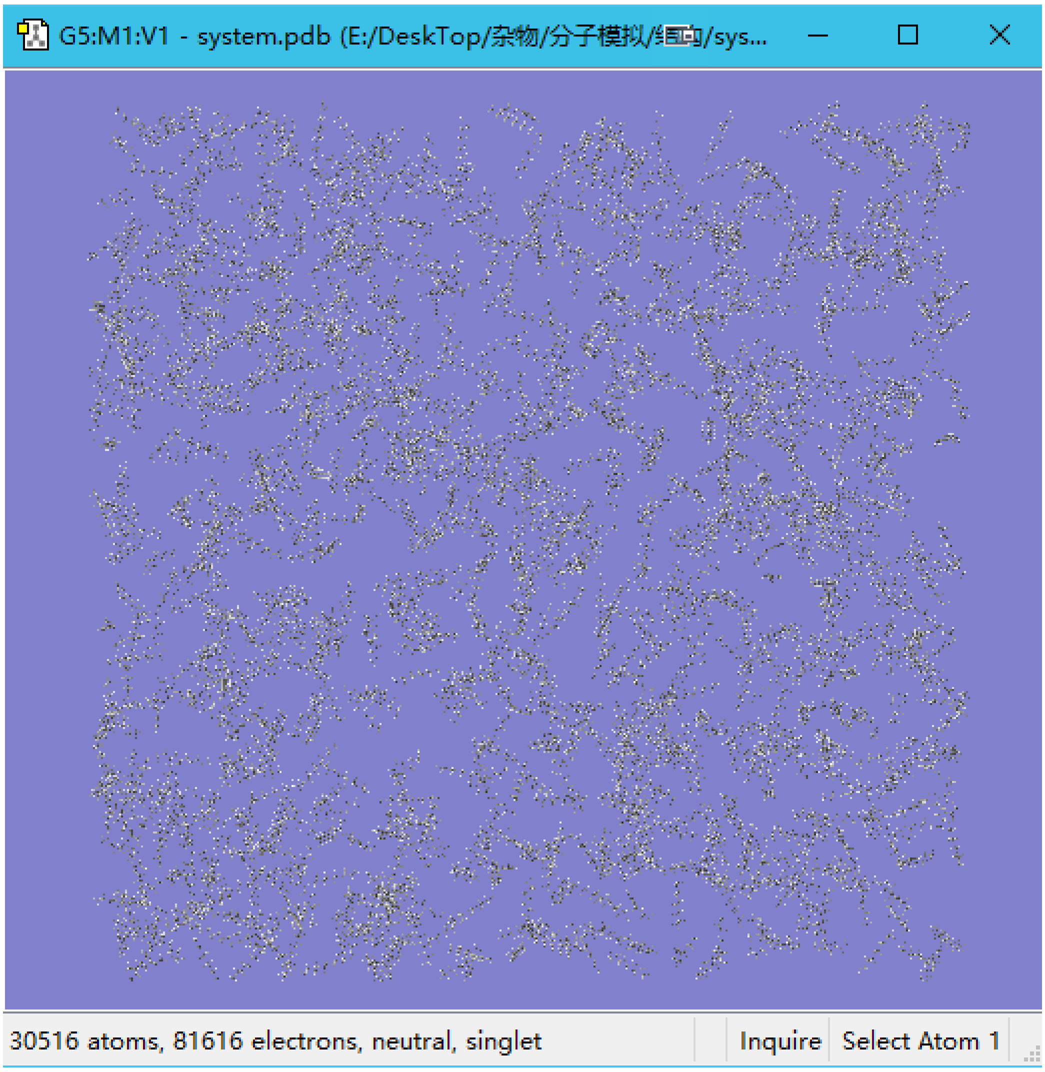
```
end structure

structure butylbenzene.pdb
  number 268
  inside box  0.0  0.0  0.0  200.0  200.0  200.0
end structure
```

- packmol的输入文件是.inp文件，使用时将packmol.exe放到工作文件夹里，通过cmd运行：

```
packmol < xxxx.inp
```

- 可以支持很复杂的结构定义，这里均相体系就很简单了. 需要指定tolerance，filetype，output，以及要填进去的东西

- 这一步会生成系统的结构文件，也就是.inp文件中指定的system.pdb

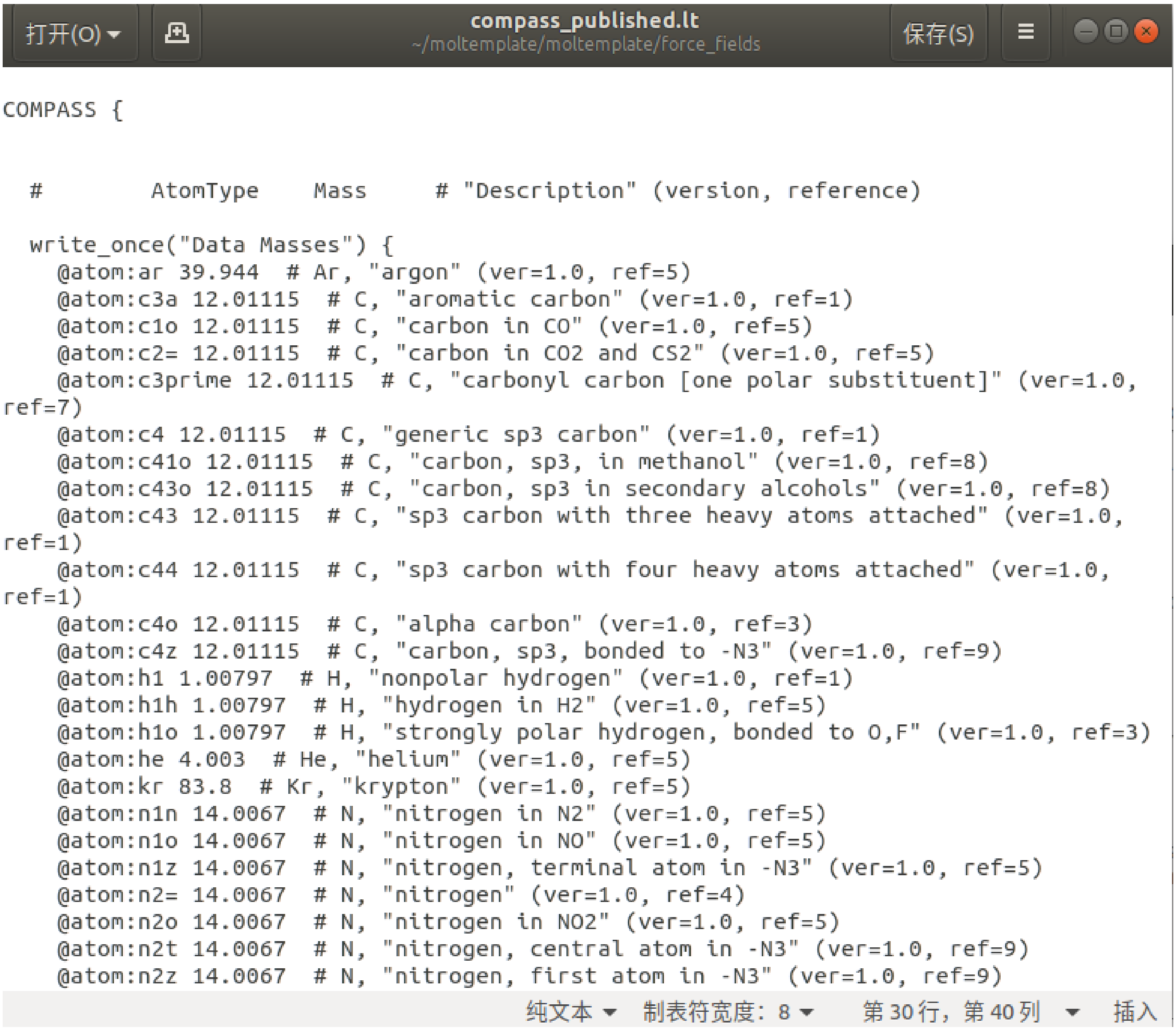

G5:M1:V1 - system.pdb (E:/DeskTop/杂物/分子模拟/[illegible]/sys...
Inquire
Select Atom 1

30516 atoms, 81616 electrons, neutral, singlet

3. 使用moltemplate给出力场信息

- moltemplate给出力场信息的方式是定义分子和系统的.lt文件，针对不同力场，moltemplate提供了对应力场的.lt文件，以Compass力场为例，moltemplate提供了compass_published.lt文件，其中定义了各种不同的原子，以及原子间成键的参数，成键类型，分子间作用力类

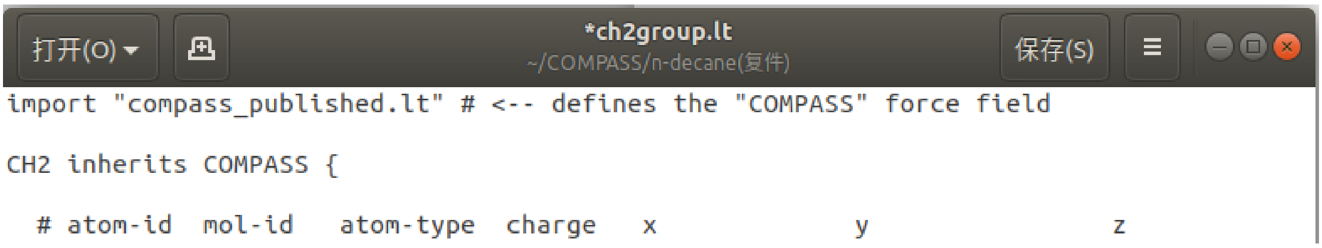
型等等，在自己定义新的分子时，只需要继承compass_published.lt文件，然后指定分子中的原子种类及原子间的连接情况即可，moltemplate会自动为其分配质量、电荷、pair参数等信息，生成lammps可接受的输入文件.



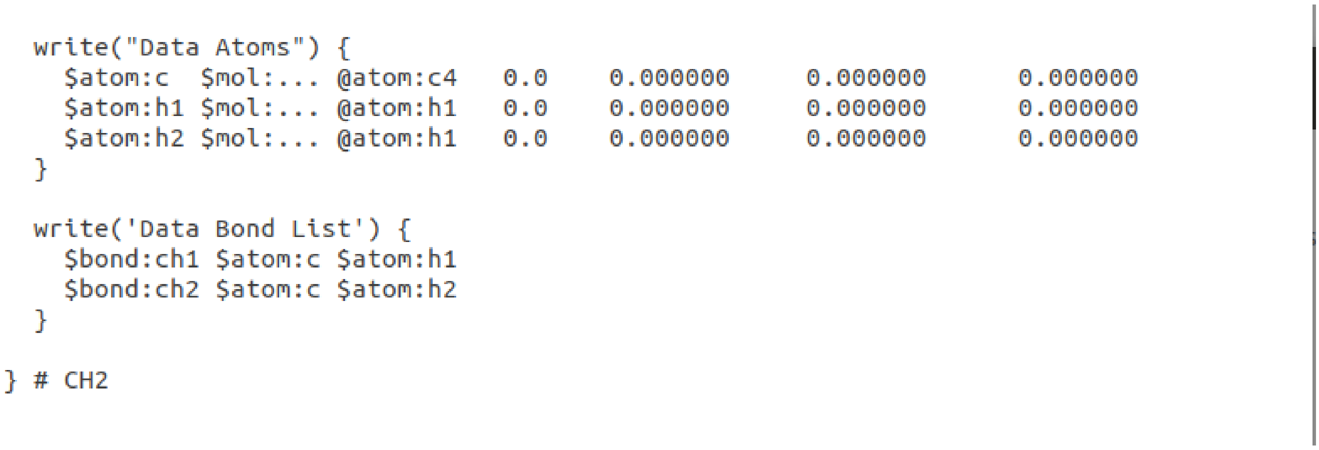
```
COMPASS {


  #        AtomType    Mass     # "Description" (version, reference)

  write_once("Data Masses") {
    @atom:ar 39.944  # Ar, "argon" (ver=1.0, ref=5)
    @atom:c3a 12.01115  # C, "aromatic carbon" (ver=1.0, ref=1)
    @atom:c1o 12.01115  # C, "carbon in CO" (ver=1.0, ref=5)
    @atom:c2= 12.01115  # C, "carbon in CO2 and CS2" (ver=1.0, ref=5)
    @atom:c3prime 12.01115  # C, "carbonyl carbon [one polar substituent]" (ver=1.0,
ref=7)
    @atom:c4 12.01115  # C, "generic sp3 carbon" (ver=1.0, ref=1)
    @atom:c41o 12.01115  # C, "carbon, sp3, in methanol" (ver=1.0, ref=8)
    @atom:c43o 12.01115  # C, "carbon, sp3 in secondary alcohols" (ver=1.0, ref=8)
    @atom:c43 12.01115  # C, "sp3 carbon with three heavy atoms attached" (ver=1.0,
ref=1)
    @atom:c44 12.01115  # C, "sp3 carbon with four heavy atoms attached" (ver=1.0,
ref=1)
    @atom:c4o 12.01115  # C, "alpha carbon" (ver=1.0, ref=3)
    @atom:c4z 12.01115  # C, "carbon, sp3, bonded to -N3" (ver=1.0, ref=9)
    @atom:h1 1.00797  # H, "nonpolar hydrogen" (ver=1.0, ref=1)
    @atom:h1h 1.00797  # H, "hydrogen in H2" (ver=1.0, ref=5)
    @atom:h1o 1.00797  # H, "strongly polar hydrogen, bonded to O,F" (ver=1.0, ref=3)
    @atom:he 4.003  # He, "helium" (ver=1.0, ref=5)
    @atom:kr 83.8  # Kr, "krypton" (ver=1.0, ref=5)
    @atom:n1n 14.0067  # N, "nitrogen in N2" (ver=1.0, ref=5)
    @atom:n1o 14.0067  # N, "nitrogen in NO" (ver=1.0, ref=5)
    @atom:n1z 14.0067  # N, "nitrogen, terminal atom in -N3" (ver=1.0, ref=5)
    @atom:n2= 14.0067  # N, "nitrogen" (ver=1.0, ref=4)
    @atom:n2o 14.0067  # N, "nitrogen in NO2" (ver=1.0, ref=5)
    @atom:n2t 14.0067  # N, "nitrogen, central atom in -N3" (ver=1.0, ref=9)
    @atom:n2z 14.0067  # N, "nitrogen, first atom in -N3" (ver=1.0, ref=9)
```

- 为了定义烷烃分子，可以先定义CH2基团和CH3基团，然后再把它拼起来组成分子，moltemplate也是基于这样的面向对象的想法设计的.下图定义了一个CH2分子，继承COMPASS力场，其中@atom是COMPASS力场文件中定义的原子类型，在这里就是c4和h1，charge可以随便写，之后moltemplate会根据力场文件重新生成. 后面的x y z是原子坐标，在完全用moltemplate生成结构文件时，必须通过计算得到.. 但是在这套技术栈之中我们就不需要指定坐标了，关键是指定这些原子的顺序，moltemplate完全按照最后系统中.lt文件中定义的各原子位置去给packmol生成的.pdb文件赋予力场信息.

- ch2：

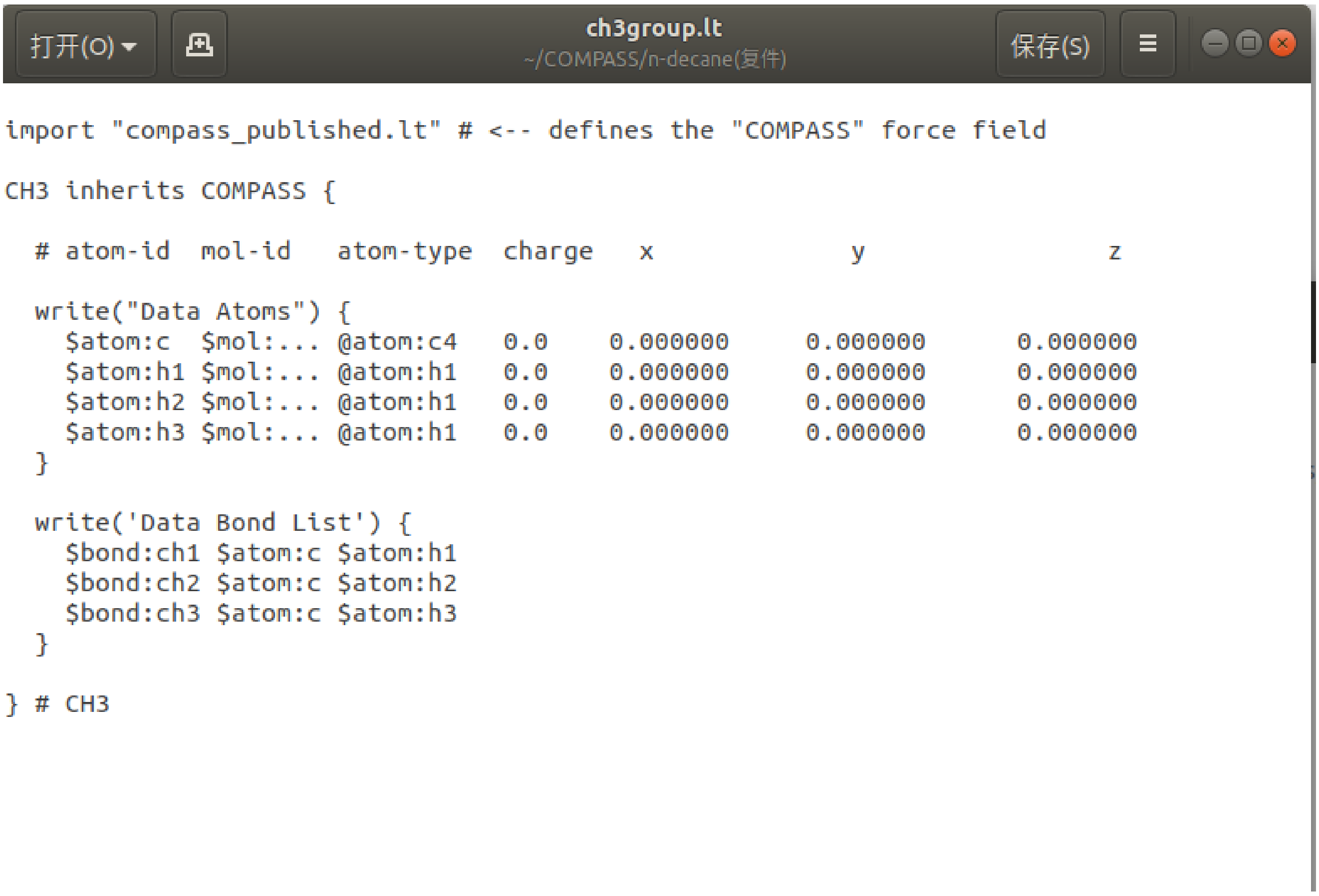


```
import "compass_published.lt" # <-- defines the "COMPASS" force field

CH2 inherits COMPASS {

  # atom-id  mol-id   atom-type  charge    x             y                z
```



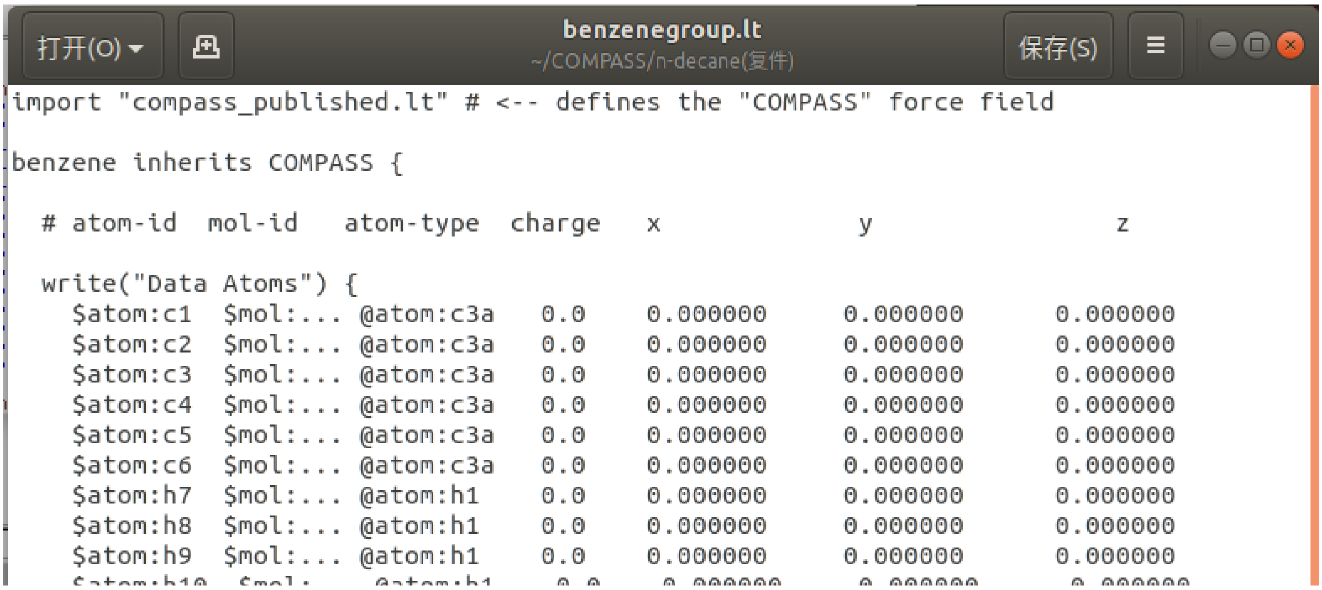
```
  write("Data Atoms") {
    $atom:c  $mol:... @atom:c4   0.0    0.000000     0.000000      0.000000
    $atom:h1 $mol:... @atom:h1   0.0    0.000000     0.000000      0.000000
    $atom:h2 $mol:... @atom:h1   0.0    0.000000     0.000000      0.000000
  }

  write('Data Bond List') {
    $bond:ch1 $atom:c $atom:h1
    $bond:ch2 $atom:c $atom:h2
  }

} # CH2
```

- ch3：

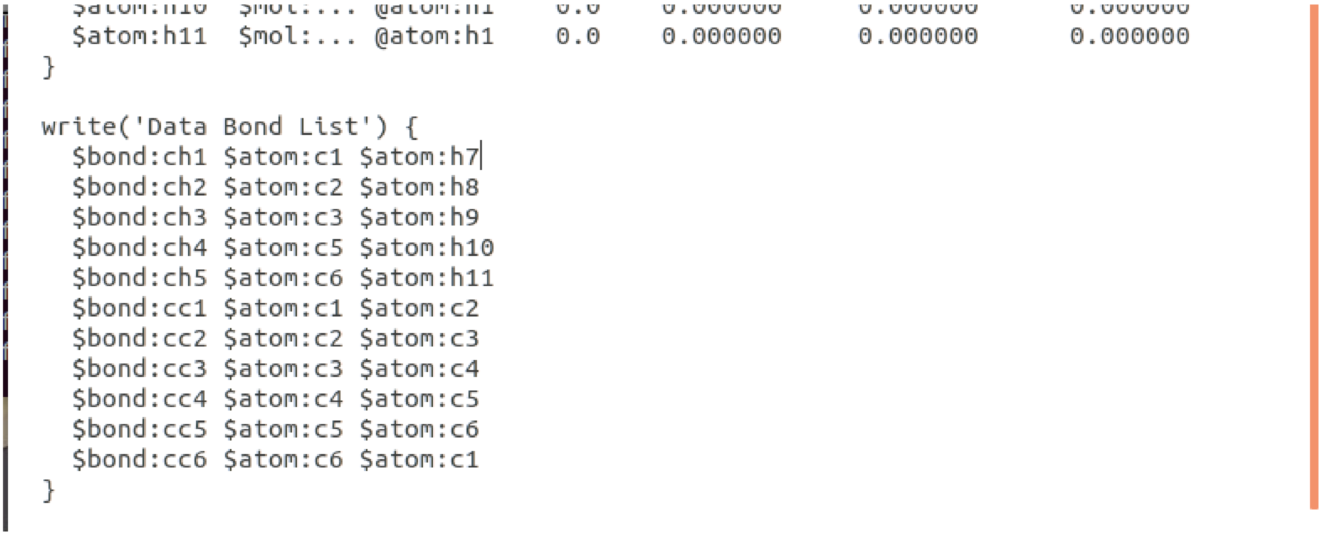


```
import "compass_published.lt" # <-- defines the "COMPASS" force field

CH3 inherits COMPASS {

  # atom-id  mol-id   atom-type  charge   x            y                z

  write("Data Atoms") {
    $atom:c  $mol:... @atom:c4   0.0    0.000000     0.000000      0.000000
    $atom:h1 $mol:... @atom:h1   0.0    0.000000     0.000000      0.000000
    $atom:h2 $mol:... @atom:h1   0.0    0.000000     0.000000      0.000000
    $atom:h3 $mol:... @atom:h1   0.0    0.000000     0.000000      0.000000
  }

  write('Data Bond List') {
    $bond:ch1 $atom:c $atom:h1
    $bond:ch2 $atom:c $atom:h2
    $bond:ch3 $atom:c $atom:h3
  }

} # CH3
```

- 苯基：（完全按照pdb文件中的顺序，注意修改原子类型）

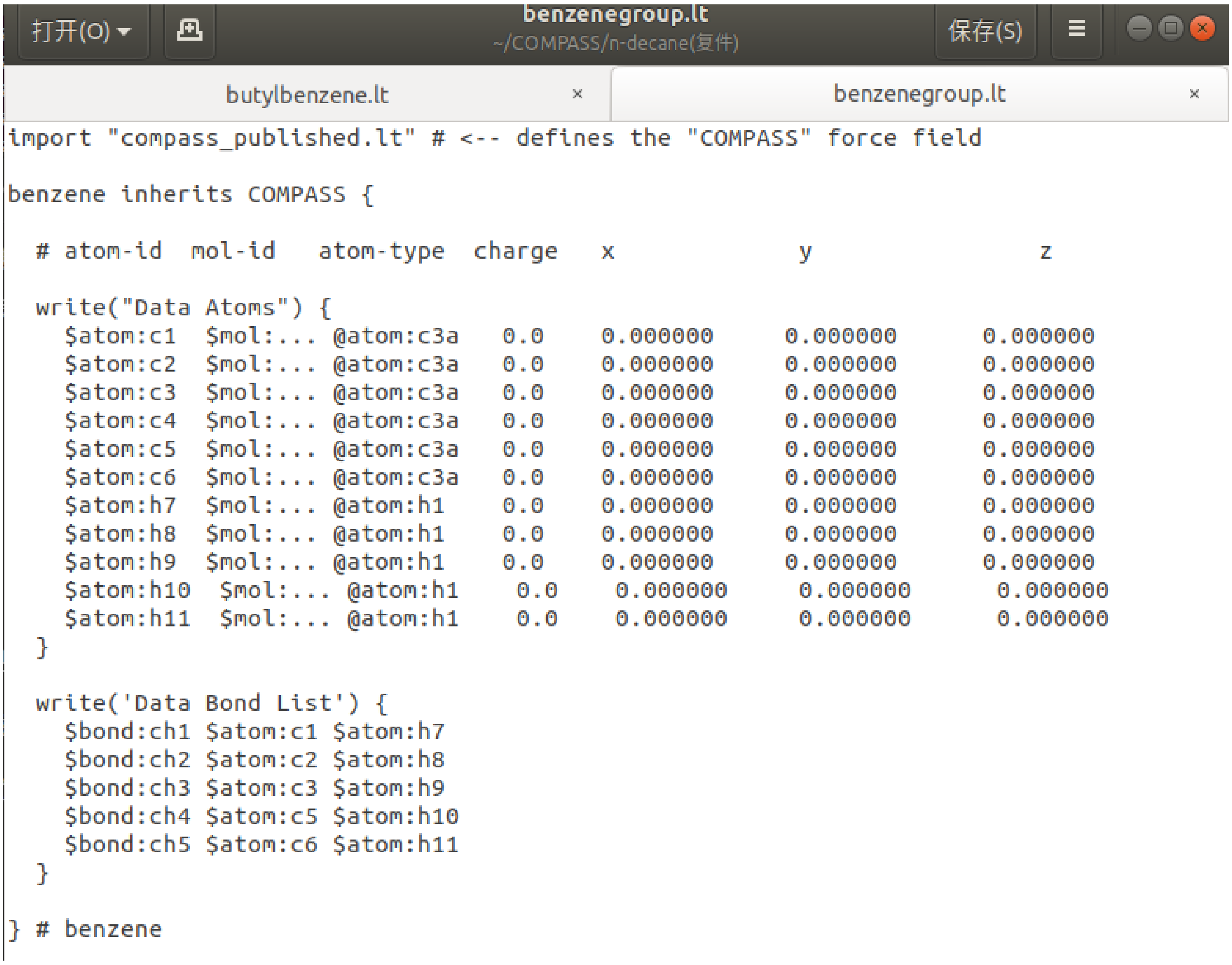


```
import "compass_published.lt" # <-- defines the "COMPASS" force field

benzene inherits COMPASS {

  # atom-id  mol-id   atom-type  charge   x            y                z

  write("Data Atoms") {
    $atom:c1  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c2  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c3  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c4  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c5  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c6  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:h7  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h8  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h9  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h10 $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
```

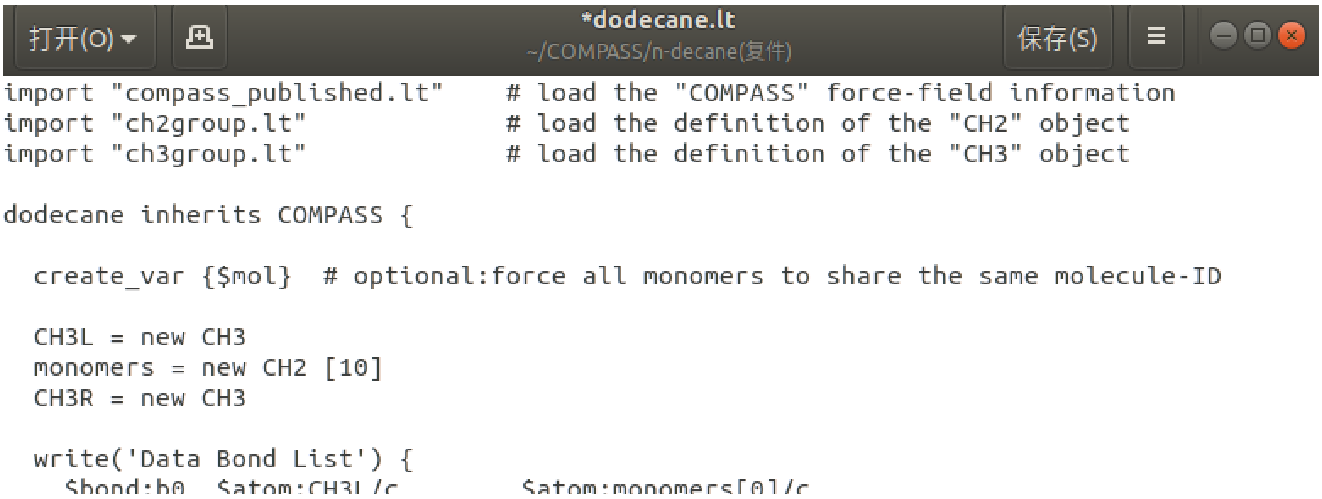


```
    $atom:h10  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h11  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
  }

  write('Data Bond List') {
    $bond:ch1 $atom:c1 $atom:h7
    $bond:ch2 $atom:c2 $atom:h8
    $bond:ch3 $atom:c3 $atom:h9
    $bond:ch4 $atom:c5 $atom:h10
    $bond:ch5 $atom:c6 $atom:h11
    $bond:cc1 $atom:c1 $atom:c2
    $bond:cc2 $atom:c2 $atom:c3
    $bond:cc3 $atom:c3 $atom:c4
    $bond:cc4 $atom:c4 $atom:c5
    $bond:cc5 $atom:c5 $atom:c6
    $bond:cc6 $atom:c6 $atom:c1
  }
```

- 定义各分子的.lt文件（定义的顺序必须和gaussview生成的pdb文件中的原子顺序一致）：

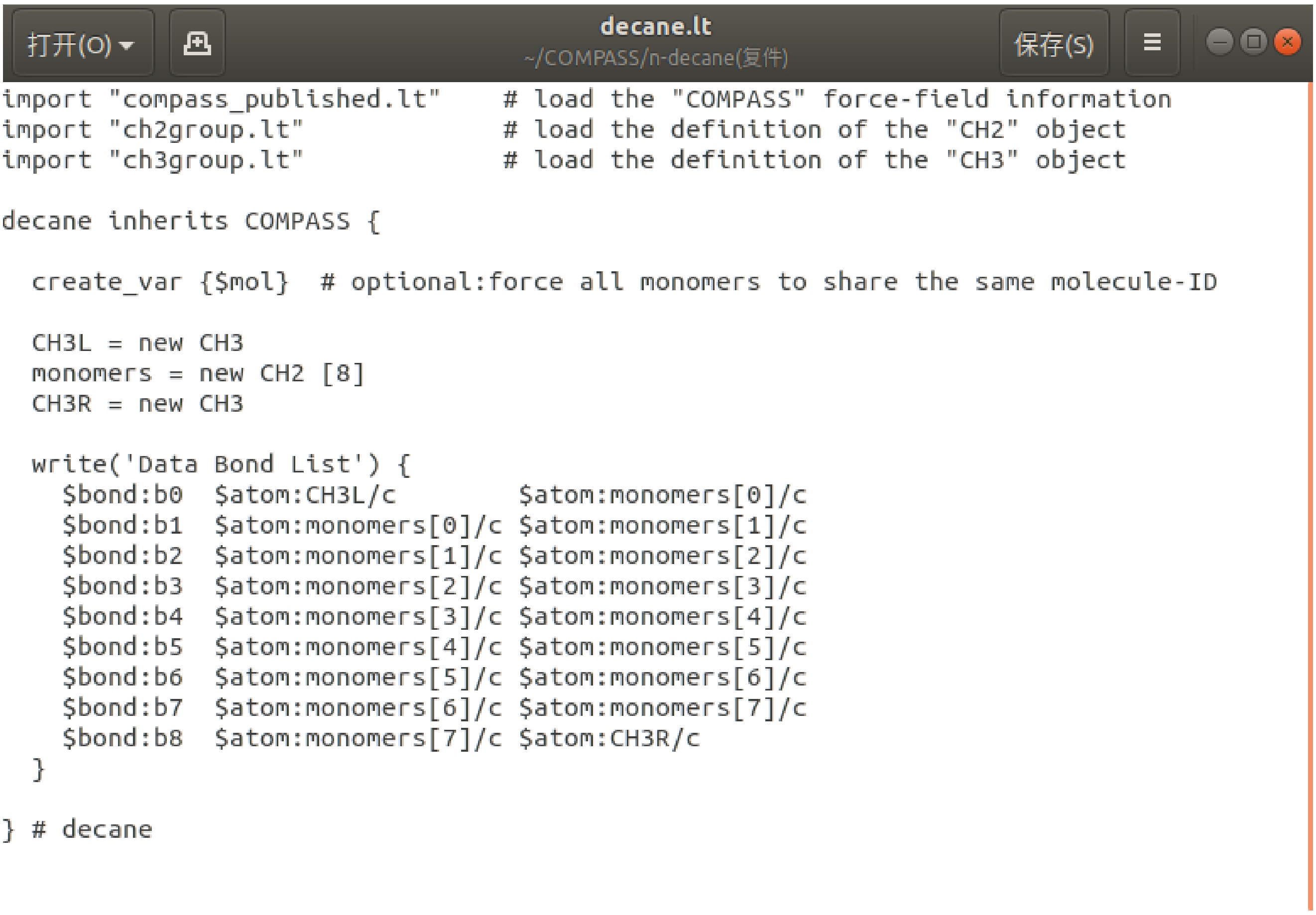


```
import "compass_published.lt" # <-- defines the "COMPASS" force field

benzene inherits COMPASS {

  # atom-id  mol-id   atom-type  charge   x            y               z

  write("Data Atoms") {
    $atom:c1  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c2  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c3  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c4  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c5  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:c6  $mol:... @atom:c3a   0.0    0.000000     0.000000      0.000000
    $atom:h7  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h8  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h9  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h10  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
    $atom:h11  $mol:... @atom:h1    0.0    0.000000     0.000000      0.000000
  }

  write('Data Bond List') {
    $bond:ch1 $atom:c1 $atom:h7
    $bond:ch2 $atom:c2 $atom:h8
    $bond:ch3 $atom:c3 $atom:h9
    $bond:ch4 $atom:c5 $atom:h10
    $bond:ch5 $atom:c6 $atom:h11
  }

} # benzene
```

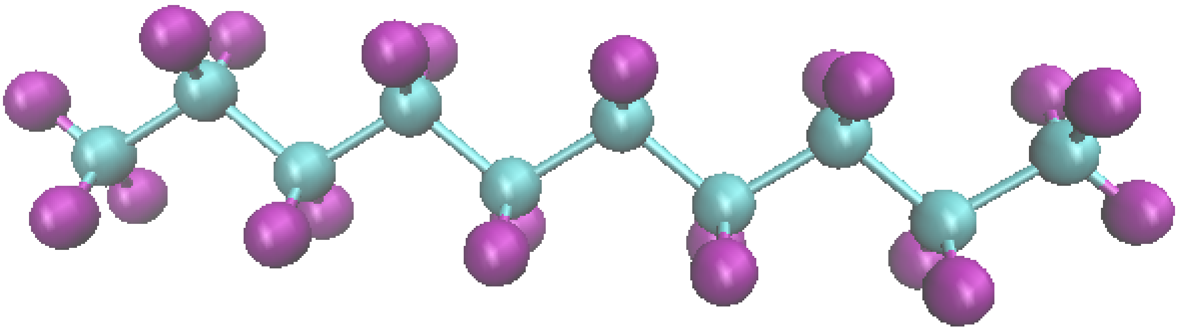


```
import "compass_published.lt"    # load the "COMPASS" force-field information
import "ch2group.lt"             # load the definition of the "CH2" object
import "ch3group.lt"             # load the definition of the "CH3" object

dodecane inherits COMPASS {

  create_var {$mol}  # optional:force all monomers to share the same molecule-ID

  CH3L = new CH3
  monomers = new CH2 [10]
  CH3R = new CH3

  write('Data Bond List') {
    $bond:b0   $atom:CH3L/c         $atom:monomers[0]/c
    $bond:b0   $atom:CH3L/c          $atom:monomers[0]/c
    $bond:b1   $atom:monomers[0]/c $atom:monomers[1]/c
    $bond:b2   $atom:monomers[1]/c $atom:monomers[2]/c
    $bond:b3   $atom:monomers[2]/c $atom:monomers[3]/c
    $bond:b4   $atom:monomers[3]/c $atom:monomers[4]/c
    $bond:b5   $atom:monomers[4]/c $atom:monomers[5]/c
    $bond:b6   $atom:monomers[5]/c $atom:monomers[6]/c
    $bond:b7   $atom:monomers[6]/c $atom:monomers[7]/c
    $bond:b8   $atom:monomers[7]/c $atom:monomers[8]/c
    $bond:b9   $atom:monomers[8]/c $atom:monomers[9]/c
    $bond:b10  $atom:monomers[9]/c $atom:CH3R/c
  }

} # decane
```

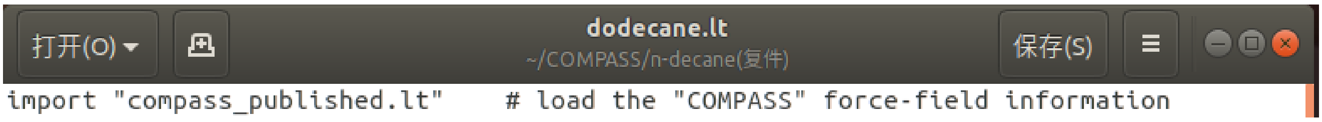
- decane：



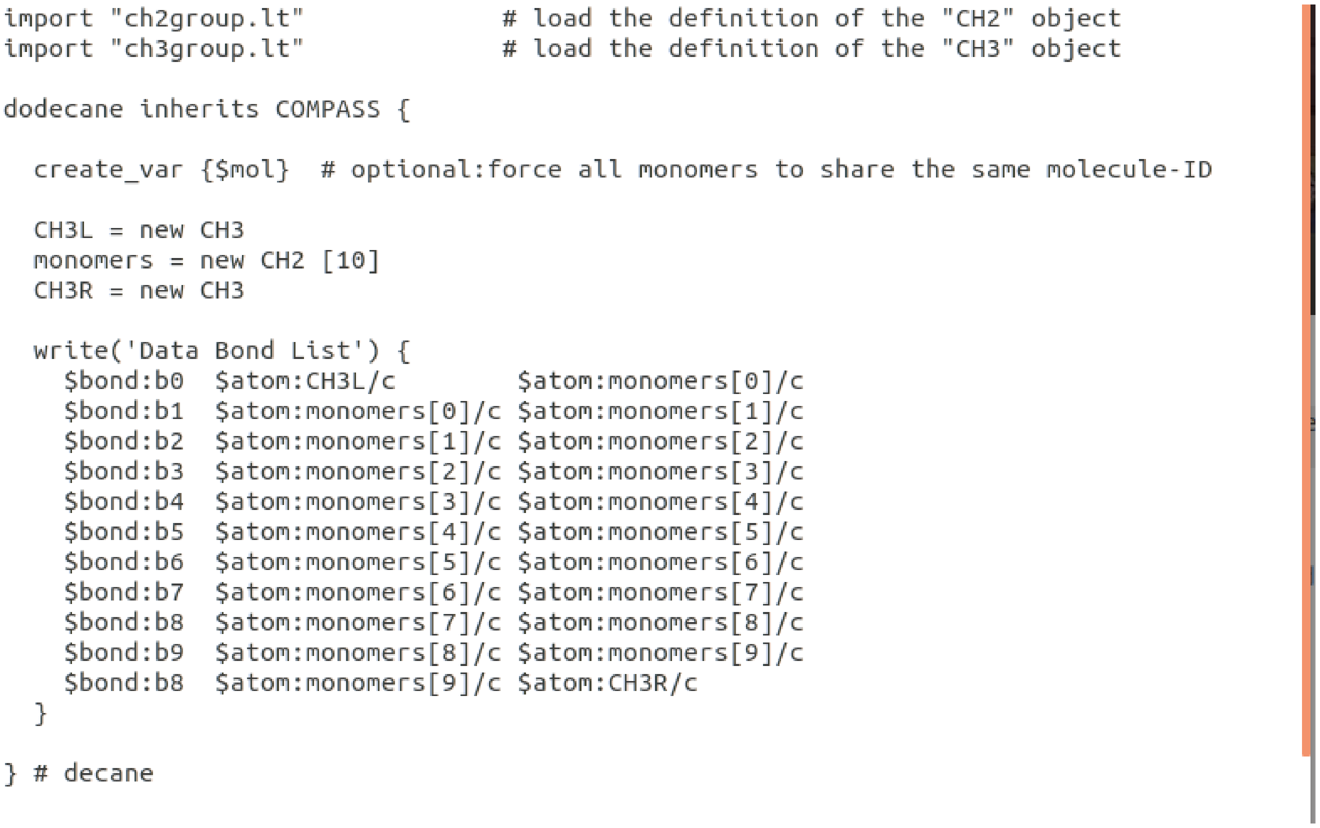
```
import "compass_published.lt"    # load the "COMPASS" force-field information
import "ch2group.lt"             # load the definition of the "CH2" object
import "ch3group.lt"             # load the definition of the "CH3" object

decane inherits COMPASS {

  create_var {$mol}  # optional:force all monomers to share the same molecule-ID

  CH3L = new CH3
  monomers = new CH2 [8]
  CH3R = new CH3

  write('Data Bond List') {
    $bond:b0   $atom:CH3L/c          $atom:monomers[0]/c
    $bond:b1   $atom:monomers[0]/c $atom:monomers[1]/c
    $bond:b2   $atom:monomers[1]/c $atom:monomers[2]/c
    $bond:b3   $atom:monomers[2]/c $atom:monomers[3]/c
    $bond:b4   $atom:monomers[3]/c $atom:monomers[4]/c
    $bond:b5   $atom:monomers[4]/c $atom:monomers[5]/c
    $bond:b6   $atom:monomers[5]/c $atom:monomers[6]/c
    $bond:b7   $atom:monomers[6]/c $atom:monomers[7]/c
    $bond:b8   $atom:monomers[7]/c $atom:CH3R/c
  }

} # decane
```



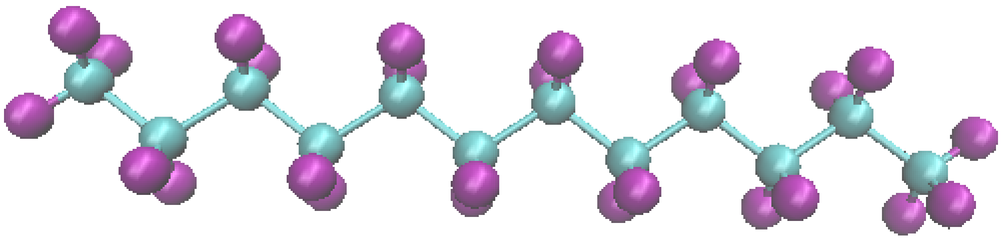
- dodecane：



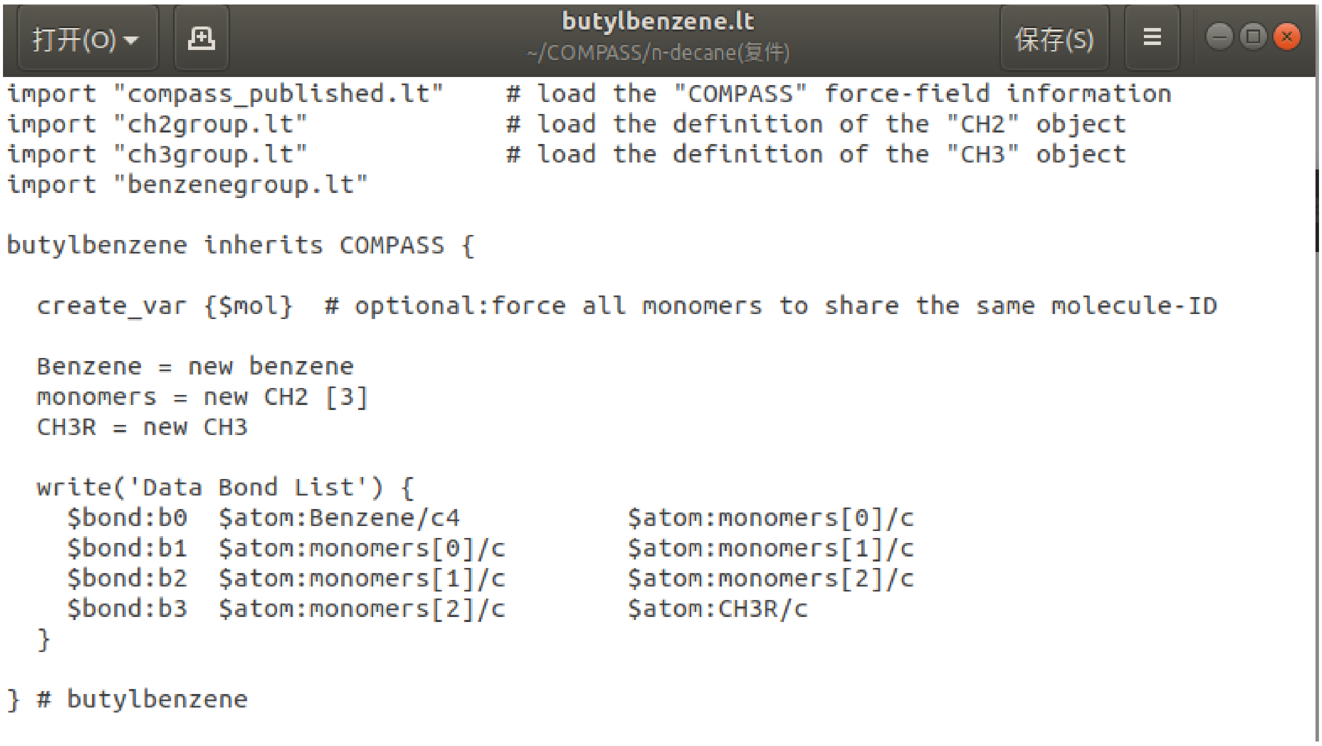
```
import "compass_published.lt"    # load the "COMPASS" force-field information
```



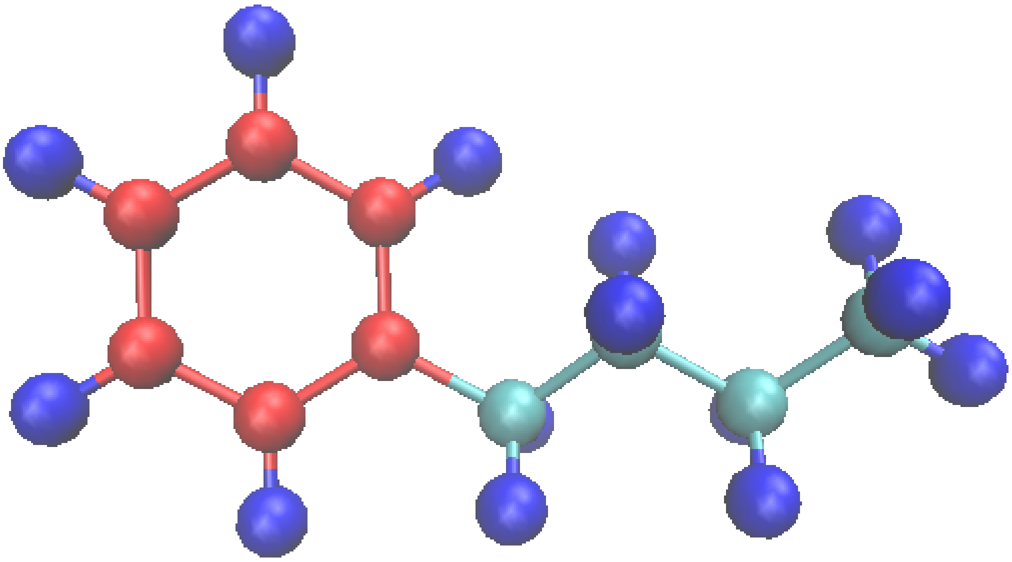
```
import "ch2group.lt"             # load the definition of the "CH2" object
import "ch3group.lt"             # load the definition of the "CH3" object

dodecane inherits COMPASS {

  create_var {$mol}  # optional:force all monomers to share the same molecule-ID

  CH3L = new CH3
  monomers = new CH2 [10]
  CH3R = new CH3

  write('Data Bond List') {
    $bond:b0  $atom:CH3L/c        $atom:monomers[0]/c
    $bond:b1  $atom:monomers[0]/c $atom:monomers[1]/c
    $bond:b2  $atom:monomers[1]/c $atom:monomers[2]/c
    $bond:b3  $atom:monomers[2]/c $atom:monomers[3]/c
    $bond:b4  $atom:monomers[3]/c $atom:monomers[4]/c
    $bond:b5  $atom:monomers[4]/c $atom:monomers[5]/c
    $bond:b6  $atom:monomers[5]/c $atom:monomers[6]/c
    $bond:b7  $atom:monomers[6]/c $atom:monomers[7]/c
    $bond:b8  $atom:monomers[7]/c $atom:monomers[8]/c
    $bond:b9  $atom:monomers[8]/c $atom:monomers[9]/c
    $bond:b8  $atom:monomers[9]/c $atom:CH3R/c
  }

} # decane
```



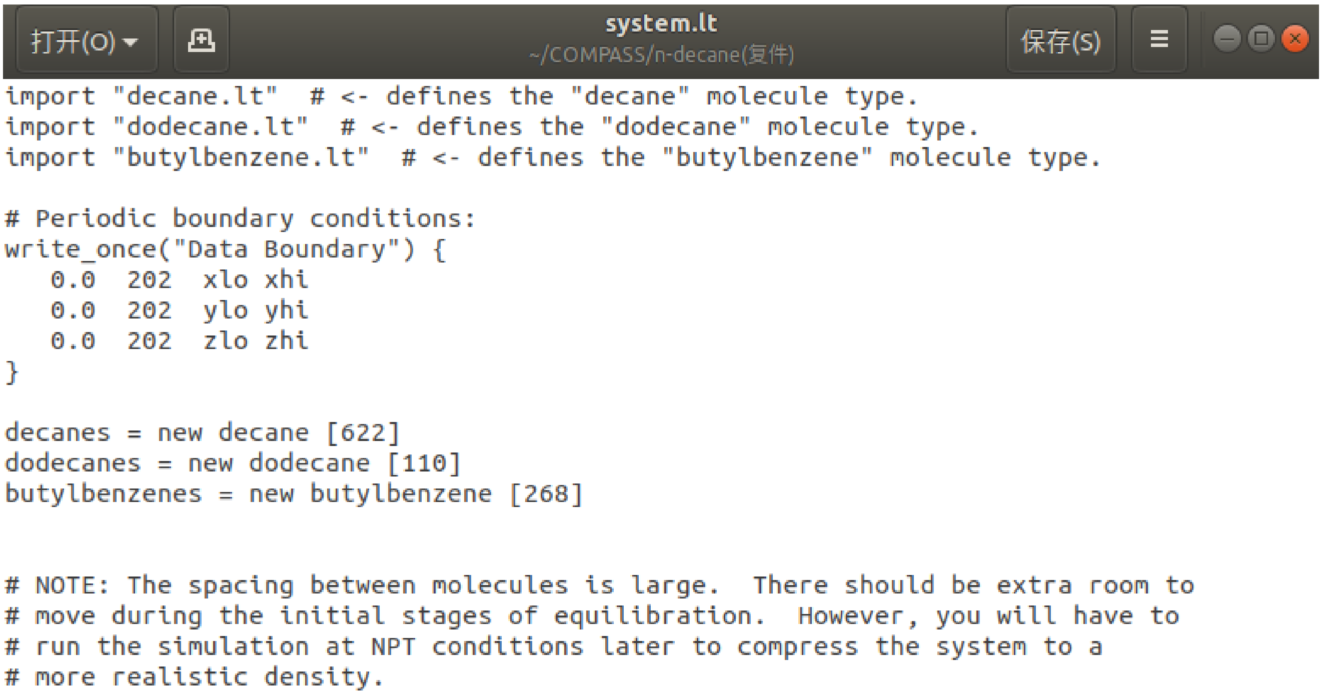
- butylbenzene：



```
import "compass_published.lt"    # load the "COMPASS" force-field information
import "ch2group.lt"             # load the definition of the "CH2" object
import "ch3group.lt"             # load the definition of the "CH3" object
import "benzenegroup.lt"

butylbenzene inherits COMPASS {

  create_var {$mol}  # optional:force all monomers to share the same molecule-ID

  Benzene = new benzene
  monomers = new CH2 [3]
  CH3R = new CH3

  write('Data Bond List') {
    $bond:b0  $atom:Benzene/c4        $atom:monomers[0]/c
    $bond:b1  $atom:monomers[0]/c     $atom:monomers[1]/c
    $bond:b2  $atom:monomers[1]/c     $atom:monomers[2]/c
    $bond:b3  $atom:monomers[2]/c     $atom:CH3R/c
  }

} # butylbenzene
```



- 定义系统.lt文件，定义顺序必须和packmol空间排布定义的顺序完全一致.

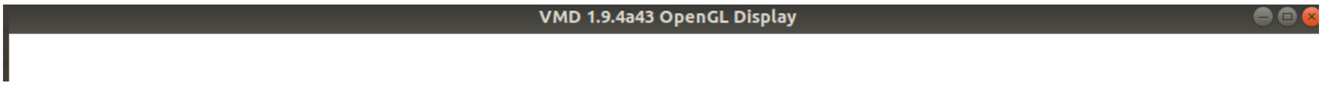


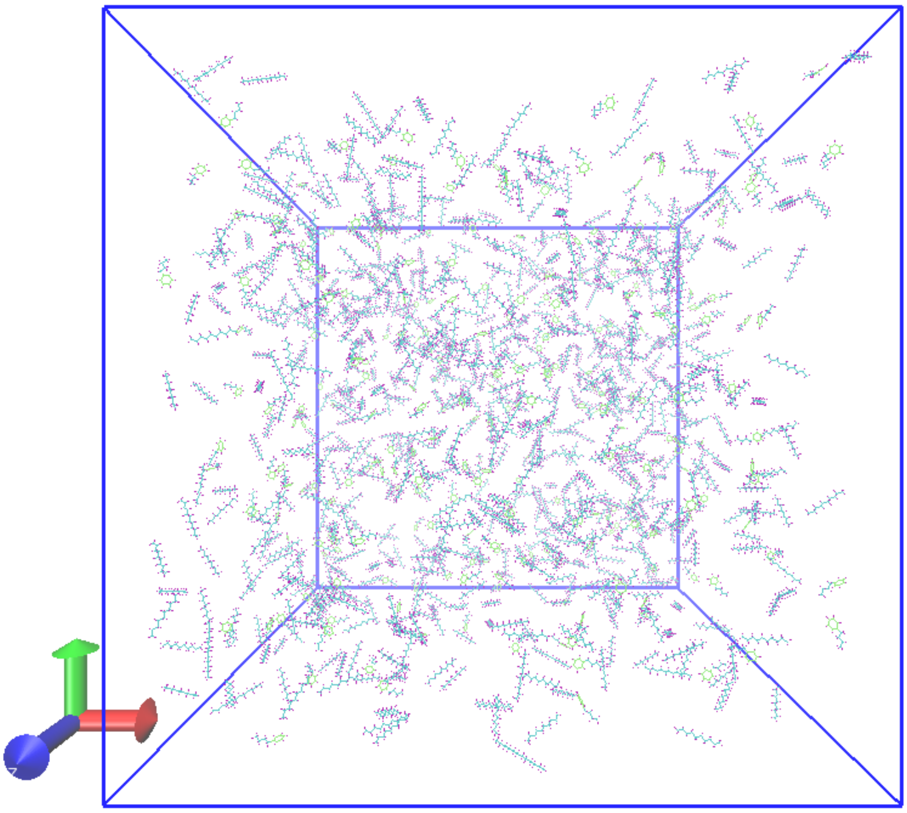
```
import "decane.lt"  # <- defines the "decane" molecule type.
import "dodecane.lt"  # <- defines the "dodecane" molecule type.
import "butylbenzene.lt"  # <- defines the "butylbenzene" molecule type.

# Periodic boundary conditions:
write_once("Data Boundary") {
   0.0  202  xlo xhi
   0.0  202  ylo yhi
   0.0  202  zlo zhi
}

decanes = new decane [622]
dodecanes = new dodecane [110]
butylbenzenes = new butylbenzene [268]


# NOTE: The spacing between molecules is large.  There should be extra room to
# move during the initial stages of equilibration.  However, you will have to
# run the simulation at NPT conditions later to compress the system to a
# more realistic density.
```

运行：

```
moltemplate.sh -pdb system.pdb system.lt
```

- 用vmd看一下生成的system.data文件：





- 此时的data文件已经包含了compass力场所需的二面角等信息，moltemplate同时生成了settings和init等文件，进行lammps in文件的参数设置. 接下来只需要写in文件即可进行lammps模拟.