MiCMoS
Milano Chemistry Molecular Simulation
Description and User Manual

Tutorials

T8. Monte Carlo: simulation of a crystal (acetanilide)

PURPOSE: In this tutorial, it is described how to prepare and equilibrate a periodic crystal of acetanilide with the Monte Carlo technique. The aim is also to get the user acquainted with the use of slave atoms for the Monte Carlo routine of MiCMoS.

REFERENCE to main manual: Sections 5.1 (**Boxcry**); 5.4 (**Pretop**); 6.2 (construction of molecular frameworks); 6.6.1 (**mcmain**); 6.6.2 (instruction file); 6.6.3 (topology and force field file); 6.6.4 (slave atom file).

FILES: You can find all the files you need to run this tutorial here:
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T8/ACANIL01.cif
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T8/acan.mci
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T8/acan.oeh
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T8/acan.sla
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T8/acan.top
The crystal and molecular structure comes from the Cambridge Structural Database entry ACANIL01, giving acanil01.*cif* as starting point. **Retcif**, **Retcor**, **Retcha** and **Crysaa** may be run in sequence as described in Tutorials T1 and T4. You will also need macros to run **Pretop**, **Boxcry** and **mcmain**. Place .*oeh* and pertinent (Windows/Unix) macros into your working directory.

If you call the run.cry macro according to

```
./run.cry acanyl01
```

it will perform the whole sequence **Retcif**, **Retcor**, **Retcha** and **Crysaa**, ending with files acanil01.*oeh* (the structure file) and acanyl01cry.*pri*, which contains information on static lattice energies. When prompted, answer 0 (normalize hydrogens), 0 (minimal output) and 0 (check the hydrogen count). See Tutorial T1 and Section 1.1 in the manual for detailed explanations. Check the results of the static energy calculation from **Crysaa** (file acanyl01.*pri*) before going on. You should find that the calculation looks fine and reasonable (no errors in acanyl01.*pri*).

This example involves a full description of a semi-rigid molecular unit with core and slave atoms. The molecular diagram below shows that the benzene ring and the N atom can be treated as a rigid fragment, while the -COCH$_3$ group is programmed to be flexible by rotation around three torsion angles (C1-N9, N9-C7 and C7-C8). This means that atoms C7, C8, O10 and their hydrogens, plus hydrogen H19, should be better defined as slaves.
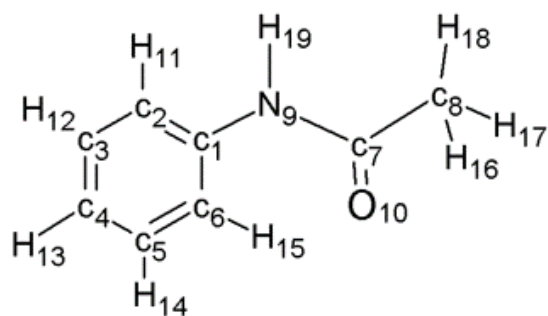
Atoms are not in the optimum sequence, though, as slaves *must* follow backbone-defining core atoms. Thus, the first thing to do is to renumber the atoms so that the first 12 are those of the rigid unit, that is, the benzene ring, its 5 hydrogens and the formerly N9 atom. This is done by editing the acanil01.*oeh* file, changing atom numbers to produce the renumbered acan.*oeh* file, which looks like as follows.
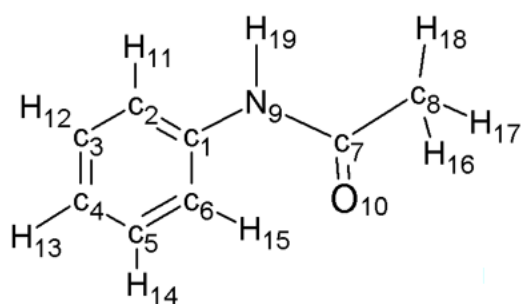
Original numbering
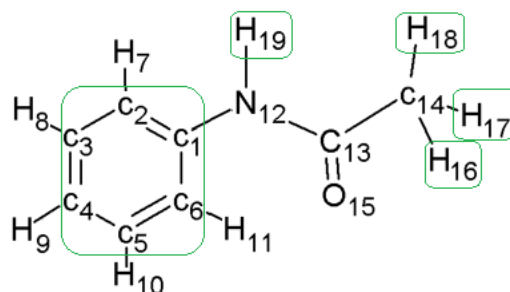
Renumbered (1-6 and 16-19 unchanged)

file acan.oeh, after renumbering of atoms

```
  acetanilide renumbered
 0
19.5090    9.3640    7.7780    90.000    90.000    90.000
 0.0
 19
  1    0.40800    0.07220    0.12710   1 12   0.3119
  2    0.35510   -0.02270    0.16810   1 12  -0.3517
  3    0.28910    0.00220    0.10910   1 12  -0.2826
  4    0.27520    0.12120    0.00820   1 12  -0.3300
  5    0.32800    0.21230   -0.03690   1 12  -0.2802
  6    0.39450    0.18890    0.02100   1 12  -0.3548
  7    0.36569   -0.11563    0.24593   1  2   0.2924
  8    0.24838   -0.07110    0.14166   1  2   0.2871
  9    0.22354    0.14237   -0.03467   1  2   0.2879
 10    0.31743    0.30306   -0.11838   1  2   0.2863
 11    0.43534    0.26049   -0.01589   1  2   0.2981
 12    0.47340    0.04200    0.19750   1 21  -0.5677
 13    0.52750    0.13190    0.21240   1 10   1.0587
 14    0.58890    0.07210    0.30420   1 13  -0.8973
 15    0.52710    0.25540    0.15670   1 27  -1.2314
 16    0.63175    0.06700    0.21650   1  3   0.3434
 17    0.60183    0.14018    0.41148   1  3   0.3379
 18    0.57725   -0.03386    0.35059   1  3   0.3056
 19    0.47853   -0.05565    0.24794   1  7   0.4864
  0
  8     8
 1.0    0.0    0.0    0.0    1.0    0.0    0.0    0.0    1.0
 0.00000    0.00000    0.00000
-1.0    0.0    0.0    0.0    1.0    0.0    0.0    0.0    1.0
 0.50000    0.50000    0.00000
 1.0    0.0    0.0    0.0   -1.0    0.0    0.0    0.0    1.0
 0.00000    0.50000    0.50000
-1.0    0.0    0.0    0.0   -1.0    0.0    0.0    0.0    1.0
 0.50000    0.00000    0.50000
-1.0    0.0    0.0    0.0   -1.0    0.0    0.0    0.0   -1.0
 0.00000    0.00000    0.00000
 1.0    0.0    0.0    0.0   -1.0    0.0    0.0    0.0   -1.0
-0.50000   -0.50000    0.00000
-1.0    0.0    0.0    0.0    1.0    0.0    0.0    0.0   -1.0
 0.00000   -0.50000   -0.50000
 1.0    0.0    0.0    0.0    1.0    0.0    0.0    0.0   -1.0
-0.50000    0.00000   -0.50000
  3
```

The structural information for slave atoms is provided in the *.sla* file that has the following content (see Manual, Section 6.6.4):

acan.sla slave atom file

```
    5
  1.3550     127.62      17.58   0  0   3   13   0   0
  1.5020     115.47     175.89   0  0   3   14   0   0
  1.2340     121.38     179.31   0  0   0   15   0   0
  1.0800     109.47     116.40   0  0   3   16  17  18
  1.0000     117.20       0.00   0  4   3   19   0   0
```

For each *i, j, k, m* sequence of atoms, each line has the *i-j* distance, the *i-j-k* angle and the *i-j-k-m* torsion angle. The numbers to be typed in can be derived from any geometry check program on the original *.cif* file (e.g. Mercury, https://www.ccdc.cam.ac.uk/solutions/csd-system/components/mercury/), or on the acan.*dat* file. The next three numbers in each line are the codes for the variation of each of the three parameters. Zero means fixed parameter,

and this is the case for all the bond lengths and for all bond angles except the 19-12-13 HNC angle, which is variable with maximum stepsize number 4 in the acan.*mci* control file (3.0 deg, see below). All torsion angles are variable, by stepsize number 3 (5.0 deg), except an improper torsion angle associated to atom 15 (carbonyl oxygen), which is kept constant to preserve the planarity of the carbonyl group (see below). The last numbers in each line are the atom sequence numbers.

Then the preliminary topology file can be prepared by the command

```
./run.pretop acan
```

Answer the dialog mode with unit factors (we do not want to rescale force constants):

```
give factors for ks,kb,kt force consts.
1 1 1
 normal end of operation
 Thank you for using MiCMoS
```

This produces an acantry.*top* file, that must be edited as usual.

acantry.top file. In red: lines to be erased; in green: lines to be edited.

```
    acetanilide renumb topology
   19
    1   -0.10849   -0.30876    0.28472   12    0.3119
    2    0.03337   -1.33436    1.22518   12   -0.3517
    3    0.13947   -1.03324    2.57459   12   -0.2826
    4    0.09887    0.28877    3.00096   12   -0.3300
    5   -0.08583    1.29802    2.07407   12   -0.2802
    6   -0.19517    1.01416    0.71709   12   -0.3548
    7    0.06036   -2.36369    0.89939    2    0.2924
    8    0.25400   -1.82842    3.29633    2    0.2871
    9    0.21077    0.52613    4.04851    2    0.2879
   10   -0.14616    2.32295    2.40923    2    0.2863
   11   -0.34595    1.81139    0.00420    2    0.2981
   12   -0.16130   -0.69629   -1.07717   21   -0.5677
   13    0.02826    0.08547   -2.16756   10    1.0587
   14    0.00414   -0.63087   -3.48836   13   -0.8973
   15    0.22250    1.30319   -2.09997   27   -1.2314
   16   -0.82812   -0.27350   -4.07661    3    0.3434
   17    0.92643   -0.44167   -4.01740    3    0.3379
   18   -0.10330   -1.69226   -3.32034    3    0.3056
   19   -0.30099   -1.67386   -1.23495    7    0.4864
    5  nslav-u
   13   0    0       0   0    0      0    0.0000
   14   0    0       0   0    0      0    0.0000
   15   0    0       0   0    0      0    0.0000
   16  17   18      0   0    0      0    0.0000
   19   0    0       0   0    0      0    0.0000
    0  ncore-v
    0  nslav-v
  131.6     0.0 volu-u,volu-v
   19  nstr-u
    1    2   1.399   4696.8    C- C
    1    6   1.394   4786.5    C- C
    1   12   1.417   4032.0    C- N
    2    3   1.387   4950.9    C- C
    2    7   1.080   3600.0    C- H
    3    4   1.390   4888.0    C- C
    3    8   1.080   3600.0    C- H
    4    5   1.383   5034.8    C- C
    4    9   1.080   3600.0    C- H
    5    6   1.391   4866.9    C- C
    5   10   1.080   3600.0    C- H
    6   11   1.080   3600.0    C- H
   12   13   1.355   5496.4    N- C
   12   19   1.000   5300.0    N- H
   13   14   1.503   2506.7    C- C
   13   15   1.235   7784.1    C- O
   14   16   1.080   3600.0    C- H
   14   17   1.080   3600.0    C- H
```

```
  14   18   1.080   3600.0   C- H
   0  nstr-v
  30  nbend-u
   1    2    3  120.00   583.8   C- C- C
   1    2    7  120.00   505.0   C- C- H
   1    6    5  119.00   576.7   C- C- C
   1    6   11  120.00   505.0   C- C- H
   1   12   13  128.00   683.1   C- N- C
   1   12   19  115.00   460.0   C- N- H
   2    1    6  120.00   583.8   C- C- C
   2    1   12  117.00   580.9   C- C- N
   2    3    4  120.00   583.8   C- C- C
   2    3    8  120.00   505.0   C- C- H
   3    2    7  120.00   505.0   C- C- H
   3    4    5  120.00   583.8   C- C- C
   3    4    9  120.00   505.0   C- C- H
   4    3    8  120.00   505.0   C- C- H
   4    5    6  121.00   590.8   C- C- C
   4    5   10  119.00   517.5   C- C- H
   5    4    9  120.00   505.0   C- C- H
   5    6   11  120.00   505.0   C- C- H
   6    1   12  124.00   646.0   C- C- N
   6    5   10  119.00   517.5   C- C- H
  12   13   14  115.00   562.3   N- C- C
  12   13   15  123.00   702.0   N- C- O
  13   12   19  117.00   460.0   C- N- H
  13   14   16  109.00   642.5   C- C- H
  13   14   17  109.00   642.5   C- C- H
  13   14   18  109.00   642.5   C- C- H
  14   13   15  121.00   691.6   C- C- O
  16   14   17  109.00   470.0   H- C- H
  16   14   18  109.00   470.0   H- C- H
  17   14   18  109.00   470.0   H- C- H
   0  nbend-v
  17  ntors-u
   6   1   2   3   50.00   -1.0   1.0   C- C- C- C
   2   1   6   5   50.00   -1.0   1.0   C- C- C- C
   2   1  12  13   50.00   -1.0   1.0   C- C- N- C
   1   2   6  12  100.00   -1.0   1.0   C- C- C- N
   1   2   3   4   50.00   -1.0   1.0   C- C- C- C
   2   1   3   7  100.00   -1.0   1.0   C- C- C- H
   2   3   4   5   50.00   -1.0   1.0   C- C- C- C
   3   2   4   8  100.00   -1.0   1.0   C- C- C- H
   3   4   5   6   50.00   -1.0   1.0   C- C- C- C
   4   3   5   9  100.00   -1.0   1.0   C- C- C- H
   4   5   6   1   50.00   -1.0   1.0   C- C- C- C
   5   4   6  10  100.00   -1.0   1.0   C- C- C- H
   6   1   5  11  100.00   -1.0   1.0   C- C- C- H
   1  12  13  14   50.00   -1.0   1.0   C- N- C- C
  12   1  13  19  100.00   -1.0   1.0   N- C- C- H
  12  13  14  16   50.00   -1.0   3.0   N- C- C- H
  13  12  14  15  100.00   -1.0   1.0   C- N- C- O
   0  ntors-v
   0  nlist-u
   0  nlist-v
  0.410   235.0    650.0    77000.0
   0  nextr
```

As usual, "u" means "solute", "v" means "solvent". Make a copy of acantry.*top* and keep working on the new file, named acan.*top*.

The atom coordinates after atom 12 and all the unnecessary bond stretch and bend potentials must be deleted.

CAUTION: remember to update the number of entries where appropriate (for example, after deleting the lines highlighted in red, the number of explicit atom coordinates is 12 and no longer 19, while `nstr-u` and `nbend-u` are all 0).

Slave atom connectivity must now be defined after *nslav-u* instructions:

```
    5  nslav-u
 13  -1    0     12    1    6    10    1.0587
 14  -1    0     13   12    1    13   -0.8973
 15  -1    0     13   14   12    27   -1.2314
 16  17   18     14   13   12     3    0.32897
 19  -1    0     12   13   14     7    0.4864
```

The meaning of that information is that atom 13 must be built by **Z-matrix procedure**, (13 -1 0) attached to atom 12 and with torsional chain made by atoms 12, 1 and 6 (see Table 6.2 in the Manual). The atom is type 10 (carbonyl carbon, Table 1.1) and its point charge parameter is given as it was in the original .*oeh* file. A similar procedure holds for atom 14 (Z-matrix, chain 13, 12, 1, type 13, amide nitrogen). Atom 15, type 27, carbonyl oxygen, is also built with the Z-matrix procedure, but it exploits an improper torsion (15, 13, 14, 12) that will be used to keep the carbonyl group planar. The three methyl hydrogens, type 3, are built over the chain 16, 14, 13, 12 using the **RX₃ procedure** (Table 6.2) and the amide hydrogen, type 7, by a 19, 12, 13, 14 chain with again the Z-matrix algorithm.

The rest of the top file has the data for the intramolecular force field. It is pointless to keep active all the 17 torsions, as the atomatic ring is rigid and we intend to focus just on the relevant ones through slave atoms. We decided that C1-N12, N12-C13 and C13-C14 bonds (new numbering) are rotatable, thus we now will define just 3 torsions and change "17" into "3".

```
3     ntors-u   torsional potentials for the 3 degrees of freedom
```
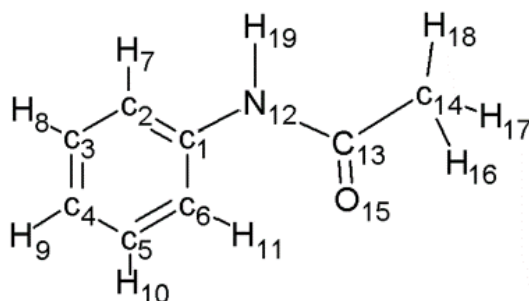
Then, you can safely erase all former lines and type the following ones in their place:

```
 13 12   1   6   10.0    1.0   4.0
 14 13  12  19   17.0   -1.0   2.0
 16 14  13  15    2.0    1.0   3.0
```

The first four entries are torsion-defining atom id numbers (C13-N12-C1-C6; C14-C13-N12-H19; H16-C14-C13-O15). Then, K, f and m parameters in $E(tors) = K\{1 + \cos[f(m \cdot \tau)]\}$ (equation (6.4) in the manual) follow, τ being the torsion angle.

The first rotation occurs around the bond N12-C1 and can be modelled using parameters of acetanilide (nº 30 in Table A7.5, $K = 10$, $f = +1$, $m = 4$).

The second rotation (C14-C13-N12-H19) should be discouraged, as reorientations that make O15 antiperiplanar with respect to C1 are difficult due to the π electron system. Moreover, we

know that chemical conjugation keeps the amide group planar, i.e., that N12, C13, C14 and O15 atoms must be constrained in the same plane. Note that we have obtained these results by combining dihedral instructions and `nslav-u` ones: (i) we use the rather high barrier suggested by Table A7.5 for aminobenzene ($K = 17$, $f = -1$, $m = 2$) (current instruction); (ii) C14 is frozen in the N12-C13-O15 plane as the slave-defining improper dihedral angle O15-C13-C14-N12 is kept fixed (see `nslav-u` and *.sla* file instructions above).

The last dihedral H16-C14-C13-O15 describes the rotation of the terminal methyl group. The same parameters as in ethanol or methanol (Table A7.5, nº 42 and 43) are a reasonable choice: $K = 2$, $f = +1$, $m = 3$, as the potential barrier against the methyl rotation is very small.

Finally, you should include a couple of `nlist-u` intramolecular contacts to protect the intermolecular contacts of the carbonyl oxygen O15 to phenyl ring ortho-hydrogens H7 and H11 with an intramolecular nonbonded potential (see manual, Sections 6.4.2, 6.6.2 and 6.6.3):

```
    2     nlist-u  intramolecular distances to prevent O atom collision
   15  7     15  11
```

Eventually, the file acan.*top* should look like:

acan.top, after editing

```
acetanilide renumb topology
12
  1   -0.10849  -0.30876   0.28472  12    0.3119
  2    0.03337  -1.33436   1.22518  12   -0.3517
  3    0.13947  -1.03324   2.57459  12   -0.2826
  4    0.09887   0.28877   3.00096  12   -0.3300
  5   -0.08583   1.29802   2.07407  12   -0.2802
  6   -0.19517   1.01416   0.71709  12   -0.3548
  7    0.06036  -2.36369   0.89939   2    0.2924
  8    0.25400  -1.82842   3.29633   2    0.2871
  9    0.21077   0.52613   4.04851   2    0.2879
 10   -0.14616   2.32295   2.40923   2    0.2863
 11   -0.34595   1.81139   0.00420   2    0.2981
 12   -0.16130  -0.69629  -1.07717  21   -0.5677
    5  nslav-u
13  -1    0    12   1    6    10    1.0587
14  -1    0    13  12    1    13   -0.8973
15  -1    0    13  14   12    27   -1.2314
16  17   18    14  13   12     3    0.32897
19  -1    0    12  13   14     7    0.4864
  0   ncore-v
  0   nslav-v
131.6    0.0 volu-u,volu-v
  0   nstr-u
  0   nstr-v
  0   nbend-u
  0   nbend-v
  3   ntors-u                        ntors-u  torsional potentials for the 3 degrees of freedom
13 12  1   6   10.0    1.0  4.0
14 13 12 19   17.0   -1.0  2.0
16 14 13 15    2.0    1.0  3.0
  0   ntors-v
  2   nlist-u                        nlist-u intramolecular distances to prevent O atom collision
15  7     15 11
  0   nlist-v
 0.410   235.0    650.0   77000.0      standard CLP parameters
  0   nextr
```

The starting crystal box can now be prepared from *.oeh* and *.sla* files by calling **Boxcry** (manual, Section 5.1).

```
./run.boxcry acan
```

The program will ask for number of repetitions along the three crystallographic directions:

```
boxcry module 3.1 oct.2018
   cell  19.509  9.364  7.778  90.00  90.00  90.00 give n. of cells on a,b,c
```

Give 2 4 5 to have an approximately cubic simulation box with 320 molecules (6080 atoms):

```
2 4 5
   acetanilid nTr,box dims,n.mols,n.atoms   2   4   5  39.0180  37.4560  38.8900  320  6080
 normal end of operation, mols. written  320
 Thank you for using MiCMoS
```

Boxcry has now prepared a file called acancry.*bxi*, which contains positions and relative orientations of all the molecules. This is what it looks like, with the slave atom information for each molecule (see also manual, Section 5.1.1 and Table 5.1):

```
 320        0
 -1.5267 -13.0302 -14.5376  -122.48   -56.03   121.46  0  1 1 1 2 2 2    1
    1.3550    127.62     17.58  0  0  3
    1.5020    115.47    175.89  0  0  3
    1.2340    121.38    179.31  0  0  0
    1.0800    109.47    116.40  0  0  3
    1.0000    117.20      0.00  0  4  3
 -8.2278  -8.3482 -14.5376   -57.52   -56.03    58.54  3  1 1 1 2 2 2    2
    1.3550    127.62     17.58  0  0  3
    1.5020    115.47    175.89  0  0  3
    1.2340    121.38    179.31  0  0  0
    1.0800    109.47    116.40  0  0  3
    1.0000    117.20      0.00  0  4  3
.................................
    8.2278  15.0618  10.6486    57.52   -56.03   -58.54  1  1 1 1 2 2 2  320
    1.3550    127.62     17.58  0  0  3
    1.5020    115.47    175.89  0  0  3
    1.2340    121.38    179.31  0  0  0
    1.0800    109.47    116.40  0  0  3
    1.0000    117.20      0.00  0  4  3
    0
    39.0180    37.4560    38.8900    90.0000    90.0000    90.0000    2    4    5
```

Along with the .*bxi* file, **Boxcry** also generates a acancry.*dat* file for visualization of the crystal structure.

The run control acan.*mci* (manual, Section 6.6.2) is set up as follows:

```
acetanilide crystal MC
#  iprint ivarib iwrh  ipots    factin
     2      0     0     0       0.7
#  cutoff  boxx    boxy    boxz    alf   bet   gam   var.indices       irbox
   15.0   0.000   0.000   0.000   0.0   0.0   0.0   1  1  1  1  1  1   1
# temp  n.moves,   ncom,    nboxc,   nwrite, nwre, npri/steps
  298.0  100000     0        0       500      0      1000
   0.30  20.0  5.0  3.0  0.0  0.  0.  0.  0.  0.
#   P     npres ianis
   1.0     900    4
```

Variability indices are non-zero for all six cell parameters; even if this is an orthorhombic structure, in principle the cell angles could be altered by the MC run. The stepsize lines specifies 0.30 and 20° for the rigid-body translations and rotations, 5° for the torsional parameters and 3° for the variation of the bending angle. The *ianis* flag is now 4 for an anisotropic variation

of the box dimensions (see also Manual, Table 6.1 in Section 6.5). Note that, at variance with liquid cases (Tutotials T6 and T7), we can directly start the simulation from a high temperature (298 K), as our starting structure corresponds to the experimental X-ray one and we do not expect to have to dispose of hard contacts.

The MC run can be started by calling **mcmain**:

```
./run.mcmain acan acancry.bxi ac1
```

where "acan" is the name of the run control and topology files (.*mci* and .*top*), acancry.*bxi* is the starting simulation box produced by **Boxcry** and "ac1" will be the prefix of all the output files.

The results can be found in the usual file ac1mc.*pri*, whereas the box corresponding to the last frame are ac1mc.*bxo* and ac1mco.*dat*.

Now open the ASCII output, ac1mc.*pri*: it is very similar to that discussed in Tutorial T6 for liquid benzene. After regular printing of atomic parameters, rescaled CLP charges and box maxteps, we found the following information:

```
N.solutes-atoms, N.solvents-atoms
    320    19     0     0
 total parameters in solutes and solvents  6720     0
 actual variables, total,solute,solvent  3520  3520     0
 ivarib   0 number of particles for P control   320.
 initial nonzero intramolecular energies
  mol., Es,Eb,Et,Enb,Tot    1      0.00      0.00      0.00    10.84     7.59
  mol., Es,Eb,Et,Enb,Tot    2      0.00      0.00      0.00    10.84     7.59
  mol., Es,Eb,Et,Enb,Tot    3      0.00      0.00      0.00    10.84     7.59
  mol., Es,Eb,Et,Enb,Tot    4      0.00      0.00      0.00    10.84     7.59
...
solute, solvent, tot intramolecular energy    2428.7      0.0    2428.7
```

We have 320 "solute" molecules, bearing 19 atoms each, for a total of 6720 variable parameters, of which only 3520 are active. Flag "*ivarib*" determines some details of how the isotermal–isobaric ensemble is handled by the Metropolis–Monte Carlo algorithm (see Section 6.6.2 and equation (6.6) in Section 6.5 in the main manual for detailed explanations). Then, for each molecule, the intramolecular contribution to the potential is displayed. Stertching (E_s), bending (E_b), torsions (E_t) and nonbonded interactions (E_{nb}), as well as total intramolecular contributions (Tot), are shown. Note that Tot is rescaled by the 0.7 fudge factor FACTIN as given in the .*mci* input file (Sections 6.4.2 and 6.6.2 in the main manual). Eventually, the total intramolecular energy of the whole simulation box is printed.

Then, the simulation is started and box/energy values are printed as usual:

```
set P, interval for P control     1.0         900
 anisotropic box change or pressure control
 Isobaric-Isothermal ensemble (IIE) P control

 MC moves initial
      900   39.021   37.460   38.890   89.998   90.006   90.030        1. box data
     1000   2433.0 -21764.8 -12329.9      0.0 -31661.7         ens data
 -21764.8      0.0      0.0 -12329.9      0.0      0.0
```

After 100 kstep, the program stops after printing relevant statistics (number of moves accepted and rejected, concerning both molecular and box degrees of freedom):

```
last step
     100000
 general,tot,acc,rej,   box,tot,acc,rej
      99889      69264      30625        111        87        24
    acetani acceptance ratio, total,box      69.34     78.38

 final result at last MC step
    1942.6 -21304.1 -11592.5      0.0 -30954.1
  19.5095  9.3861  7.7773   89.83   90.44   90.11

 Intermolecular energies
   LP energies, u,v,uv -21304.15      0.00      0.00
 Coul energies, u,v,uv -11592.52      0.00      0.00
 Total LP,Coul,total E -21304.15 -11592.52 -30954.12
   box dipole energy        0.00

    acetani final Ecoh,Et per mol.,vbox,dens  -102.8   -96.7  56964.40   1.261
```

Note that the total sum of moves (99,889+111, molecules+box) is 100,000, the total number of steps. In other words, the moves ratio is 99.9:0.1 in favor of molecular degrees of freedom. Final "per mole" energies are printed, as well as the predicted box volume and density. The last information concerns the distribution of steps over parameters, that is, for each parameter is displayed the number of steps in which that parameter has been varied. The output ends with 3250 entries, which sum up to the total of 99,889 moves involving molecular degrees of freedom.

```
distribution of steps over parameters
   27  33  26  37  33  29  26  20  28  38  28  26  34  34  30  31  27  30  33  25
   21  32  34  26  20  33  33  30  25  20  30  35  15  30  27  26  21  24  19  31
...
...
   37  26  23  16  23  20  33  20  34  32  25  31  17  32  31  19  41  29  36  29
 normal end of operation
```

Please note that this is just an illustrative run, optimal to be ended a few minutes. A bit longer simulations ($\geq 10^6$ steps) should be set up to ensure that the system is fully equilibrated.

In summary:

1) Run **Retcif**, **Retcor**, **Retcha**, **Crysaa** on acanil01.*cif* to get acanil01.*oeh*;
2) Renumber atoms to have the first ones in the rigid part, obtain acan.*oeh*;
3) Prepare distances, angles and torsions for slave atoms by any geometry check program, for example by running Mercury (https://www.ccdc.cam.ac.uk/solutions/csd-system/components/mercury/) on the original .*cif* file;
4) Prepare the sla file (by hand, using templates), with actual values of the geometrical paramters and indication of variable parameters;
5) Launch **Pretop** to prepare a tentative .*top* file. Make a copy of this file and call it acan.*top*.
6) Edit acan.*top* to delete stretch /bend potentials and non-rigid atoms, and to insert codes for the construction of slave atoms and torsion potential functions;
7) Run **Boxcry** on the acan.*oeh* file to obtain the starting box (acancry.*bxi*);
8) Prepare the acan.*mci* run control file by editing one of the many templates;
9) Run the MC module with acan.*top*, acan.*mci* and acancry.*bxi*.