## MiCMoS Milano Chemistry Molecular Simulation Description and User Manual

# Tutorials

## **T10.** Molecular Dynamics simulation of crystals

**PURPOSE**: In this tutorial, it is described how to prepare and equilibrate the P2<sub>1</sub>2<sub>1</sub>2 RT phase of pyridone with the Molecular Dynamics technique.

**REFERENCE** to main manual: Sections 5.4 (*Pretop*); 6.2 (construction of molecular frameworks); 7.6.1 (*mdmain*); 7.6.2 (instruction file, *.mdi*); 7.6.3 (input box file, *.dat*); 7.6.4 (topology and force field file, *.top*).

**FILES:** You can find all the files you need to run this tutorial here: https://sites.unimi.it/xtal\_chem\_group/images/MiCMoS\_package/T10/PYRIDO11.cif https://sites.unimi.it/xtal\_chem\_group/images/MiCMoS\_package/T10/pyrd.mdi The starting structure file for pyridone (PYRIDO11.cif) has been downloaded from the Cambridge Structural Data Centre. You should produce a valid .*oeh* file, as well as a preliminary static energy analysis, as described in Tutorials T1 and T4. This means that you have to launch in sequence *Retcif, Retcor, Retcha* and *Crysaa*: you can do this directly with the available macro **run.cry** (see below). You will also need macros to run *Pretop, Boxcry* and *mdmain*. Place .*cif* files and pertinent (Windows/Unix) macros into your working directory.

The procedure for the MD simulation of a crystal structure can be straightforward with minimal user intervention in most cases. The preparation of an *.oeh* file from a standard *.cif* file has been carried out several times in former tutorials (see T1, T2, T4, T5 and T8) and should be well known at this time. From the *.oeh* file, *Pretop* generates a topology file that can be applied usually with only minor human intervention, needed for special torsions (none if the molecule is rigid). Templates for the *.mdi* run control file and topologies are available and intervention may only concern the optimization of the relaxation parameters. The *Boxcry* module prepares a crystal box, namecry.*dat*, which can be input directly to the MD module *mdmain* without having to go through a preliminary Monte Carlo equilibration or minimization.

**CAUTION**: This is certainly true if we accept that starting experimental structures are more or less correct and correspond to well–behaved (meta)stable potential energy minima (at least). Indeed, we do not expect significant steric clashes, misplaced atoms or ill–positioned molecules from good–quality X-ray structures. However, always keep in mind the programmers' motto – *garbage in, garbage out*. Ensuring that your starting structure is correct is the first mandatory step of any computer simulation.

Since MD topology files are usually rather complex, the *Pretop* module produces a file called NAMEtry.*top* in the first place, which is then typically renamed ad NAME.*top*. This is cautionary to avoid an inadvertent overlay if corrections are to be inserted or, worse, by a successive run of the *Pretop* module that would destroy the previous .*top* file.

In MD simulations, a good choice of many parameters is essential to obtain physically meaningful results: force field constants, temperature and pressure control, cutoff, box dimensions, etc. (see manual, Section 7). The examples given in this tutorial give average and more or less adequate values, but cannot always be taken as absolute indications, since these choices may be quite different for different chemical systems. The MiCMoS environment provides two largely tested systems for the treatment of small organic molecules, the CLP scheme and a LJC scheme, but allows the introduction of user-defined parameters, both for intra- and intermolecular potentials.

First, make a copy of the starting PYRIDO11.cif entry in the CSD:

#### cp PYRIDO11.cif pyrid.cif

This molecule is strictly rigid so the MD run can be started almost immediately by the following command sequence. When the procedure is standard and there are no loopholes, the **run.cry** macro present in batch directory of the package combines **Retcif**, **Retcor**, **Retcha** and **Crysaa** deleting all unnecessary output files. Call the basic program sequence with the command:

#### ./run.cry pyrd

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. You will end with pyrid.*oeh* and pyrid.*dat* file bearing CLP (modified extended Hückel) charges. Check the results of the static energy calculation from *Crysaa* (file pyrdcry.*pri*) before going on. You should find that the calculation looks fine and reasonable (no errors in pyrdcry.*pri*).

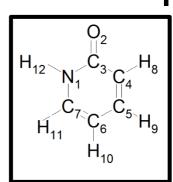
Now prepare the topology file:

#### ./run.pretop pyrd

For crystals with molecules constrained in a packing environment the force constants need not be upgraded, so use 1., 1., 1. rescaling factors when prompted. You have now a tentative pyridtry.*top* file, which is shown below.

File pyridtry.top,	with the	molecular	scheme and	atom	numherina
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This .*top* file has all the stretching and bending force field parameters needed for the MD run. The labels at the right of each force field line (C-C, C-C-C, etc.) are just indicative but are not used.

Before proceeding, copy pyridtry. top into pyrid. top and keep editing this latter.

**CAUTION**: when dealing with flexible molecules, torsional potential must be updated according to Table A7.5 in the Appendix of the main manual. In any case, even in the case of rigid pyridone, a safe practice is to always inspect closely all assigned torsions. Actually, the automatic *Pretop* procedure assigns zero energy at zero torsion angle, but sometimes chooses the atom numbers corresponding to 180°.

This is exactly the case for torsion around the endocyclic N1-C3 bond (the first ntors-u instruction).

7 1 3 2 50.00 -1.0 1.0 C- N- C- O

This corresponds to torsion C7–N1–C3–O2, which should be maximally stable when the torsion angle is 180°. That granted, recall that 50.0, –1.0 and +1 are *K*, *f* and *m* values in *E*(*tors*) =  $K\{1 + \cos[f(m \cdot \tau)]\}$  (see manual, Section 7.4.1 and Figure A7.1b in Section A7.3, Appendix): the problem is that f = –1 and m = +1 stabilize torsions of 0° and destabilize those at 180°. Therefore, this instruction must be corrected. You have two choices. The simplest one is to re–define the torsion by choosing an endocyclic cis–chain, for which the potential stabilizing 0° conformers is correct:

7 1 3 **4** 50.00 -1.0 1.0 C- N- C- **C** 

Another equivalent possibility is to maintain the atom chain identities, and to correct the functional to have 0° conformations destabilized and 180° ones stabilized:

7 1 3 2 50.00 **1.0** 1.0 C-N-C-O

Check by yourself all other torsions: you should agree in that all other parameters are correct. The pyrid.top file is now ready for entering Dynamics. Before that, we have to define the simulation box. We can call *Boxcry* to do that from the .*oeh* file:

#### ./run.boxcry pyrid

The program will print:

```
boxcry module 3.1 oct.2018
cell 13.657 5.912 5.701 90.00 90.00 90.00 give n. of cells on a,b,c
```

Give 2 5 5 to have an approximately cubic simulation box with 200 pyridone molecules in file pyridcry.*dat*.

```
#PYRIDO11 'P nTr,box dims,n.mols,n.atoms 2 5 5 27.3140 29.5600 28.5050 200 2400
normal end of operation, mols. written 200
Thank you for using MiCMoS
```

File pyridcry.*bxi* is also produced, but is for Monte Carlo but is not used in MD. Note that the crystal box is kept rather small in this short example.

Now prepare the run control file pyrid.*mdi* according to the following instructions. Have a look to the manual (Section 7.6.2) for a detailed description and meaning of all parameters.

p	yridone 1	PYRID011	clp po	otential	mini	mal ba	rostat					
#	n.steps	irvel	ipri	ibox ids	tr	timest	ep ieng	t ibias	+Ebias	Nbias	tinor	n tinof
	10000	0	0	1 0		0.002	0	0				
#	cutoffu	cutoffv	cutoff	Euv facti	n i	pots	ianh	inano				
	15.0	0.0	0.0	0.0		0	0	0				
#	N(T)	Tset Ts	tart Tr	celax 0/	1/2	weak/s	tiff/CS	VR				
	250	298 2	298	0.6	0							
#	N(P)	Pset co	omprs	0/lianis	ipr	ww	iextst	r + str	all 22,	33, 1	2 13 2	23, GPa
	300	1.0	0.35	1	0	0.0	0					
#	N(com)	nwbox	nwre	npri								
	50	200	200	100								

**CAUTION**: With one simulation box edge of 27.3 Å, the maximum cutoff allowed is 15 Å (must not exceed 0.55 times any of the three box lengths).

All other parameters should be obvious to the user who has gone through the preceding tutorials or has studied the manual; note that inano is zero, meaning that we are dealing with an unconfined periodic simulation box, as it should be. All the other values are more or less standard, with the only exceptions of N(T), Trelax, N(P) and comprs, that may need adjustment; as a rough guide, comprs is sensitive to the strength of crystal forces and may need smaller values in a hydrocarbon than in a strongly hydrogen-bound crystal that may tolerate a large pressure-volume jump (this is not a strict rule, though).

The comprs parameter is the first suspect in case of crash of the simulation. Then in order of frequency come a wrong assignment or rescaling of force constants (that may be evident from the starting values of intramolecular energies), and a badly prepared starting computational box. The latter case is more frequent for liquids than for crystals.

The actual MD run is started by the command

## ./run.mdmain pyrid pyridcry.dat py1

The prefix "pyrid" identifies input .*top* and .*mdi* files, pyridcry.*dat* is the starting simulation box and py1 will be the prefix of all the output files. These are: py1md.*pri* (regular printout), py1mdo.*dat* (last frame of the trajectory), py1mdc.*dat* (full trajectory) and py1md.*ene* (energu trajectory).

Now, open the py1md.*pri* printfile. You can check the total number of degrees of freedom (d.o.f.):

N.mols, N.atoms, (u-v), Mws	200	12	0	0	95.10	0.00
n. of atomic degrees of	freedom,		7200.		0.	7197.

We have 200 molecules consisting of 12 atoms each. Every molecule has 6 rigid body d.o.f. accounting for translations and rotations of the whole backbone, plus  $3 \times 12 - 6$  internal d.o.f. due to intramolecular vibrations. Overall, the total number of d.o.f. is thus 200 x 12 x 3 =

7200. As we fix the centre of mass of the simulation box, the effective number of d.o.f. is 7197.

The last lines of the py1md.*pri* file summarize intermolecular energies, final unit cell parameters, and density, with corresponding percent changes from the starting estimates:

Intermolecular energies 0.00 LP energies, u,v,uv,ubar,vbar -9321.76 0.00 0.00 0.00 Coul energies, u,v,uv,ubar,vbar -6482.69 0.00 0.00 0.00 0.00 final box edges, multiplicities 26.466 29.647 29.782 2 5 5 final unit cell 13.233 5.929 5.956 90.0 90.0 90.0 1.352 %edges, abs angles, %density variations -3.1 0.3 4.5 -0.0 -0.0 -0.0 -1.51 -79.0 final cohesive Ens, solute, solvent, solvation 0.0 0.0 cohesive energy variations -0.7 0.0 0.0

You see that this short run changes only marginally the cell parameters. Temperature and pressure oscillate around the preset values. To have a look at them, you can resort to Unix grep command, as explained in the Tutorial T9:

grep 'nmove,Pset, Pcurrent' py1md.pri grep 'old and new temperatures' py1md.pri grep 'ens data' py1md.pri

for pressure, temperature and energies, respectively. Results are:

Pressures as a function of the simulation step:

300	nmove,Pset,	Pcurrent	1.000	13.3
600	nmove,Pset,	Pcurrent	1.000	399.0
900	nmove,Pset,	Pcurrent	1.000	492.1
9300	nmove,Pset,	Pcurrent	1.000	-109.0
9600	nmove,Pset,	Pcurrent	1.000	1.9
9900	nmove,Pset,	Pcurrent	1.000	145.7

Temperatures as a function of the simulation step:

25	0 old	and	new	temperatures	208.8	262.3	0.0	0.0	208.8	262.4	
50	0 old	and	new	temperatures	241.4	275.3	0.0	0.0	241.5	275.5	
75	0 old	and	new	temperatures	258.2	282.1	0.0	0.0	258.3	282.2	
950	0 old	and	new	temperatures	303.8	300.3	0.0	0.0	304.0	300.5	
975	0 old	and	new	temperatures	286.9	293.6	0.0	0.0	287.0	293.7	
1000	0 old	and	new	temperatures	302.7	299.9	0.0	0.0	302.9	300.0	

Energies as a function of the simulation step:

100 1816.4 1367.3 998.1	0.0	0.0	0.0	0.0	0.0	-9174.3	-7000.9	-11993.6	-80.9	1.372 ens data
200 2054.6 1314.8 1194.1	0.0	0.0	0.0	0.0	0.0	-9605.7	-6866.2	-11908.4	-82.4	1.372 ens data
300 2002.1 1401.0 1215.7	0.0	0.0	0.0	0.0	0.0	-9513.9	-6731.0	-11626.1	-81.2	1.372 ens data
9800 3147.5 2373.2 1565.0	0.0	0.0	0.0	0.0	0.0	-9245.5	-6536.2	-8696.1	-78.9	1.354 ens data
9900 3185.4 2386.5 1612.2	0.0	0.0	0.0	0.0	0.0	-9266.6	-6561.9	-8644.5	-79.1	1.352 ens data
10000 3030.9 2439.8 1652.0	0.0	0.0	0.0	0.0	0.0	-9321.8	-6482.7	-8681.7	-79.0	1.352 ens data

As for energies, from left to right: step number; stretching, bending and torsion energies of the solute; a dummy zero; stretching, bending and torsion energies of the solvent; a dummy zero; Lennard–Jones intermolecular energies; Coulomb intermolecular energies; total energies; cohesive energies per molecule per asymmetric unit; total density, in g/mL. All

energies are expressed in kJ/mol. From the .*top* file, we see that we have 12 stretching d.o.f. and 18 bending d.o.f., for a total of 200 x 12 = 2400 stretching d.o.f. and 200 x 18 = 3600 bending d.o.f.. Final internal stretching and bending energies are  $\sim$  3000 kJ/mol and  $\sim$  2400 kJ/mol, corresponding to 1.2 kJ/mol per d.o.f. (stretching) and 0.7 kJ/mol per d.o.f. (bending). These both comply well with the  $\frac{1}{2}$  RT estimate at 298 K (1.2 kJ/mol per d.o.f.).