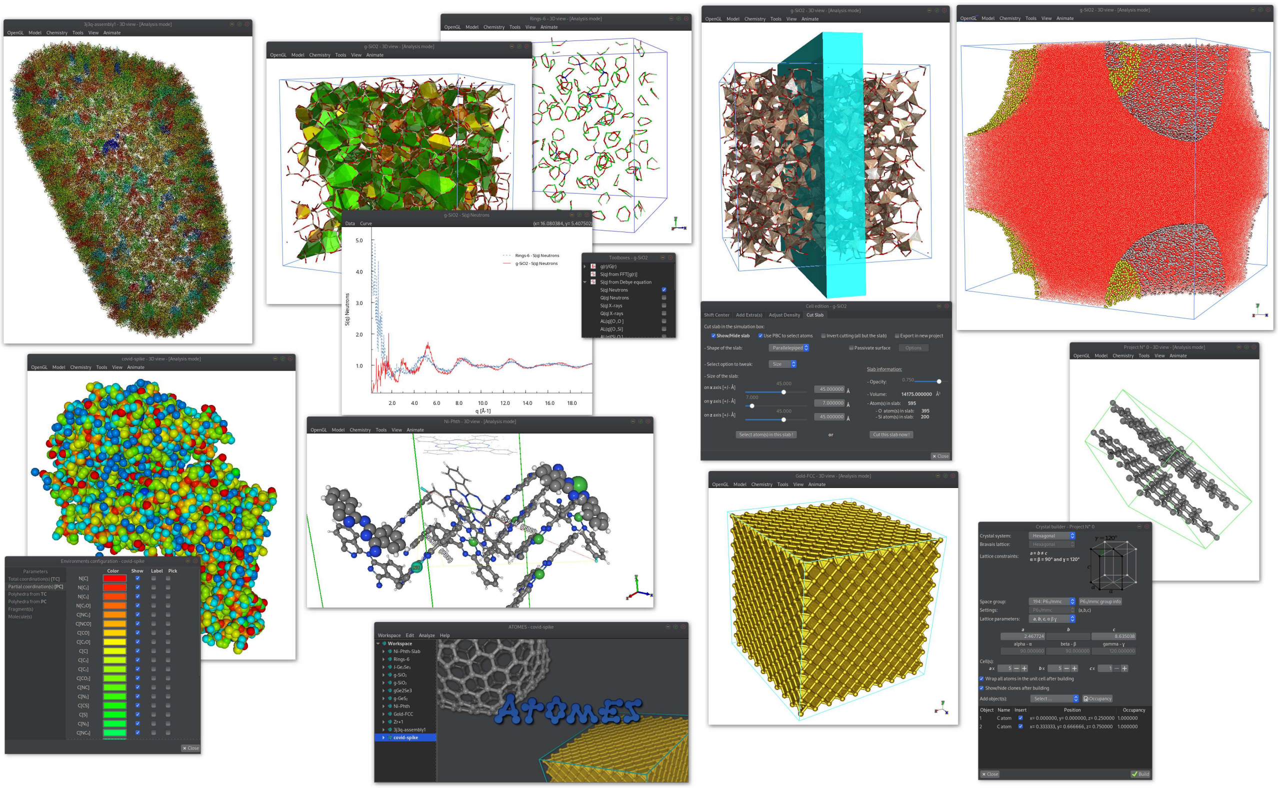
atomes

https://atomes.ipcms.fr



atomes: user manual

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Introduction

atomes is a cross-platform Free (Open Source) computational material science tool box. It regroups a comprehensive panel of specialized edition tools, several assistants dedicated to the preparation of numerical experiments, and, a large number of physico-chemical analysis. Advanced visualization utilities and capabilities being available at each stage of the process **atomes** introduces innovative 3D rendering possibilities and intuitive applications of the calculation results.

atomes is designed to analyze, to visualize and to create/edit large three-dimensional atomic scale models, and can handle MD trajectories from hundreds of thousands, up to millions, of atoms. Using OpenMP parallelization, file processing, coordination and physico-chemical analysis make use of the advantages of modern CPUs and their multiple cores. Consequently when importing atomic coordinates several properties are analyzed on the fly regardless of the size, in number of atoms or MD steps, and the periodicity of the system.
atomes offers a workspace that allows to have many projects opened simultaneously. The different projects in the workspace can exchange data: analysis results, atomic coordinates ...

atomes also provides an advanced input preparation system for further calculations using well known molecular dynamics codes:

- Classical MD : DL-POLY [1] and LAMMPS [2]
- *ab-initio* MD : CPMD [3] and CP2K [4]
- QM-MM MD : CPMD [3] and CP2K [4]

To prepare the input files for these calculations is likely to be the key, and most complicated step towards MD simulations. **atomes** offers a user-friendly assistant to help and guide the user step by step to achieve this crucial step.

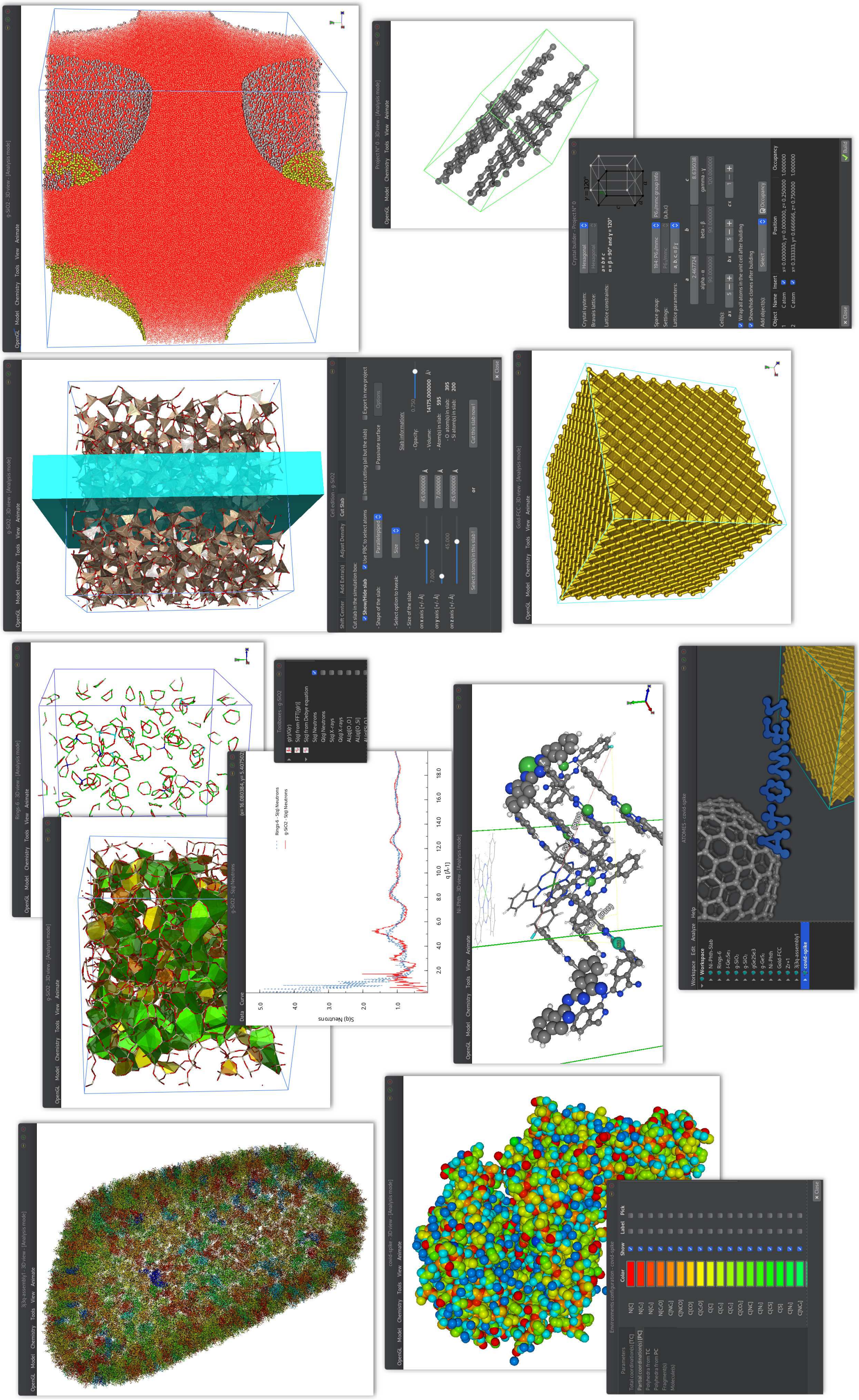


Figure 1.1 *Overview of the* **atomes** *program.*

Programming framework

atomes is developed in C, GLSL (OpenGL shading language), and FORTRAN90. The GTK [5] library is used to create the **G**raphical **U**ser **I**nterface, and the OpenMP [6] API for parallel programming is used to take advantage of the CPU's cores.
The 3D rendering is performed, via the GtkGLArea widget, using modern OpenGL language [7], and the Epoxy library is used to ensure the OpenGL function pointer management. Also the FFmpeg [8] library is used to encode video from off-screen OpenGL rendering.

2.1 Supported platforms

The GTK library is a highly portable programming interface which allows **atomes** to be a cross-platform software. Linux, MacOS (Sonoma 14.4.1 - M3 Max processor) and Microsoft Windows (10, 11) versions of the program are available.

2.2 Dependencies and requirements

Library	Version	
	Min. required	Recommended
GTK+	3.16 / 4.60	3.22 + / 4.60 +
FFmpeg	3.1	3.41 +
Epoxy	1.3	1.43 +
OpenMP	4.5	4.5 +

Table 2.1 *Libraries used by* **atomes**.

Features

3.1 Main window

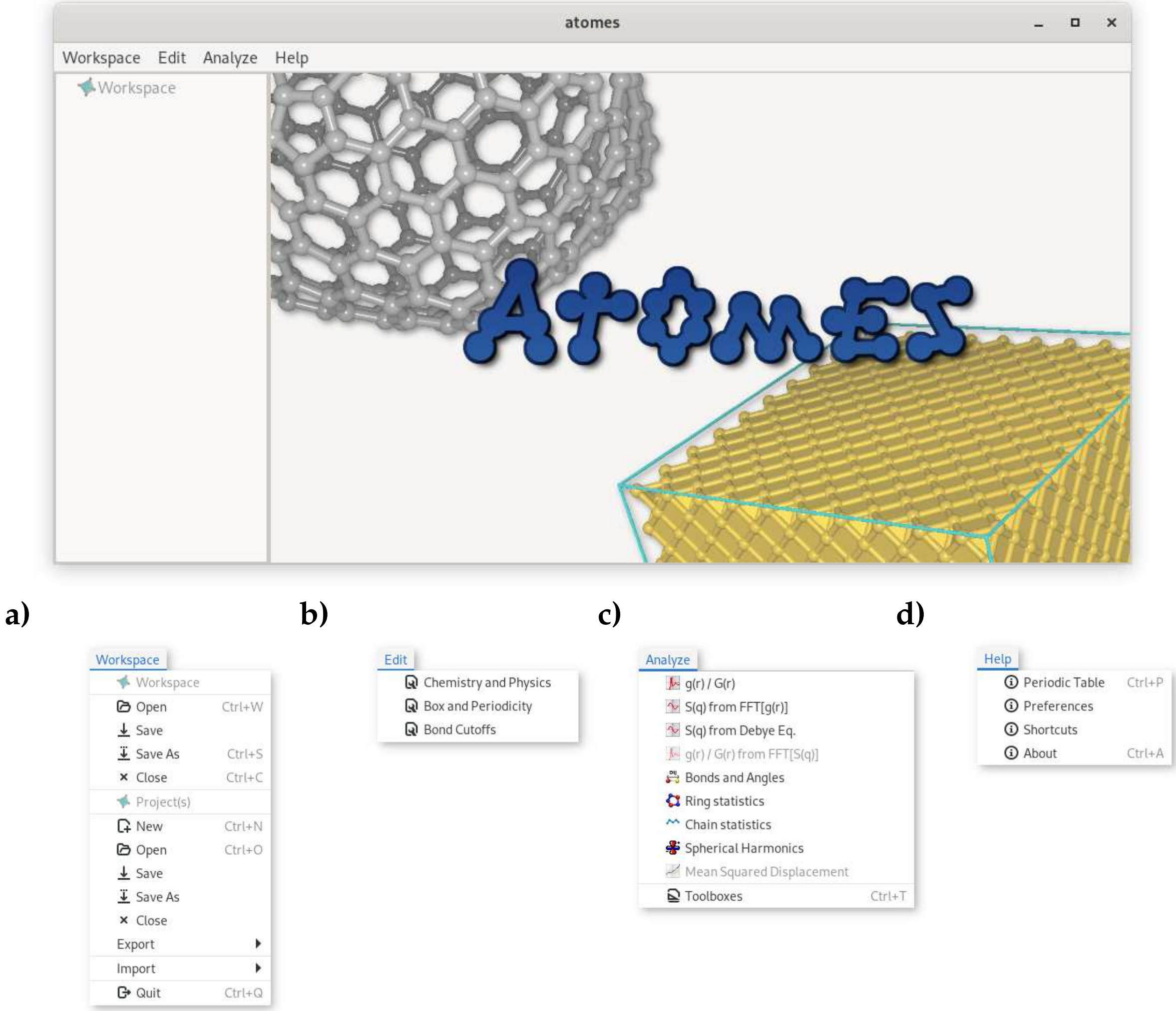


Figure 3.1 *Main window of the* **atomes** *program.*

The main interface of the **atomes** program [Fig. 3.1-a] gives access to:

- The "`Workspace menu`" [Fig. 3.1-b] to open and save files, including **atomes** workspace and project files.
- The "`Edit menu`" [Fig. 3.1-c] to adjust chemical / physical of a system to be studied/edited.
- The "`Compute menu`" [Fig. 3.1-d] to run some analysis on the **active** project (see section 3.5 for details).
- The "`Help menu`" [Fig. 3.1-e] to access the documentation, a periodic table and define user preferences (see section 3.9 for details).

atomes allows to build, edit, study, analyse and compare multiple systems within the same instance of the program. Each system (molecule(s)/material ...) is defined in a data structure called **project**, **atomes** projects (*.apf files) can be opened/saved separately, the list of opened project(s) appears in the left side of the main window in a browsable tree-like structure. The entire list of project(s) displayed in this part of the main window is a data structure called **workspace**, and **atomes** workspace files (*.awf files) can also be opened and saved, allowing to back up the entire list of projects at once, preserving the possible connections, data exchanges, between each projects.
An illustration is presented in figure 1.1, many different projects being opened in the workspace. To each of these project is assigned an OpenGL 3D window, few of them being visible in figure 1.1. Double-clicking on the "`Workspace`" word at the top root of the tree, the list of all projects appears in the right side window. This list includes, in bold green font, the name of the **active** project (see section 3.5 for details).

Keyboard shortcuts

- Workspace:

  Ctrl + w : open workspace

  Ctrl + s : save workspace as

  Ctrl + c : close workspace

- Project:

  Ctrl + n : create new project

  Ctrl + o : open project

- Misc:

  Ctrl + t : show curve toolboxes

  Ctrl + p : open periodic table

  Ctrl + a : show about dialog

  Ctrl + q : quit

- On any file dialog:

  Ctrl + l : open command line

3.2 Workspace and project tree

In **atomes** each project, as soon as it is created and whether it is new (empty) or contains atomic coordinates, is immediately:

- inserted into the workspace tree: a branch will appear bearing the project name [Fig. 3.2].
- assigned an OpenGL window for visualization, analysis and edition.
- the "`Toolboxes`" dialog [Fig. 4.2] is refreshed, and if required open, to present the data of this project.

Figure 3.2 illustrates the structure of project tree branch in the **atomes** workspace.

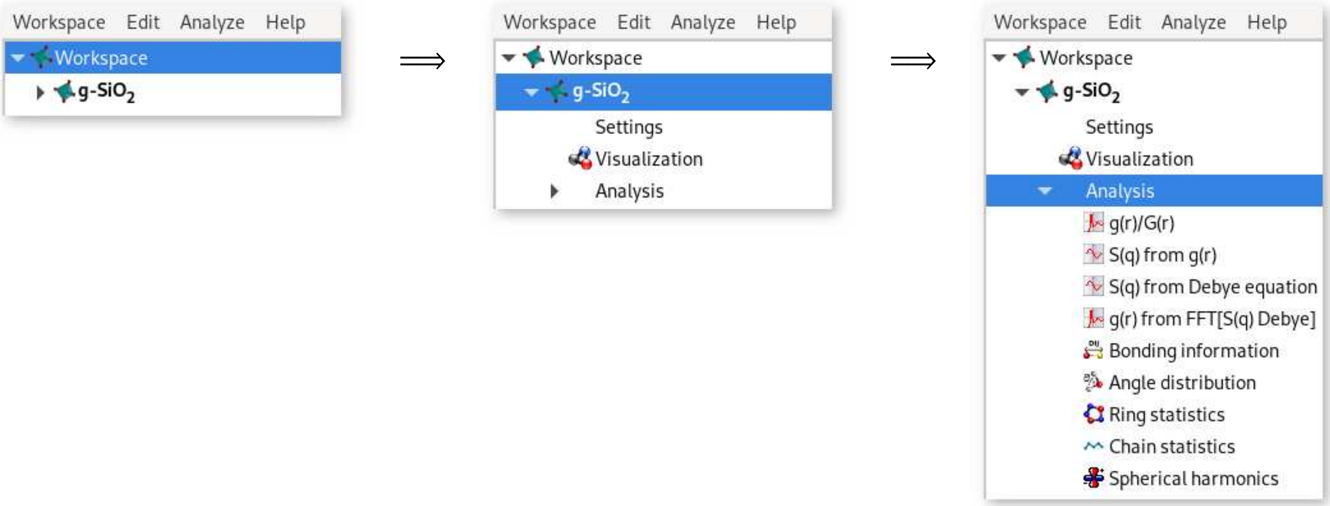


Figure 3.2 *Project tree in the* **atomes** *program.*

On each line/tree branch in the workspace tree the double-click with the left button of the mouse has an effect:

- "`Workspace`" line: displays workspace information, lists all opened project(s) and gives the name of the **active** project in bold green font [Fig. 1.1].
- "`Project's name`" line: activates the project (see section 3.5 for details), when the project is **active** its name is displayed in bold font.
- "`Settings`" line: provides general information about the project.
- "`Visualization`" line: open/close the OpenGL visualization window, and display OpenGL/hardware information.
- Each of the calculation lines (ex: "`g(r)/G(r)`"): if the calculation was performed for that project displays summary of the calculation, used parameters, and results.

As illustrated in figure 3.3 the right click of the mouse display a menu basically reproduces the Workspace menu [Fig. 3.1-b], but also introduces two new buttons to activate the project (see section 3.5 for details) and edit its name.

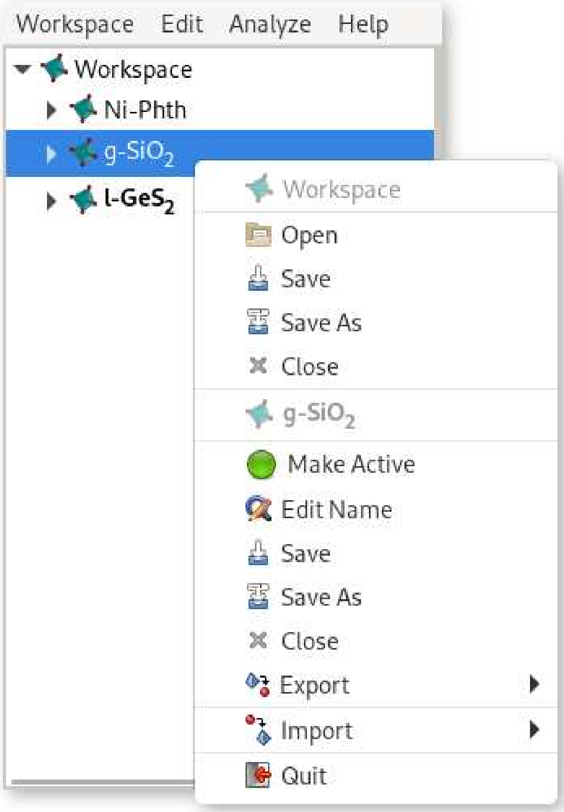


Figure 3.3 *Mouse left click menu in the workspace tree of the* **atomes** *program.*

The name of the project supports Pango markup[9]:

- for $_{\text{underscore}}$
- for $^{\text{exponent}}$
- <i> </i> for *italic*
-   for **bold**
- <u> </u> for underline
- <tt> </tt> for `monospace`

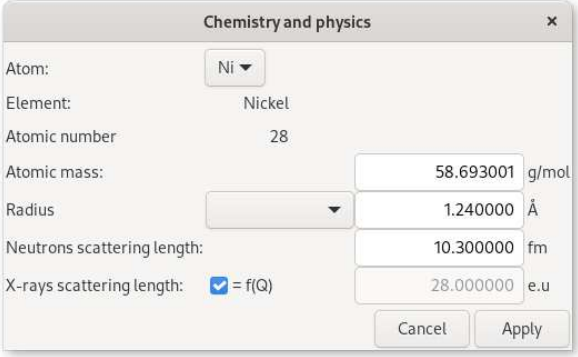
and more ... see: https://docs.gtk.org/Pango/pango_markup.html

3.3 Files

3.3.1 Importing atomic coordinates

The list of the supported format of atomic coordinates is presented in appendix A. ISAACS files contains all the information required to prepare analysis and visualization. For the other file formats, and after reading the atomic coordinates, dialog boxes appears automatically in the following order:

1) The "`Chemistry and physics`" dialog [Fig. 3.4]



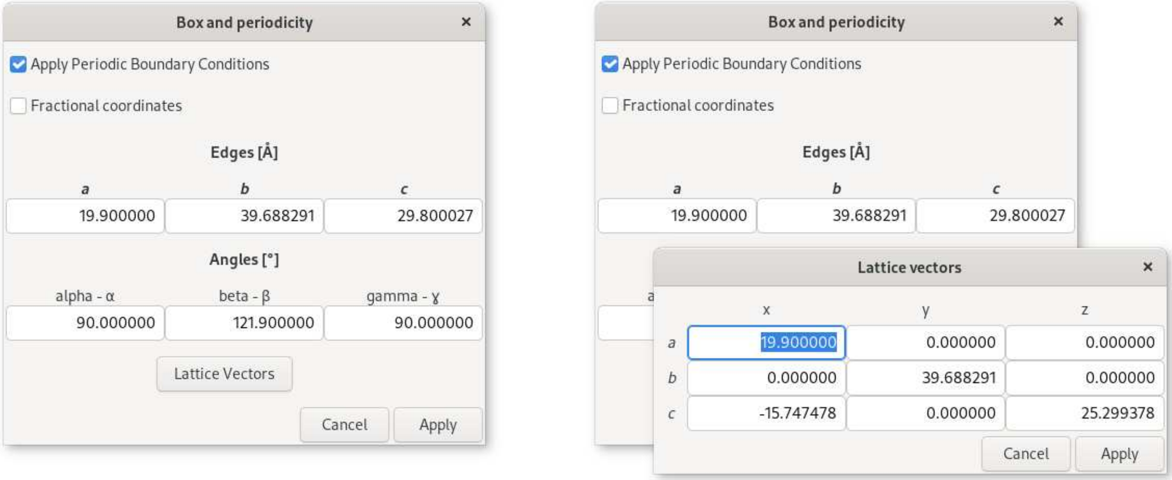
Atom: Ni
Element: Nickel
Atomic number 28
Atomic mass: 58.693001 g/mol
Radius 1.240000 Å
Neutrons scattering length: 10.300000 fm
X-rays scattering length: ☑ = f(Q) 28.000000 e.u

Figure 3.4 *The "`Chemistry and physics`" dialog in the* **atomes** *program.*

This dialog allows to tweak the chemical and physical properties of the elements found in the coordinates file (see figure 3.4).
Particular attention should be given to the selection of the neutrons and X-rays scattering length, for the former parameters are included in **atomes** (see chapter F), for the latter two possibilities are offered to the user:

- Use the exact Q dependent method to compute X-rays S(Q) related properties.
- Use an approximation with the X-rays scattering length equal to the atomic number of the element.

2) The "`Box and periodicity`" dialog [Fig. 3.5]



☑ Apply Periodic Boundary Conditions
☐ Fractional coordinates

Edges [Å]

a	b	c
19.900000	39.688291	29.800027

Angles [°]

alpha - α	beta - β	gamma - γ
90.000000	121.900000	90.000000

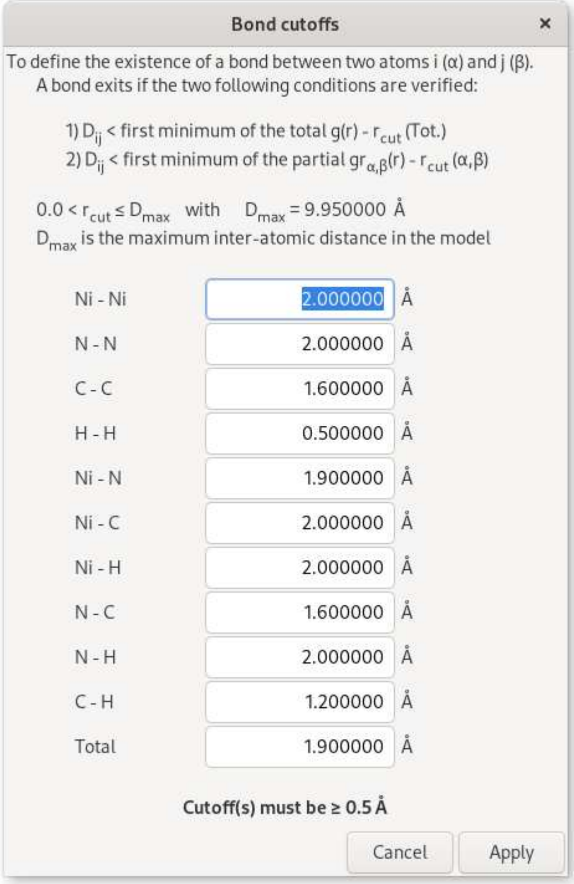
Lattice vectors

	x	y	z
a	19.900000	0.000000	0.000000
b	0.000000	39.688291	0.000000
c	-15.747478	0.000000	25.299378

Figure 3.5 *The "`Box and periodicity`" dialog in the* **atomes** *program.*

This dialog allows to define the periodicity and if needed adjust the model box proportions, or lattice vectors (see [Fig. 3.5]).

3) The "`Bond cutoffs`" dialog [Fig. 3.6]



To define the existence of a bond between two atoms i (α) and j (β).
A bond exits if the two following conditions are verified:

1) D_{ij} < first minimum of the total g(r) - r_{cut} (Tot.)
2) D_{ij} < first minimum of the partial $gr_{\alpha,\beta}(r)$ - r_{cut} (α,β)

$0.0 < r_{cut} \leq D_{max}$ with $D_{max} = 9.950000$ Å
D_{max} is the maximum inter-atomic distance in the model

Ni - Ni	2.000000	Å
N - N	2.000000	Å
C - C	1.600000	Å
H - H	0.500000	Å
Ni - N	1.900000	Å
Ni - C	2.000000	Å
Ni - H	2.000000	Å
N - C	1.600000	Å
N - H	2.000000	Å
C - H	1.200000	Å
Total	1.900000	Å

Cutoff(s) must be ≥ 0.5 Å

Figure 3.6 *The "`Bond cutoffs`" dialog in the* **atomes** *program.*

This dialog allows to adjust the cutoff distances used to define the existence or absence of chemical bonds (see figure 3.6), both for the calculations (see section 3.5) sensitive to these parameters and for the 3D visualization in the OpenGL window (see section 3.6).
As soon as the "`Bond cutoffs`" dialog closes **atomes** will have everything required to setup the 3D model and the OpenGL window will appear.

The 3 dialog boxes "`Chemistry and physics`", "`Box and periodicity`" and "`Bond cutoffs`" can be re-opened again later on using the "`Edit`" menu [Fig. 3.1-c]. However in that case only the **active** project parameters can to be modified. Therefore remember to activate the project you want to edit before using the edit menu.

3.3.2 Reading atomes project file(s)

The **atomes** project file allows to store:

- The atomic coordinates, including MD trajectories.
- The results/data of all calculations performed within **atomes**.
- The results of all modifications of the calculations data, including graph windows (see chapter 4).
- The parameters of the OpenGL window, so that when re-opened the project appears exactly as it was when saved.

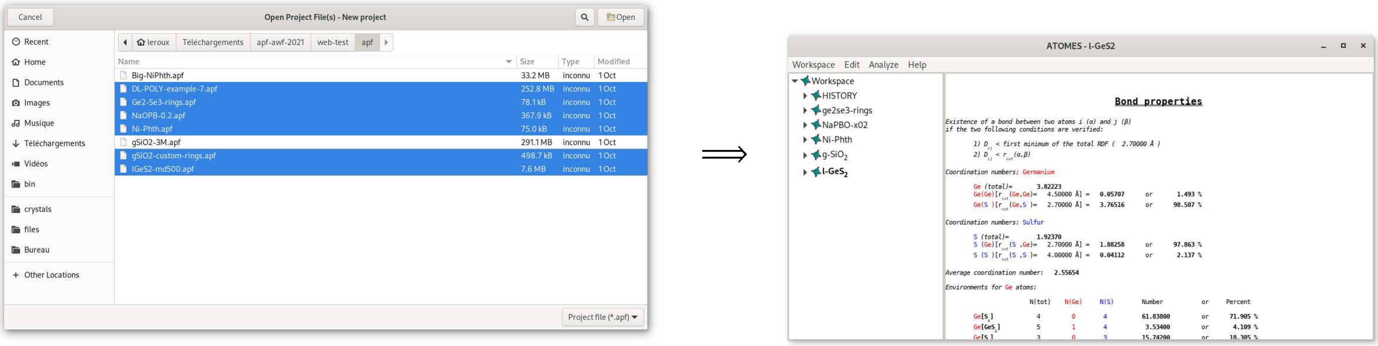
The main idea being to be able to resume work exactly where it was before saving the **atomes** project file.

The **atomes** project files have the extension: **.apf**

To open **atomes** project file(s) use the "`Open Project File(s)`" dialog [Fig. 3.7]. This can be done using alternatively:

- The workspace menu.
- The right click menu obtained with the mouse button of the workspace tree.
- The keyboard shortcut Ctrl + o on top of the **atomes** program main window.

Many **atomes** project files can be opened simultaneously, simply select all projects to be opened in the "`Open Project File(s)`" dialog, click "`Open`" and they will appear in the workspace tree:



Name	Size	Type	Modified
Big-NiPhth.apf	33.2 MB	inconnu	1 Oct
DL-POLY-example-7.apf	252.8 MB	inconnu	1 Oct
Ge2-Se3-rings.apf	78.1 kB	inconnu	1 Oct
NaOPB-0.2.apf	367.9 kB	inconnu	1 Oct
Ni-Phth.apf	75.0 kB	inconnu	1 Oct
gSiO2-3M.apf	291.1 MB	inconnu	1 Oct
gSiO2-custom-rings.apf	498.7 kB	inconnu	1 Oct
lGeS2-md500.apf	7.6 MB	inconnu	1 Oct

```
                    Bond properties

Existence of a bond between two atoms i (α) and j (β)
if the two following conditions are verified:

        1) D_ij < first minimum of the total RDF (  2.70000 Å )
        2) D_ij < r_cut(α,β)

Coordination numbers: Germanium

        Ge (total)=       3.82223
        Ge(Ge)[r_cut(Ge,Ge)=   4.50000 Å] =   0.05707      or       1.493 %
        Ge(S )[r_cut(Ge,S )=   2.70000 Å] =   3.76516      or      98.507 %

Coordination numbers: Sulfur

        S (total)=        1.92370
        S (Ge)[r_cut(S ,Ge)=   2.70000 Å] =   1.88258      or      97.863 %
        S (S )[r_cut(S ,S )=   4.00000 Å] =   0.04112      or       2.137 %

Average coordination number:   2.55654

Environments for Ge atoms:

                       N(tot)    N(Ge)    N(S)       Number          or      Percent

        Ge[S_4]          4         0        4       61.83800         or      71.905 %
        Ge[GeS_4]        5         1        4        3.53400         or       4.109 %
        Ge[S ]           3         0        3       15.74200         or      18.305 %
```

Figure 3.7 *The "`Open Project File(s)`" dialog in the* **atomes** *program.*

Later on when using the **atomes** program remember that any window specifically dedicated to a project will have the name of this project in its title bar.

3.3.3 Reading atomes workspace file(s)

The **atomes** workspace file allows to store:

- A collection of **atomes** projects.
- The relations between these projects, data exchanges, comparisons ...

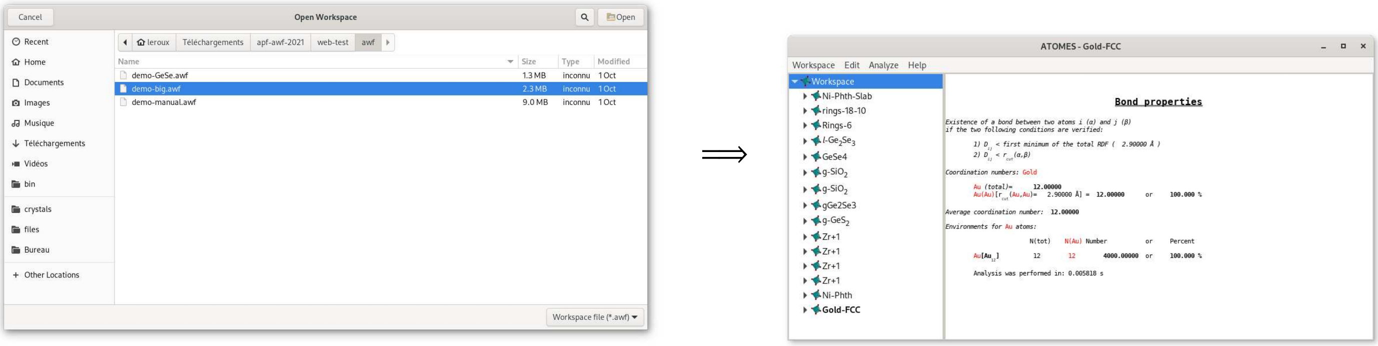
Again the idea is to be able to resume work exactly where it was before saving the **atomes** workspace file.

The **atomes** workspace files have the extension: **.awf**

To open **atomes** workspace file use the "`Open Workspace`" dialog [Fig. 3.8].
This can be done using alternatively:

- The workspace menu.
- The right click menu obtained with the mouse button of the workspace tree.
- The keyboard shortcut Ctrl + w on top of the **atomes** program main window.

Only a single **atomes** workspace file can be opened at a time, if needed close the opened workspace, then open the new one:



Name	Size	Type	Modified
demo-GeSe.awf	1.3 MB	inconnu	1 Oct
demo-big.awf	2.3 MB	inconnu	1 Oct
demo-manual.awf	9.0 MB	inconnu	1 Oct

```
                         Bond properties

Existence of a bond between two atoms i (α) and j (β)
if the two following conditions are verified:

     1) D_ij < first minimum of the total RDF (  2.90000 Å )
     2) D_ij < r_cut(α,β)

Coordination numbers: Gold

     Au (total)=      12.00000
     Au(Au)[r_cut(Au,Au)=   2.90000 Å] =  12.00000      or     100.000 %

Average coordination number:  12.00000

Environments for Au atoms:

                    N(tot)    N(Au) Number          or     Percent

     Au[Au_12]       12        12       4000.00000  or     100.000 %

     Analysis was performed in: 0.005818 s
```

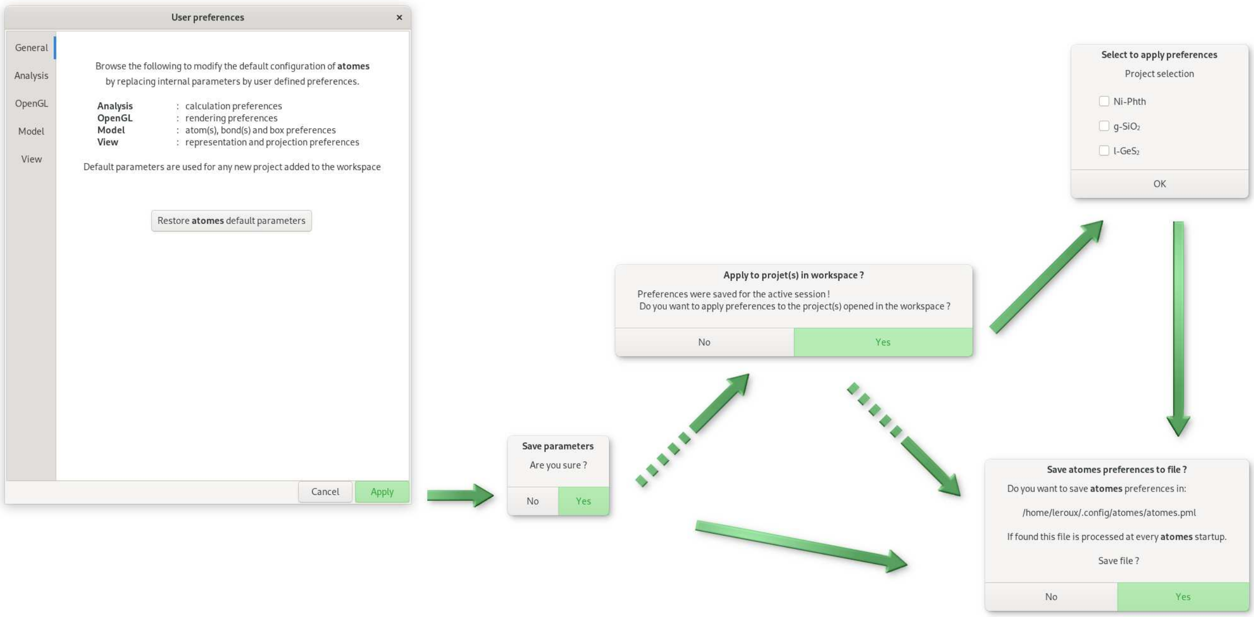
Figure 3.8 *The "`Open Workspace`" dialog in the* **atomes** *program.*

3.4 User preferences

The "`User preferences`" dialog that can be opened via the "`Help`" menu of the main window allows to adjust **atomes** internal options for all projects to be opened in **atomes** workspace, configuration options include:

- Analysis option
- OpenGL rendering options
- Model atom(s), bond(s), label(s) and model box options
- Representation, projection, background, axis and selection options

As illustrated in the next pages it is possible to configure the default behavior of several parts of the software.



Browse the following to modify the default configuration of **atomes**
by replacing internal parameters by user defined preferences.

Analysis : calculation preferences
OpenGL : rendering preferences
Model : atom(s), bond(s) and box preferences
View : representation and projection preferences

Default parameters are used for any new project added to the workspace

Are you sure ?

Preferences were saved for the active session !
Do you want to apply preferences to the project(s) opened in the workspace ?

Do you want to save **atomes** preferences in:

/home/leroux/.config/atomes/atomes.pml

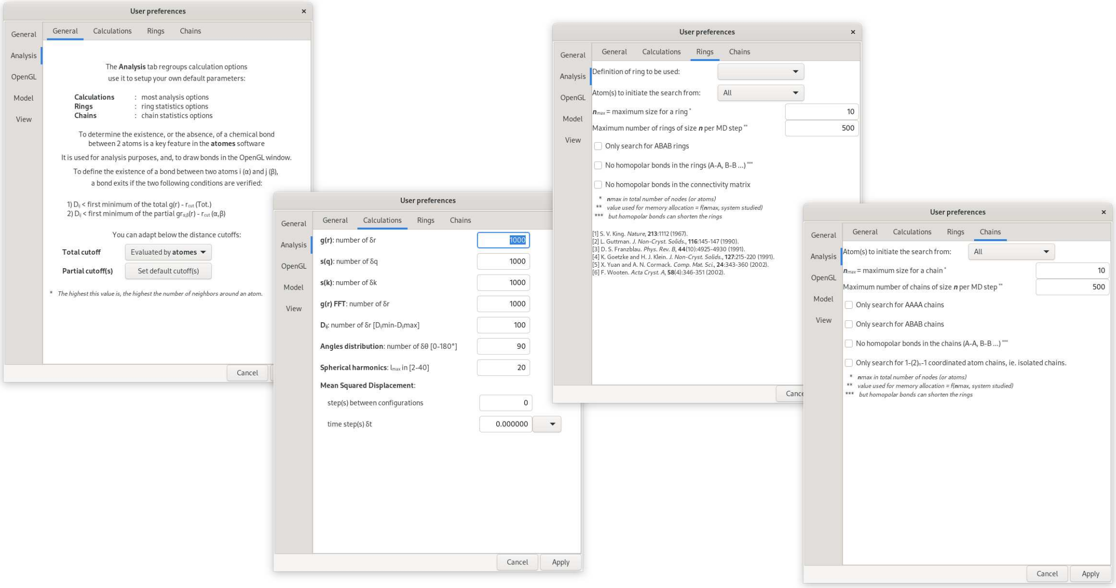
If found this file is processed at every **atomes** startup.

Save file ?

Figure 3.9 *The "`User preferences`" dialog in the* **atomes** *program.*

When clicking on "`Apply`", and after confirmation, the options defined in the "`User preferences`" dialog are applied to the active session of **atomes**. Afterwards options can be stored in a XML file named "`atomes.pml`" (which exact location depends on your operating system), if found this file will be process at every **atomes** startup to ensure for user selected options to be used. Optionaly if projects are opened in **atomes** workspace it is possible to apply selected options to any of these projects.
Note that you can restore **atomes** default internal parameters at any time from the "`General`" tab.

3.4.1 Analysis options



The **Analysis** tab regroups calculation options
use it to setup your own default parameters:

Calculations : most analysis options
Rings : ring statistics options
Chains : chain statistics options

To determine the existence, or the absence, of a chemical bond between 2 atoms is a key feature in the **atomes** software

It is used for analysis purposes, and, to draw bonds in the OpenGL window.

To define the existence of a bond between two atoms i (α) and j (β), a bond exits if the two following conditions are verified:

1) D_{ij} < first minimum of the total g(r) - r_{cut} (Tot.)
2) D_{ij} < first minimum of the partial $gr_{\alpha,\beta}(r)$ - r_{cut} (α,β)

You can adapt below the distance cutoffs:

Total cutoff: Evaluated by **atomes**
Partial cutoff(s): Set default cutoff(s)

* *The highest this value is, the highest the number of neighbors around an atom.*

g(r): number of δr: 1000
s(q): number of δq: 1000
s(k): number of δk: 1000
g(r) FFT: number of δr: 1000
D_{ij}: number of δr [D_{ij}min-D_{ij}max]: 100
Angles distribution: number of δθ [0-180°]: 90
Spherical harmonics: l_{max} in [2-40]: 20
Mean Squared Displacement:
step(s) between configurations: 0
time step(s) δt: 0.000000

Definition of ring to be used:
Atom(s) to initiate the search from: All
n_{max} = maximum size for a ring *: 10
Maximum number of rings of size *n* per MD step **: 500
☐ Only search for ABAB rings
☐ No homopolar bonds in the rings (A-A, B-B ...) ***
☐ No homopolar bonds in the connectivity matrix

* *nmax in total number of nodes (or atoms)*
** *value used for memory allocation = f(nmax, system studied)*
*** *but homopolar bonds can shorten the rings*

[1] S. V. King. *Nature*, **213**:1112 (1967).
[2] L. Guttman. *J. Non-Cryst. Solids.*, **116**:145-147 (1990).
[3] D. S. Franzblau. *Phys. Rev. B*, **44**(10):4925-4930 (1991).
[4] K. Goetzke and H. J. Klein. *J. Non-Cryst. Solids.*, **127**:215-220 (1991).
[5] X. Yuan and A. N. Cormack. *Comp. Mat. Sci.*, **24**:343-360 (2002).
[6] F. Wooten. *Acta Cryst. A*, **58**(4):346-351 (2002).

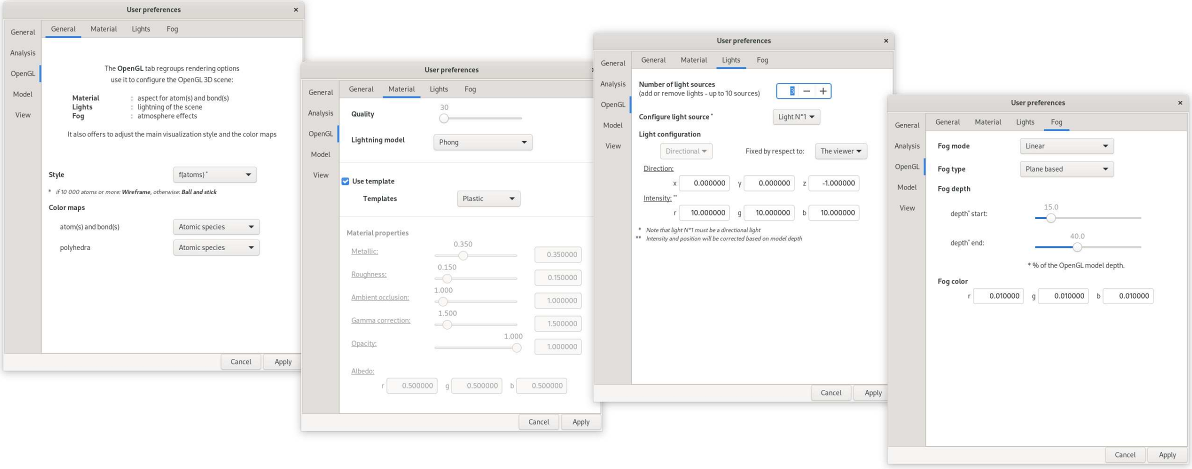
Atom(s) to initiate the search from: All
n_{max} = maximum size for a chain *: 10
Maximum number of chains of size *n* per MD step **: 500
☐ Only search for AAAA chains
☐ Only search for ABAB chains
☐ No homopolar bonds in the chains (A-A, B-B ...) ***
☐ Only search for 1-$(2)_n$-1 coordinated atom chains, ie. isolated chains.

* *nmax in total number of nodes (or atoms)*
** *value used for memory allocation = f(nmax, system studied)*
*** *but homopolar bonds can shorten the rings*

Figure 3.10 *The "*`Analysis preferences`*" dialog in the* **atomes** *program.*

Analysis options tabs 3.10 cover physico-chemical analysis parameters required to perform the corresponding calculations. The "`General`" page offers to specify how first neighbor atoms are determined in the **atomes** software.

3.4.2 OpenGL rendering options



The **OpenGL** tab regroups rendering options
use it to configure the OpenGL 3D scene:

Material : aspect for atom(s) and bond(s)
Lights : lightning of the scene
Fog : atmosphere effects

It also offers to adjust the main visualization style and the color maps

Style: f(atoms) *

* *if 10 000 atoms or more:* ***Wireframe****, otherwise:* ***Ball and stick***

Color maps
atom(s) and bond(s): Atomic species
polyhedra: Atomic species

Quality: 30
Lightning model: Phong
☑ **Use template**
Templates: Plastic

Material properties
Metallic: 0.350 0.350000
Roughness: 0.150 0.150000
Ambient occlusion: 1.000 1.000000
Gamma correction: 1.500 1.500000
Opacity: 1.000 1.000000
Albedo: r 0.500000 g 0.500000 b 0.500000

Number of light sources
(add or remove lights - up to 10 sources): 3
Configure light source *: Light N°1
Light configuration
Directional   Fixed by respect to: The viewer
Direction: x 0.000000 y 0.000000 z -1.000000
Intensity: ** r 10.000000 g 10.000000 b 10.000000

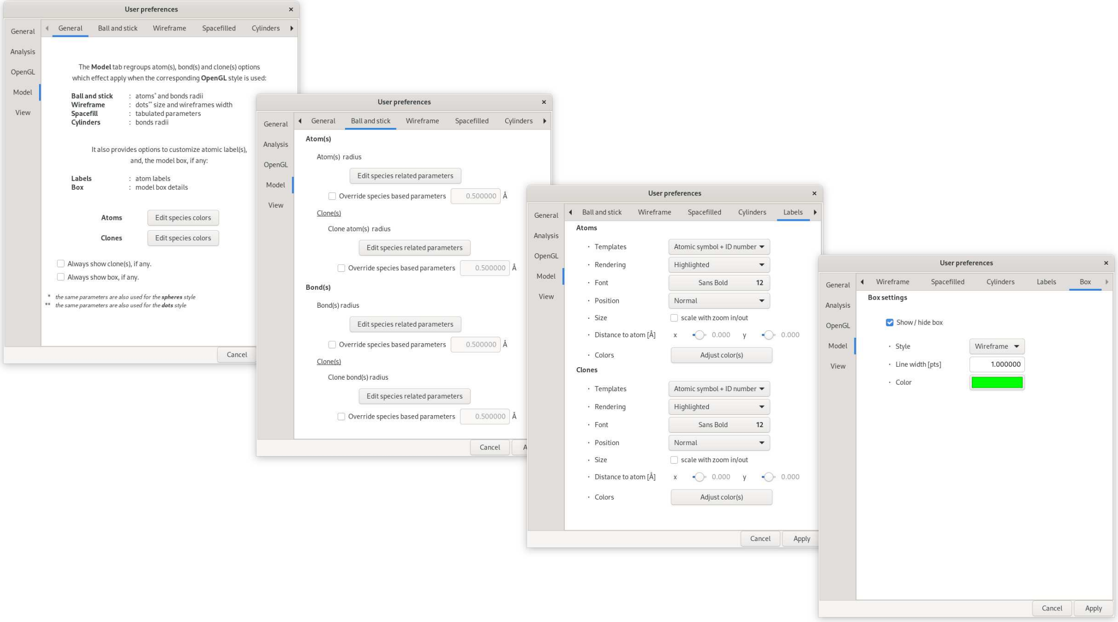
* *Note that light N°1 must be a directional light*
** *Intensity and position will be corrected based on model depth*

Fog mode: Linear
Fog type: Plane based
Fog depth
depth* start: 15.0
depth* end: 40.0
* % of the OpenGL model depth.
Fog color: r 0.010000 g 0.010000 b 0.010000

Figure 3.11 *The "*`OpenGL preferences`*" dialog in the* **atomes** *program.*

Rendering can be entirely configured using this tab, including style and colormpas, material aspect, lights and fog options that can be adjusted to user preferences.

3.4.3 Model options



The **Model** tab regroups atom(s), bond(s) and clone(s) options which effect apply when the corresponding **OpenGL** style is used:

Ball and stick : atoms* and bonds radii
Wireframe : dots** size and wireframes width
Spacefill : tabulated parameters
Cylinders : bonds radii

It also provides options to customize atomic label(s), and, the model box, if any:

Labels : atom labels
Box : model box details

Atoms Edit species colors
Clones Edit species colors

☐ Always show clone(s), if any.
☐ Always show box, if any.

* *the same parameters are also used for the **spheres** style*
** *the same parameters are also used for the **dots** style*

Atom(s)
Atom(s) radius
Edit species related parameters
☐ Override species based parameters 0.500000 Å
Clone(s)
Clone atom(s) radius
Edit species related parameters
☐ Override species based parameters 0.500000 Å
Bond(s)
Bond(s) radius
Edit species related parameters
☐ Override species based parameters 0.500000 Å
Clone(s)
Clone bond(s) radius
Edit species related parameters
☐ Override species based parameters 0.500000 Å

Atoms
- Templates: Atomic symbol + ID number
- Rendering: Highlighted
- Font: Sans Bold 12
- Position: Normal
- Size: ☐ scale with zoom in/out
- Distance to atom [Å]: x 0.000 y 0.000
- Colors: Adjust color(s)

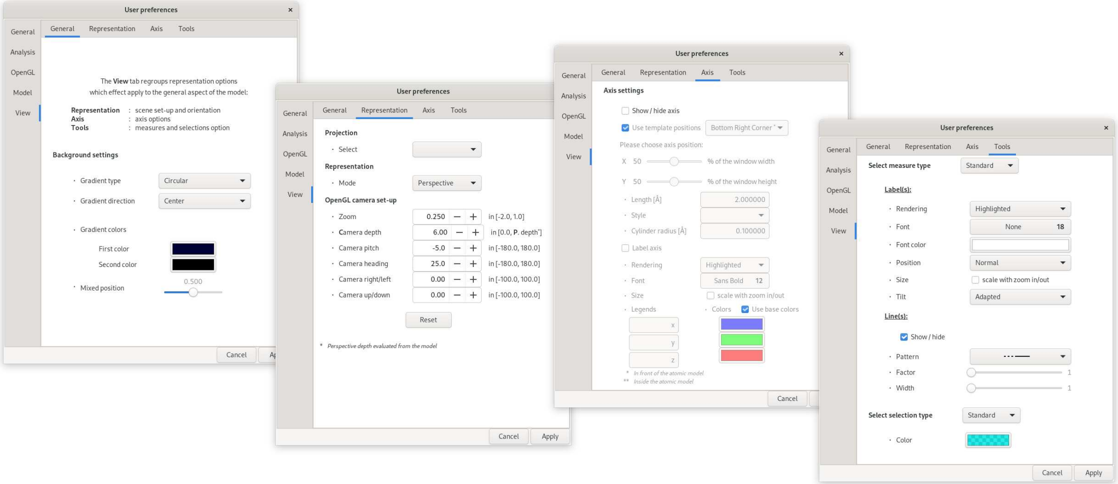
Clones
- Templates: Atomic symbol + ID number
- Rendering: Highlighted
- Font: Sans Bold 12
- Position: Normal
- Size: ☐ scale with zoom in/out
- Distance to atom [Å]: x 0.000 y 0.000
- Colors: Adjust color(s)

Box settings
☑ Show / hide box
- Style: Wireframe
- Line width [pts]: 1.000000
- Color: 🟩

Figure 3.12 *The "`Model preferences`" dialog in the* **atomes** *program.*

This tab allows to configure model style from atomic species color to atom and bond radii for any rendering style available in the **atomes** software. Atom and clone labels as well as model box layout can also be configured.

3.4.4 Representation options



The **View** tab regroups representation options which effect apply to the general aspect of the model:

Representation : scene set-up and orientation
Axis : axis options
Tools : measures and selections option

Background settings
- Gradient type: Circular
- Gradient direction: Center
- Gradient colors
  - First color
  - Second color
- Mixed position: 0.500

Projection
- Select

Representation
- Mode: Perspective

OpenGL camera set-up
- Zoom: 0.250 in [-2.0, 1.0]
- Camera depth: 6.00 in [0.0, P. depth*]
- Camera pitch: -5.0 in [-180.0, 180.0]
- Camera heading: 25.0 in [-180.0, 180.0]
- Camera right/left: 0.00 in [-100.0, 100.0]
- Camera up/down: 0.00 in [-100.0, 100.0]

* *Perspective depth evaluated from the model*

Axis settings
☐ Show / hide axis
☑ Use template positions: Bottom Right Corner *
Please choose axis position:
X 50 % of the window width
Y 50 % of the window height
- Length [Å]: 2.000000
- Style
- Cylinder radius [Å]: 0.100000

☐ Label axis
- Rendering: Highlighted
- Font: Sans Bold 12
- Size: ☐ scale with zoom in/out
- Legends: x, y, z
- Colors: ☑ Use base colors

* *In front of the atomic model*
** *Inside the atomic model*

Select measure type: Standard

Label(s):
- Rendering: Highlighted
- Font: None 18
- Font color
- Position: Normal
- Size: ☐ scale with zoom in/out
- Tilt: Adapted

Line(s):
☑ Show / hide
- Pattern
- Factor: 1
- Width: 1

Select selection type: Standard
- Color

Figure 3.13 *The "`View preferences`" dialog in the* **atomes** *program.*

This tab offers configuration options to defined default background, representation, axis layout and measurement information layout.

3.5 Analyzing models using atomes

atomes can compute the following structural characteristics of a 3D structure model:

- Radial distribution functions g(r) (RDFs) [10] including °:
  - Total RDFs for neutrons and X-rays.
  - Partial RDFs.
  - Bhatia-Thornton RDFs [11]

  ° Radial distribution functions can be computed by i) direct real space calculation and/or ii) Fourier transforming of the structure factor calculated using the Debye formalism [12]

- Structure factors S(q) [12] including °°:
  - Total structure factors S(q) for neutrons and X-rays.
  - Total Q(q) [12, 13] for neutrons and X-rays.
  - Partial S(q):
    - Faber-Ziman [14] partial S(q)
    - Ashcroft-Langreth [15, 16, 17] partial S(q)
    - Bhatia-Thornton [18] partial S(q)

  °° Structure factors can be computed by i) Fourier transforming of the radial distribution functions and/or ii) using the Debye formalism [12]

- Interatomic bond properties
  - Coordination numbers
  - Atomic near neighbor distribution
  - Fraction of links between tetrahedra
  - Fraction of tetrahedral units
  - Bond lengths distribution for the first coordination sphere
- Distribution of Bond angles
- Distribution of Dihedral angles
- Ring statistics, according to several definitions:
  - All closed paths (no rules)
  - King's rings [19, 20]
  - Guttman's rings [21]
  - Primitive rings [22, 23] (or Irreducible [24])
  - Strong rings [22, 23]

  And including options to:
  - search only for ABAB rings
  - exclude rings with homopolar bonds (A-A or B-B) from the analysis

Ring statistics is presented according to the R.I.N.G.S. method [25].

- Chain statistics, including options to:
    - search only for AAAA chains
    - search only for ABAB chains
    - exclude chains with homopolar bonds (A-A or B-B) from the analysis
    - search only for 1-$(2)_n$-1 chains
- Spherical harmonics invariant, Q_l, as local atomic ordering symmetry identifiers [26]
    - Average Q_l for each chemical species
    - Average Q_l for a user specified structural unit
- Mean Square Displacement of atoms (MSD)
    - Atomic species MSD
    - Directional MSD (x, y, z, xy, xz, yz)
    - Drift of the center of mass

See appendix E to learn more about the physics and the chemistry behind these calculations.

The calculations presented in this list can only be performed on the **active** project, ie. the project which name appears in the title bar of the **atomes** program main window, in bold font in the **atomes** workspace tree and in green bold font in the workspace information dialog [Fig. 1.1].
For more about running calculation using **atomes** see chapter 4.

3.6 Visual analysis using atomes

Each model in the **atomes** workspace is assigned an OpenGL window that provides an interactive experience to visualize and analyze its properties. Isolated configurations as well as entire molecular dynamics trajectories can be visualized.
Among the possibilities of the OpenGL window:

- Advanced color map options, for both atoms and polyhedra.
- Advanced coordination(s) visualization options (total, partial, fragments, molecules).
- Advanced coordination polyhedra visualization options.
- Measurement tools.
- Advanced layout system for atomic labels, measurements, MD box and model axis.
- Image and movie rendering, including an intuitive interface to movie encoding that allows to record every interaction/modification made to the OpenGL window.
- Advanced OpenGL configuration options.

For a complete description of these features see chapter 5.

3.7 Visual edition and model creation using atomes

Using **atomes** "`Crystal builder`" it is possible to build crystalline structures or even super-structures. Also if the model description contains a box, then cell edition options become available:

- Wrap atoms in original cell
- Shift cell center
- Add extra cell(s)
- Create super cell
- Change the model density
- Cut slabs or extract atoms from the model.

And if the model contains only a single configuration (and not a molecular dynamics trajectory), or when an empty project is created, the atom(s) edition options/mode become available:

- Motion (random or selected atom(s))
- Replacement (random or selected atom(s))
- Removal (random or selected atom(s))
- Insertion

For a complete description of these features see chapter 6.

3.8 Preparing MD calculations in atomes

atomes provides input creation assistants for well known molecular dynamics codes:

- CPMD [3]
- CP2K [4]
- DL-POLY [1]
- LAMMPS [2]

For a complete description of these features see chapter 7.

Physico-chemical analysis in atomes

In this chapter examples will be illustrated using an **atomes** workspace presented in figure 4.1, this workspace contains 3 different projects, liquid GeSe systems with a similar chemistry yet obtained using a different set of DFT-GGA functionals. [27]

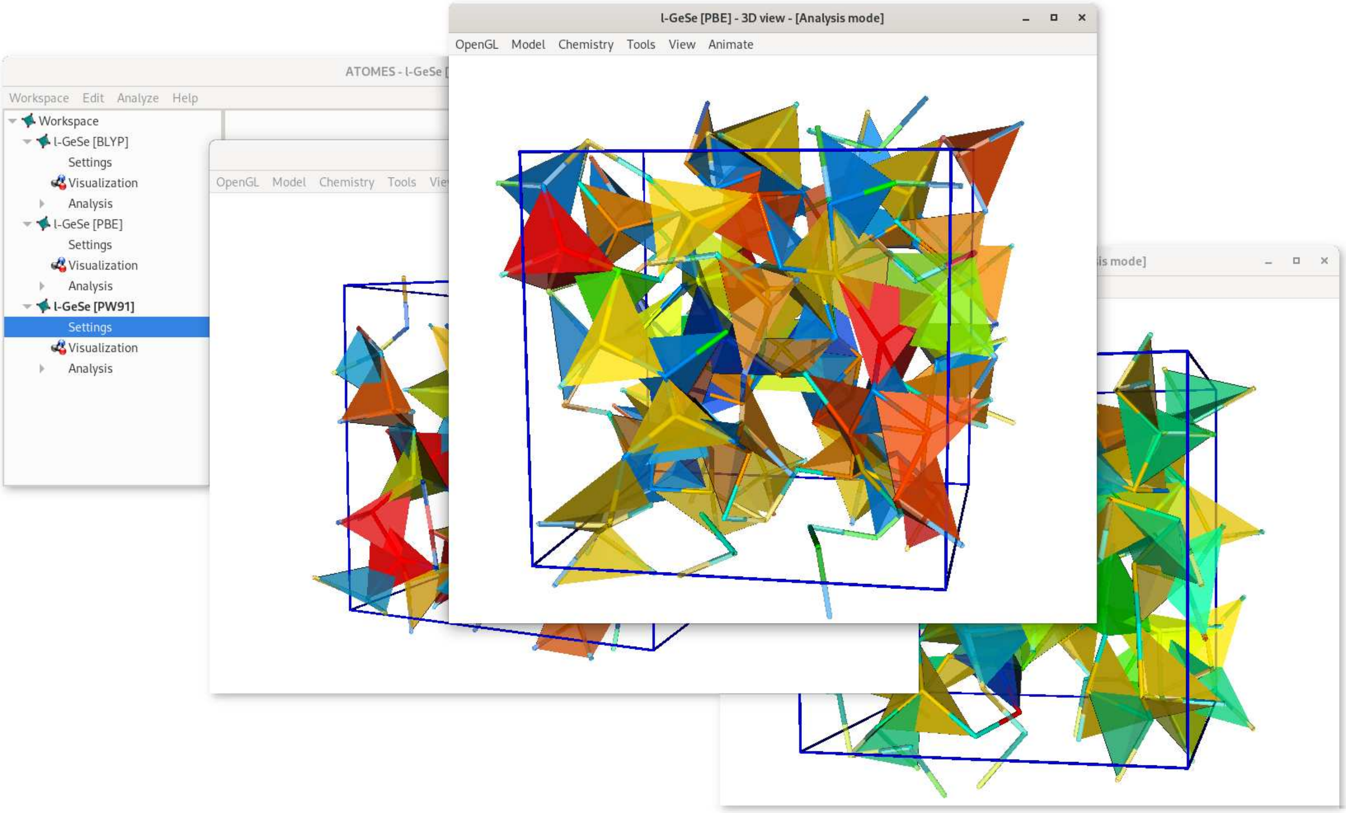


Figure 4.1 *Example workspace to illustrate the analysis capabilities of the* **atomes** *programs containing 3 projects, named "*`l-GeSe [BLYP]`*", "*`l-GeSe [PBE]`*" and "*`l-GeSe [PW91]`*".*

When a project is opened in the **atomes** workspace, and if this project is the **active** project, then it it possible to compute the properties presented in section 3.5, and the

parameter(s) of the calculation(s) can be adjusted via the associated dialog boxes accessible by using the "`Analyze`" menu [Fig. 3.1-d].
Some of the calculations of the "`Analyze menu`" are immediately available when a project is opened, other require some condition(s) to be full-filled before being accessible:

1. g(r)/G(r): requires a model box to be described.
2. S(q) from FFT[g(r)]: requires 1 to be completed.
3. S(q) from Debye equation: requires a model box to be described.
4. g(r)/G(r) from FFT[S(q)]: requires 3 to be completed.
5. Bonds and angles: no conditions.
6. Ring statistics: no conditions.
7. Chain statistics: no conditions.
8. Spherical harmonics: requires 5 to be completed.
9. Mean Squared Displacement: requires the project have more than 1 configuration (MD trajectory).

4.1 Visualisation of the results of the calculations

When a particular structural characteristic is computed results can be directly displayed in the main **atomes** windows [Fig. 3.1-a]. In addition the visualization mode of most of the computed characteristics can be controlled the "`Toolboxes`" dialog:

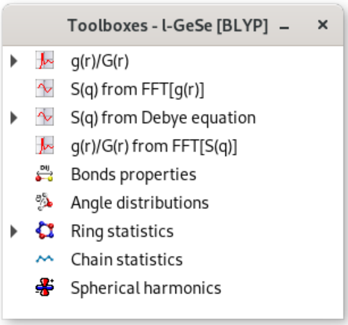


Figure 4.2 *The "`Toolboxes`" dialog in the* **atomes** *program.*

The "`Toolboxes`" dialog contains a tree that becomes browsable for a particular calculation when that calculation is completed successfully.
If closed the "`Toolboxes`" dialog can be opened alternatively using:

- The last button of the "`Analyze menu`" called "`Toolboxes`" [Fig. 3.1-d].

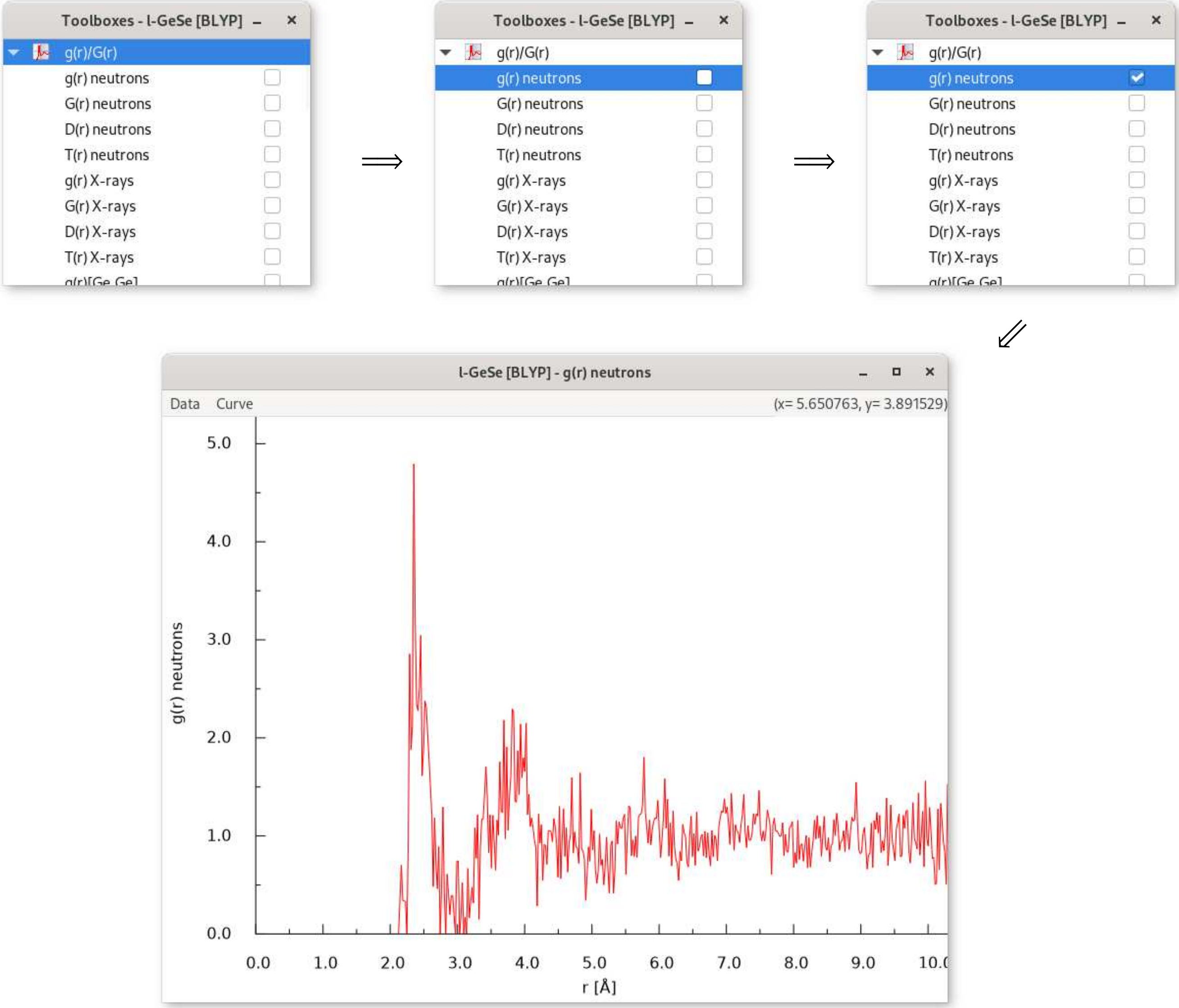


Figure 4.3 *Interaction with the "`Toolboxes`" dialog in the* **atomes** *program.*

- The Ctrl + t keyboard shortcut over the main window of the **atomes** program.

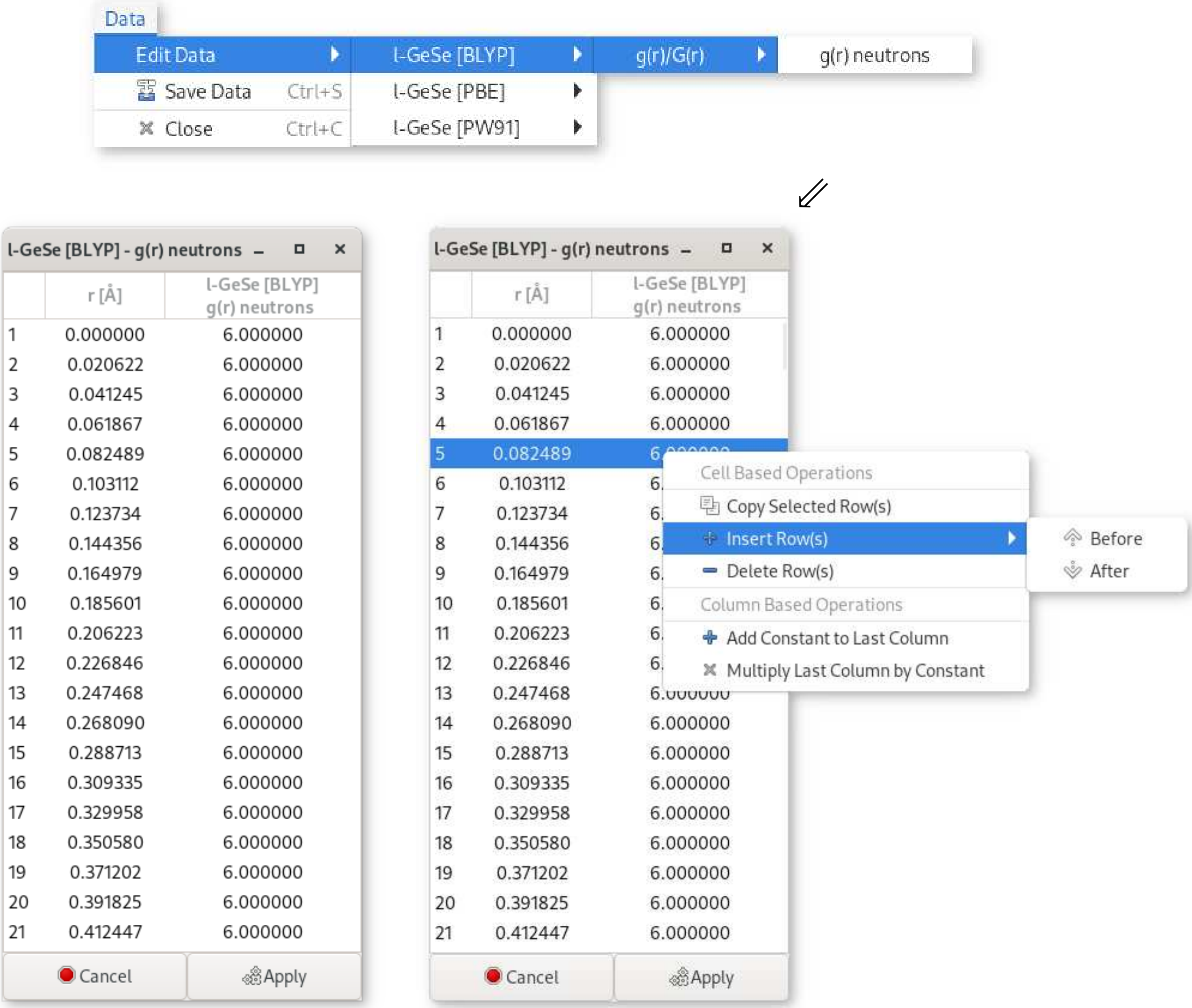
When a button in an interaction menu is activated [Fig. 4.3] the corresponding result is instantaneously displayed as a curve or a histogram [Fig. 4.3] depending on the nature of the computed structural characteristic, in figure 4.2 the g(r) for the project "`l-GeSe [PW91]`" for the example workspace in figure 4.1.

4.2 Data and plot edition

atomes offers editing tools which allows to edit/save/export the data from the calculations, and configure the layout of the graphs showing result of the calculations. These tools are available from both the contextual menu [Fig. 4.8] and the top menu of any graph window [Fig. 4.3].

4.2.1 Data edition

As illustrated in figure 4.4 it is possible to edit any of the data set presented in the graph window in a spreadsheet like environment (including a contextual menu accessible using the right button of the mouse).



	r [Å]	l-GeSe [BLYP] g(r) neutrons
1	0.000000	6.000000
2	0.020622	6.000000
3	0.041245	6.000000
4	0.061867	6.000000
5	0.082489	6.000000
6	0.103112	6.000000
7	0.123734	6.000000
8	0.144356	6.000000
9	0.164979	6.000000
10	0.185601	6.000000
11	0.206223	6.000000
12	0.226846	6.000000
13	0.247468	6.000000
14	0.268090	6.000000
15	0.288713	6.000000
16	0.309335	6.000000
17	0.329958	6.000000
18	0.350580	6.000000
19	0.371202	6.000000
20	0.391825	6.000000
21	0.412447	6.000000

	r [Å]	l-GeSe [BLYP] g(r) neutrons
1	0.000000	6.000000
2	0.020622	6.000000
3	0.041245	6.000000
4	0.061867	6.000000
5	0.082489	6.000000
6	0.103112	6.
7	0.123734	6.
8	0.144356	6.
9	0.164979	6.
10	0.185601	6.
11	0.206223	6.
12	0.226846	6.
13	0.247468	6.000000
14	0.268090	6.000000
15	0.288713	6.000000
16	0.309335	6.000000
17	0.329958	6.000000
18	0.350580	6.000000
19	0.371202	6.000000
20	0.391825	6.000000
21	0.412447	6.000000

Figure 4.4 *Top: The "`Data`" and the "`Edit Data`" menus in the top menu of the graph window. Bottom: the "`Data Edition`" window and the associated contextual menu.*

4.2.2 Plot edition

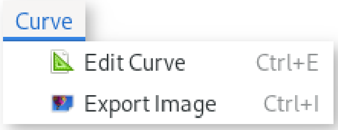
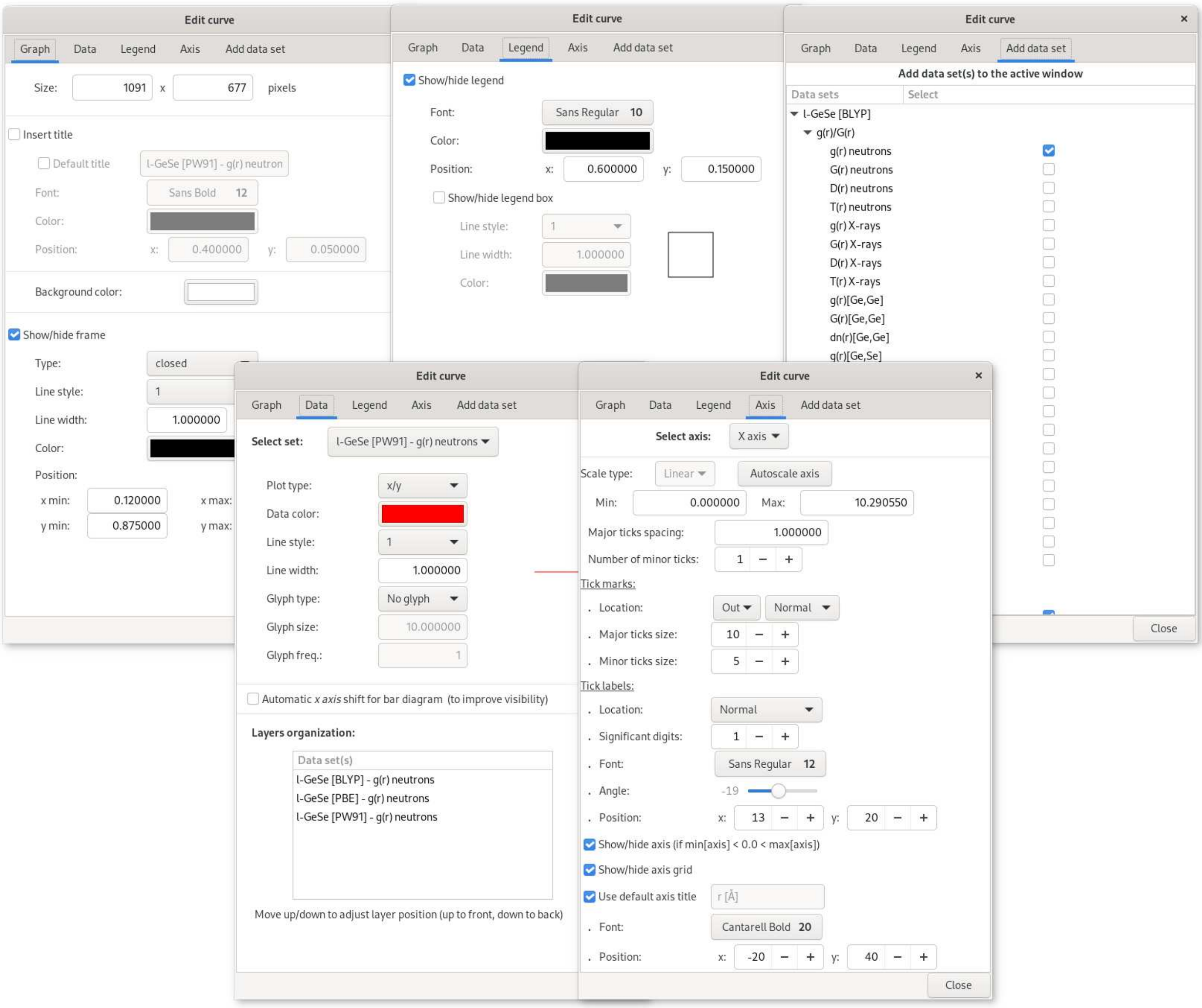


Figure 4.5 *The "`Curve`" menu, and the corresponding buttons in the contextual menu of the graph window in the* **atomes** *program.*

Using the data plot editing tool [Fig. 4.6] it is possible to configure the layout of the selected graph, as well as the layout each data set which happen to be plotted on the graph, it is also possible to configure X and Y axis layout and/or position.



Size: 1091 x 677 pixels
☐ Insert title
☐ Default title l-GeSe [PW91] - g(r) neutron
Font: Sans Bold 12
Color:
Position: x: 0.400000 y: 0.050000
Background color:
☑ Show/hide frame
Type: closed
Line style: 1
Line width: 1.000000
Color:
Position:
x min: 0.120000 x max:
y min: 0.875000 y max:

☑ Show/hide legend
Font: Sans Regular 10
Color:
Position: x: 0.600000 y: 0.150000
☐ Show/hide legend box
Line style: 1
Line width: 1.000000
Color:

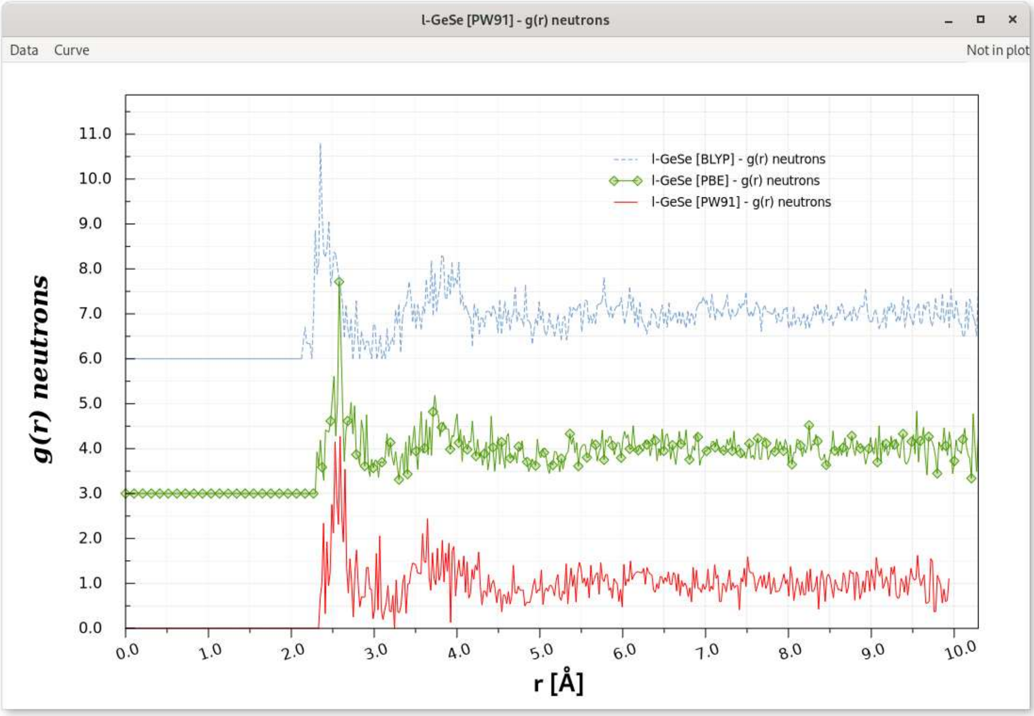
Add data set(s) to the active window
Data sets Select
l-GeSe [BLYP]
g(r)/G(r)
g(r) neutrons ☑
G(r) neutrons ☐
D(r) neutrons ☐
T(r) neutrons ☐
g(r) X-rays ☐
G(r) X-rays ☐
D(r) X-rays ☐
T(r) X-rays ☐
g(r)[Ge,Ge] ☐
G(r)[Ge,Ge] ☐
dn(r)[Ge,Ge] ☐
g(r)[Ge,Se] ☐

Select set: l-GeSe [PW91] - g(r) neutrons
Plot type: x/y
Data color:
Line style: 1
Line width: 1.000000
Glyph type: No glyph
Glyph size: 10.000000
Glyph freq.: 1
☐ Automatic *x axis* shift for bar diagram (to improve visibility)
Layers organization:
Data set(s)
l-GeSe [BLYP] - g(r) neutrons
l-GeSe [PBE] - g(r) neutrons
l-GeSe [PW91] - g(r) neutrons
Move up/down to adjust layer position (up to front, down to back)

Select axis: X axis
Scale type: Linear Autoscale axis
Min: 0.000000 Max: 10.290550
Major ticks spacing: 1.000000
Number of minor ticks: 1
Tick marks:
. Location: Out Normal
. Major ticks size: 10
. Minor ticks size: 5
Tick labels:
. Location: Normal
. Significant digits: 1
. Font: Sans Regular 12
. Angle: -19
. Position: x: 13 y: 20
☑ Show/hide axis (if min[axis] < 0.0 < max[axis])
☑ Show/hide axis grid
☑ Use default axis title r [Å]
. Font: Cantarell Bold 20
. Position: x: -20 y: 40

Figure 4.6 *The data plot editing tool box in the* **atomes** *program.*

Furthermore depending on the calculation several data sets can be selected and plotted together with the main data set of the active window. Data plot edition in the **atomes** program is illustrated with the example in figure 4.7.



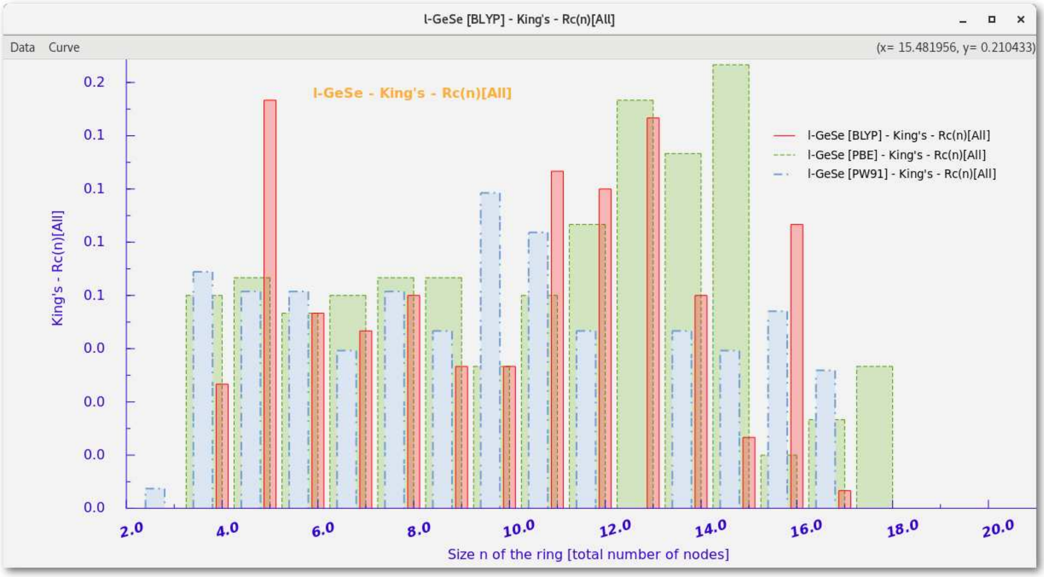


Figure 4.7 *Examples of data plot edition in the* **atomes** *program.*

4.3 Mouse interaction with the data plot

4.3.1 Right button contextual menu

To use the right button of the mouse over the graph window allows to open a contextual menu [Fig. 4.8].

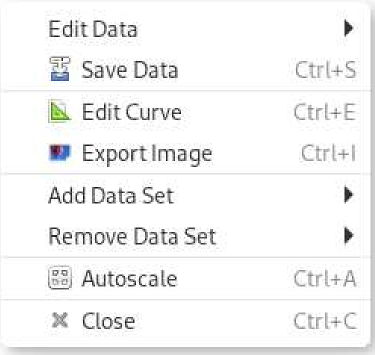


Figure 4.8 *Mouse contextual menu over the graph window in the* **atomes** *program.*

This menu allows the following actions:

1. Edit Data : essentially reproduces the "`Edit data`" submenu from the graph window's top menu [Fig. 4.9-a].
2. Save Data (see section 4.2)
3. Edit Curve (see section 4.2)
4. Export Image (see section 4.2)
5. Add Data Set: allows to add data set(s) to the graph window, this extra data set from a similar kind of calculation can come either from the same project or any other project opened in the workspace. The submenu list of available data set(s) compatible with the present graph/calculation in the workspace and offers shortcuts to insert each of them in the graph [Fig. 4.9-b].
6. Remove Data Set: allows to remove data set(s) from the graph window. Only data sets that were actually added to the graph window can be removed and not the initial data set of the graph window (in this example case the "`g(r) neutrons`" for "`l-GeSe [PW91]`" project [Fig 4.9-c].
7. Autoscale: offers to autoscale the x and y axis for the entire set(s) of data presented in the graph window.
8. Close: closes the graph window.

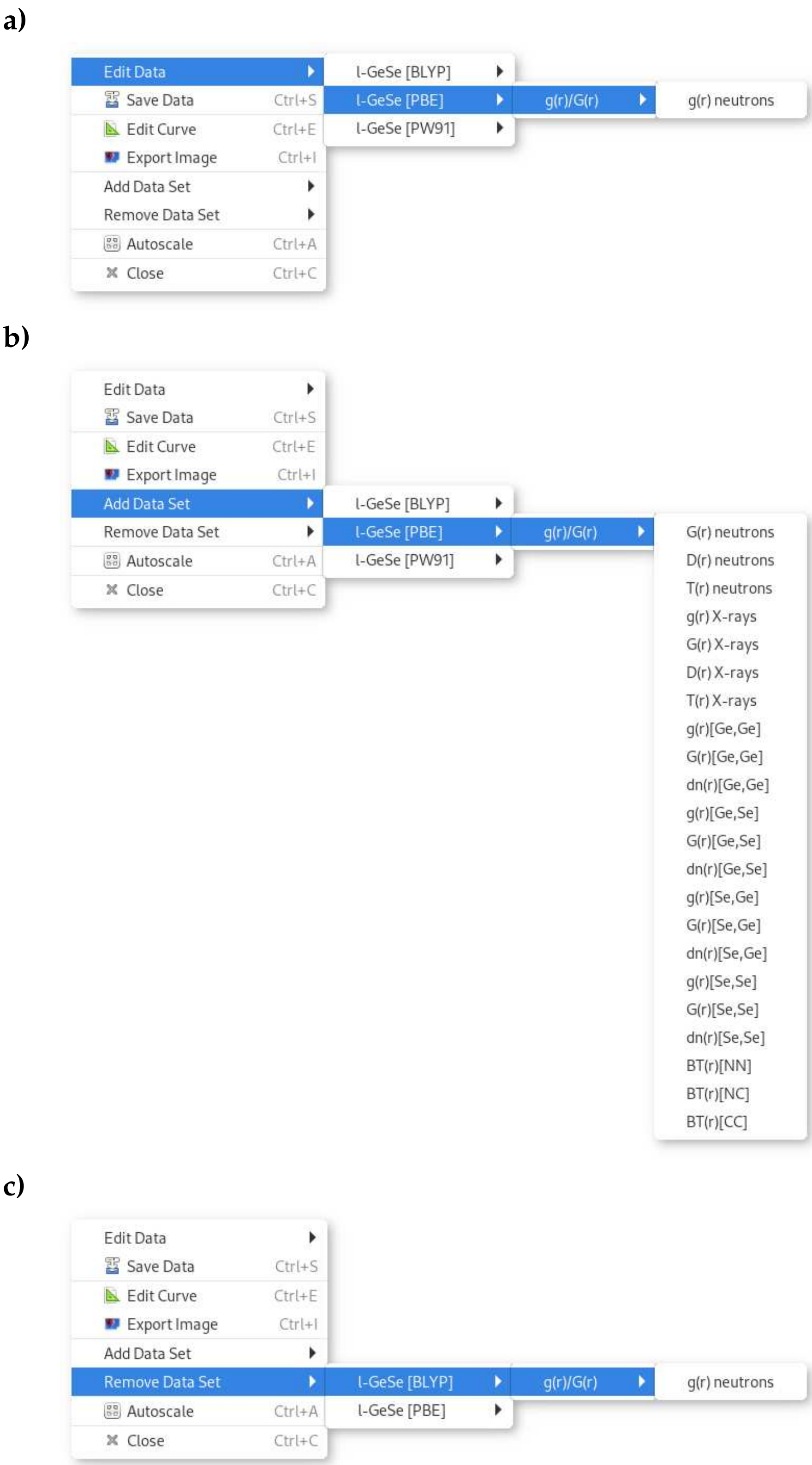


Figure 4.9 *The "`Edit Data`" a), "`Add Data Set`" b) and "`Remove Data Set`" c) sub-menus in the graph window contextual menu for the example workspace [Fig. 4.1].*

4.3.2 Left button zoom in and out

Using the mouse over the graph window it is possible to zoom in and out, by pressing the left button and then and move up/down/left/right while keeping the button pressed. Then a rectangle will be drawn over the window [Fig. 4.10], starting at the point where the button was first pressed, and ending at the point the mouse is hanging over. The effect of the zoom action will be specified by a text inscription at the origin point of the rectangle, and by the color of the rectangle:

- Zoom in(x) and in(y): direction from bottom left to top right, and red color.
- Zoom in(x) and out(y): direction from top left to bottom right, and violet color.
- Zoom out(x) and in(y): direction from bottom right to top left, and blue color.
- Zoom out(x) and out(y): direction from top right to bottom left, and green color.

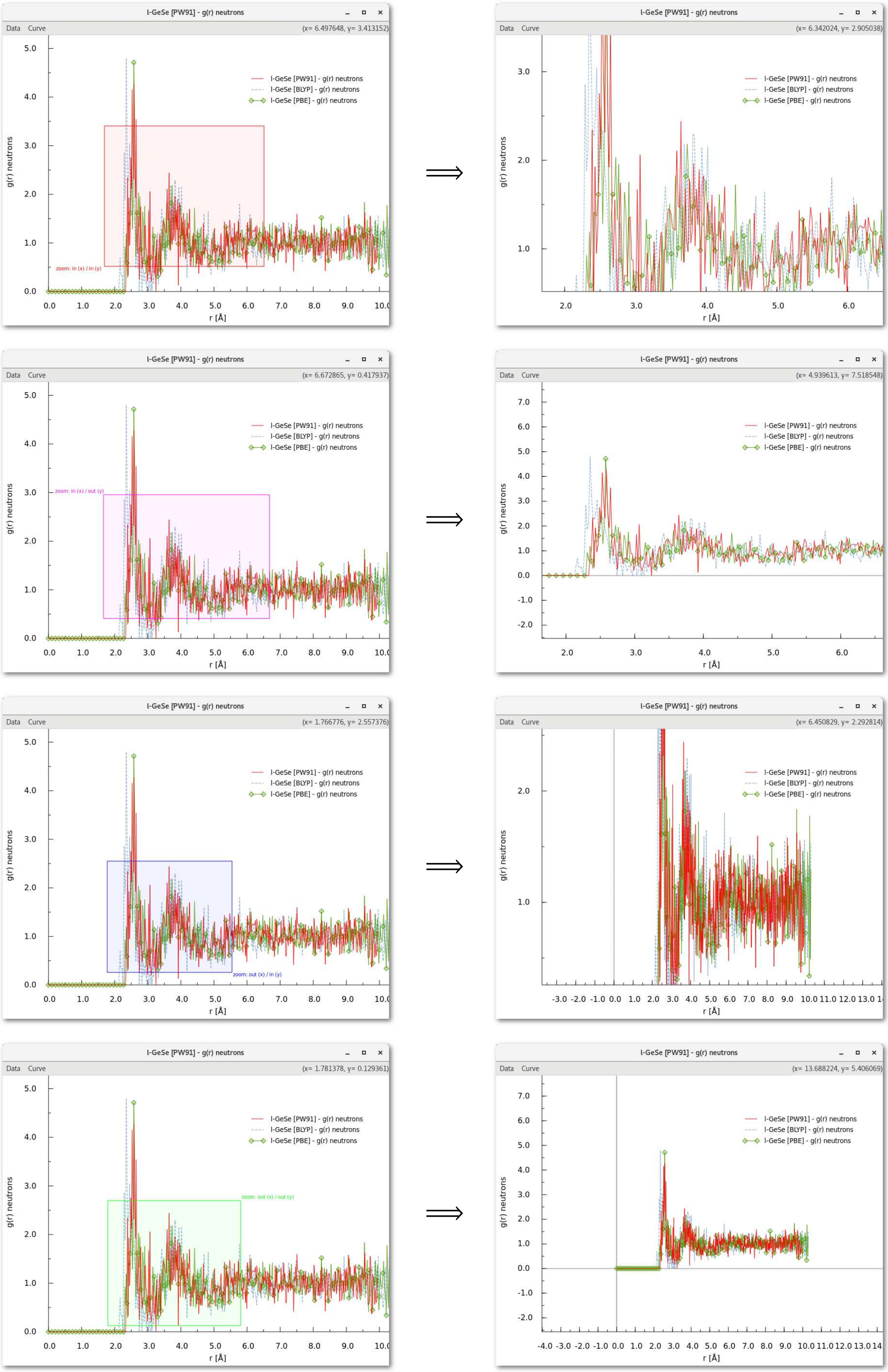


Figure 4.10 *The mouse left button zoom in/out of the graph window in the* **atomes** *program.*

4.4 Saving the data

Results computed by **atomes** can be easily saved using the standard copy and paste method (for the results presented in the edition window [Fig. 4.4] or in the main **atomes** window [Fig. 3.1]) or using the "`Data menu`" [Fig. 4.4]. It is possible to export data either in a raw ASCII format (simple two columns file with x and y) or in the Xmgrace format which can be used immediately in the Grace WYSIWYG 2D plotting tool [28] for further analysis.

Note that if more than one data sets are presented on the same graph window, then all data sets will be written in the same file when saving the data. Thus, for a particular calculation, if all data sets are added to the graph window using the data plot editing tool [Fig. 4.6], then all the data result of this analysis can be saved at once. This is true for both ASCII and Xmgrace file formats.

4.5 Keyboard shortcuts

- Combined keys shortcuts:

  Ctrl + a : Autoscale

  Ctrl + c : Close curve window

  Ctrl + e : Open the data plot editing tool box [Fig. 4.6]

  Ctrl + i : Export image

  Ctrl + s : Save / export data

Visual analysis in atomes

In this chapter examples will be illustrated using an **atomes** workspace presented in figure 5.1, this workspace contains 3 different projects:

- a molecular surface of Nickel-Phthalocyanine molecules with 512 atoms.
- a SiO_2 glass with 3000 atoms.
- a GeS_2 glass molecular dynamics trajectory with 500 MD steps and 258 atoms.

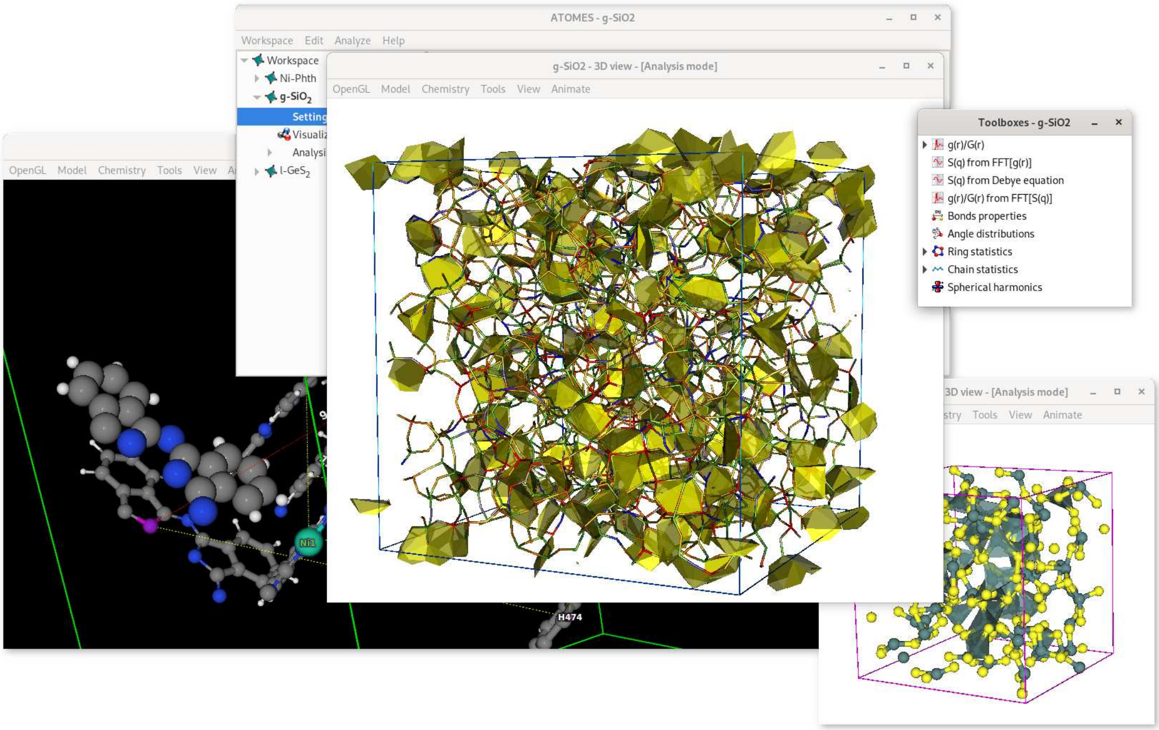


Figure 5.1 *Example workspace to illustrate the visualization capabilities of the* **atomes** *program containing 3 projects, named "*`Ni-Phth`*", "*`g-SiO`$_2$*" and "*`l-GeS`$_2$*".*

5.1 Window top bar menu

In order to present the functionalities available in the OpenGL window, we will browse the top bar menu [Fig. 5.1] and present each submenu one after the other.

5.1.1 The "`OpenGL`" menu

Figure 5.2 *The "`OpenGL`" menu and the attached submenus.*

The "`OpenGL`" menu is detailed in figure 5.2. The behavior of the "`Render`" menu [Fig. 5.2-c], and the "`Quality`" menu [Fig. 5.2-d], as well as of the "`Render image`" button being pretty intuitive the following only detail the behavior of the "`Style menu`", the "`Color scheme(s)`" menu [Fig. 5.2-b], and the "`Material and lights`" button.

5.1.1.1 The "`Style`" menu

Using the "`Style`" menu it is possible to define to **default style** of the model representation, the options are among the most commonly used in chemistry. Changing the **default style** from this menu will update several parts of the OpenGL window and associated menus. For instance selecting the "`Ball and stick`" option will update the first tab of "`Atom(s) configuration`" dialog [Fig. 5.6] to display atomic radius and the "`Bond(s)`" menu [Fig. 5.5] to present the "`Radius(ii)`" and offer a shortcut to modify their values.
It is possible to define local style(s) to improve the visual representation, however this is only possible using the mouse, see section 5.2.2.1, and changing the **default style** of the model using the "`Style`" menu will reset/erase any local style(s) value(s) to the default.

5.1.1.2 The "`Color scheme(s)`" menu

In the **atomes** program when the file is opened most of the bonding properties are calculated "on-the-fly", allowing to gain insights on the atomic coordinations, as well as the number of fragments and the different molecules in the model.
Therefore before using the "`Color scheme(s)`" menu it is important to be familiar with the following definitions:

- **Total coordination** = total number of first neighbor atoms around the atom.
- **Partial coordination** = number of atoms of each chemical species around the atom.
- **Fragments** = isolated molecular objects in the model.
- **Molecules** = the different topological objects in the model.
- **Coordination polyhedra** = structure drawn by linking the atoms of the first coordination sphere for a particular atom. Requires the considered atom to have 3 neighbors, then the atom it-self is used as a point to build the polyhedra, or more.

The "`Color scheme(s)`" menu allows to change the Color Map (CM) for both atoms and coordination polyhedra, based on the bonding analysis performed using the bond cutoff(s) specified by the user. An illustration is provided in figure 5.3 for the "`Ni-Phth`" project of the example workspace, note that is this model the molecule on the top is missing a hydrogen atom compared to the one that composed the surface.
The colors of each objects can be modified/adapted via the appropriate menus/dialogs (see sections 5.1.2 and 5.1.3).

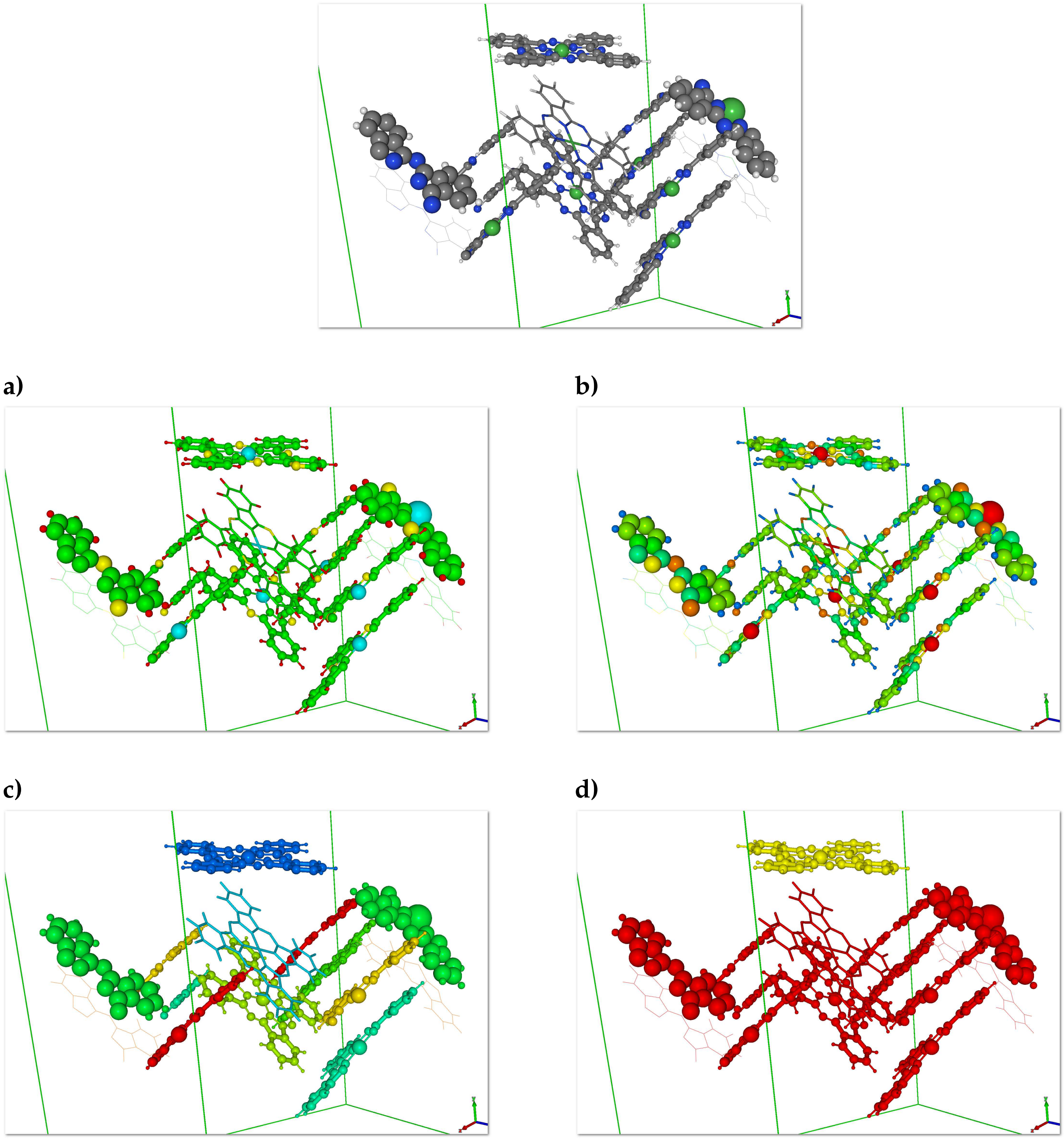


Figure 5.3 *The standard Colors Maps (CM) for the atoms accessible using the "*`Color scheme(s)`*" menu. Top standard colors using the chemical species,* **a)** *Total coordinations as CM,* **b)** *Partial coordinations as CM,* **c)** *Fragments as CM and* **d)** *Molecules as CM.*

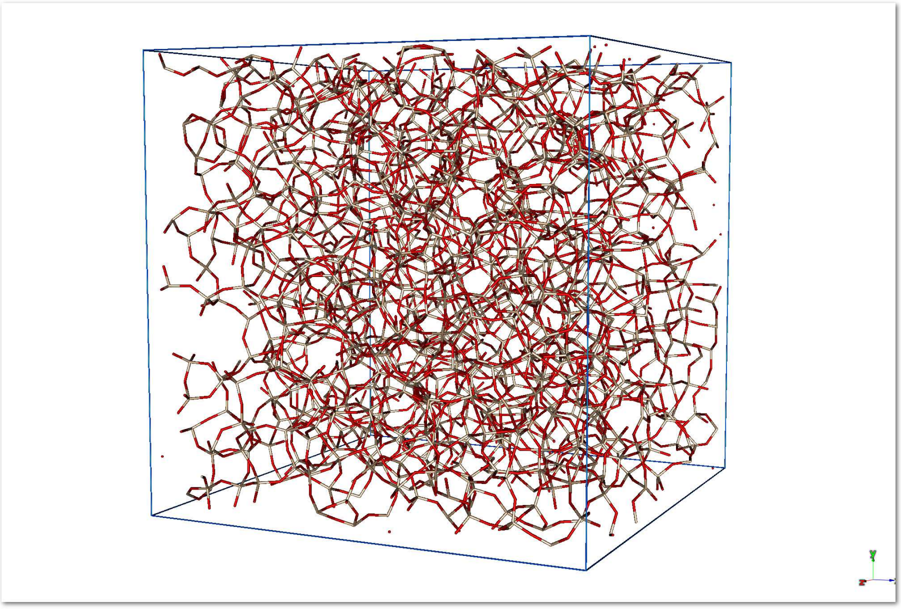
Using a custom color map

Alternatively to the CMs proposed by the **atomes** program it is possible to apply a user defined CM to the OpenGL model, this option is accessible via the "`Custom`" button of the "`Atoms & bonds`" menu [Fig. 5.2-b]. In that case it is required to read a file (having the extension "*.dat") that contains the numerical data to be used as color scale. This file must be a simple (Unix like) text file with as many lines as:

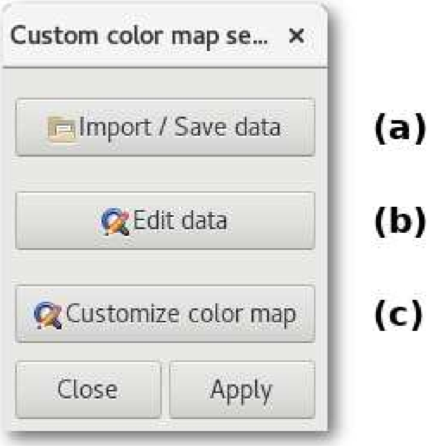
Total number of MD steps × Total number of atoms

Indeed the new colors can be applied to the entire MD trajectory.
An example is provided hereafter for the silica glass model:

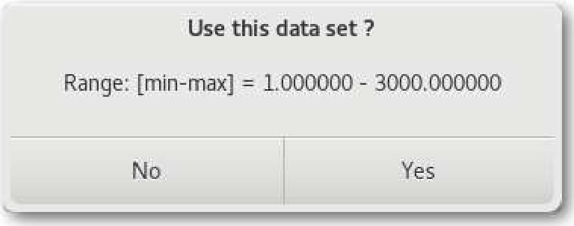
1. In the initial setup the chemical species are used as color map:



2. When the "`Custom`" button is pressed for the atoms CMs, the "`Custom color map setup`" dialog appears:



3. **(a)** The "`Import / Save data`" button allows to import your data file to create the color map. If the data file is processed successfully then **atomes** will propose to use it and a confirmation dialog will pop-up:

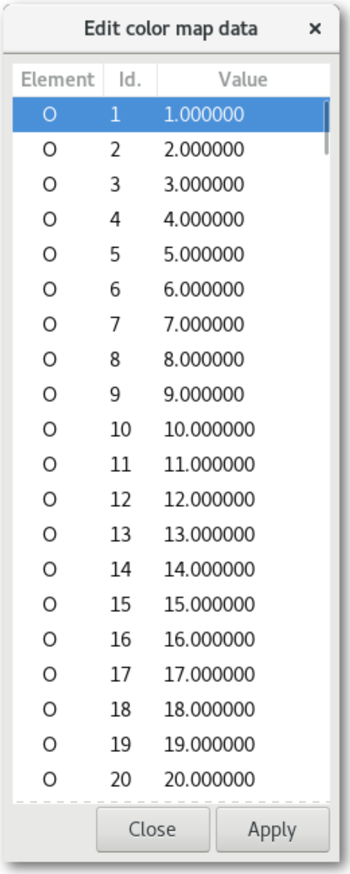


Use this data set ?

Range: [min-max] = 1.000000 - 3000.000000

For this example the data points are simply the atom indices from 1 to 3000.

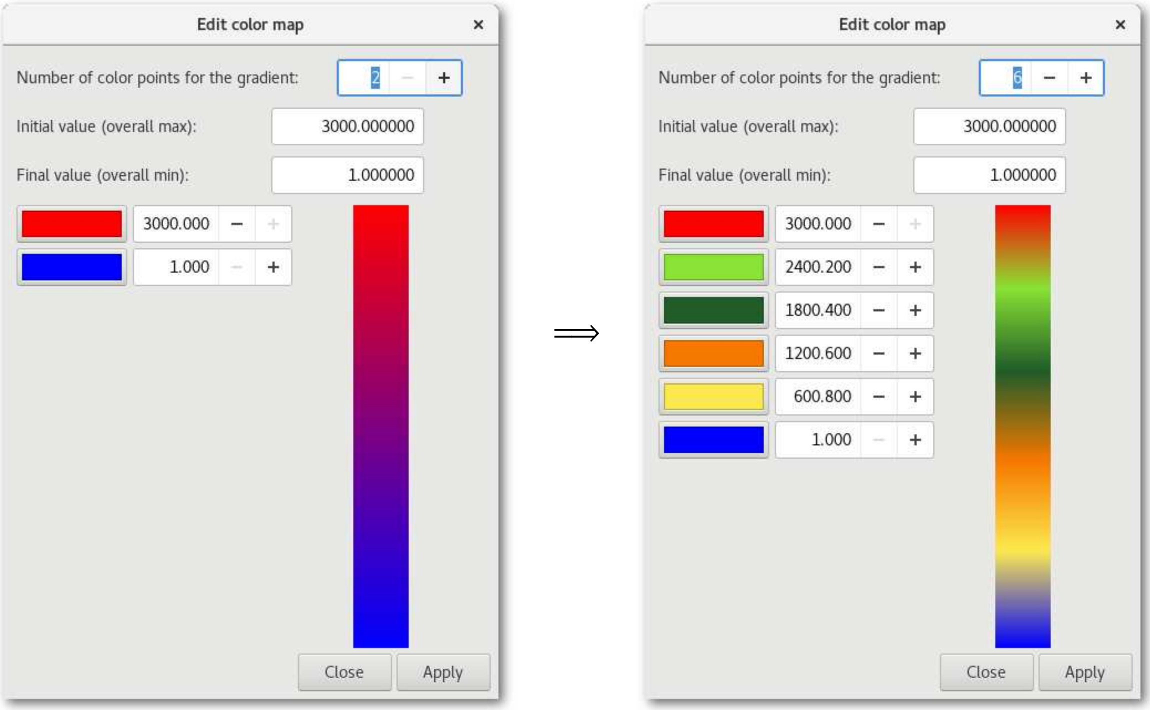
4. **(b)** Afterwards using the "`Edit data`" button it becomes possible to edit the data in a basic spreadsheet like mode, so that values for a particular atom can be checked and/or modify if needed:



Edit color map data

Element	Id.	Value
O	1	1.000000
O	2	2.000000
O	3	3.000000
O	4	4.000000
O	5	5.000000
O	6	6.000000
O	7	7.000000
O	8	8.000000
O	9	9.000000
O	10	10.000000
O	11	11.000000
O	12	12.000000
O	13	13.000000
O	14	14.000000
O	15	15.000000
O	16	16.000000
O	17	17.000000
O	18	18.000000
O	19	19.000000
O	20	20.000000

5. **(c)** And using the "`Customize color map`" button is possible to customize the color map, initially a gradient of red an blue between the maxima and the minima of the values in the data set is used, but you can easily add or remove point(s), and adjust the corresponding color to enhance the visual representation of your model:



Edit color map

Number of color points for the gradient: 2

Initial value (overall max): 3000.000000

Final value (overall min): 1.000000

🟥	3000.000
🟦	1.000

Edit color map

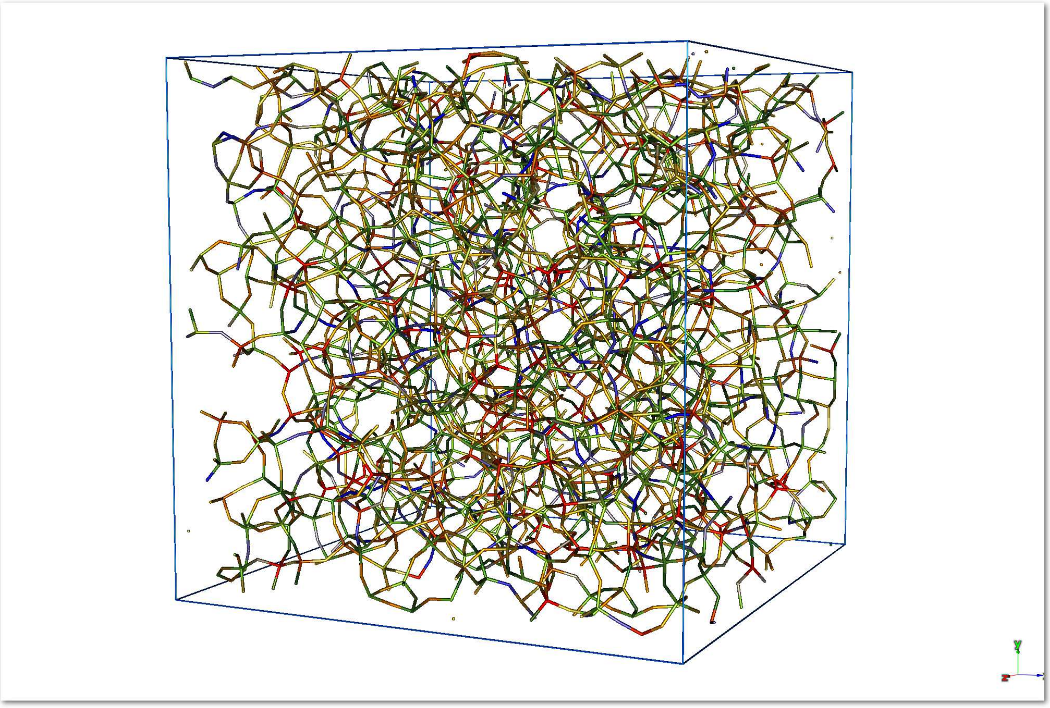
Number of color points for the gradient: 6

Initial value (overall max): 3000.000000

Final value (overall min): 1.000000

🟥	3000.000
🟩	2400.200
🟩	1800.400
🟧	1200.600
🟨	600.800
🟦	1.000

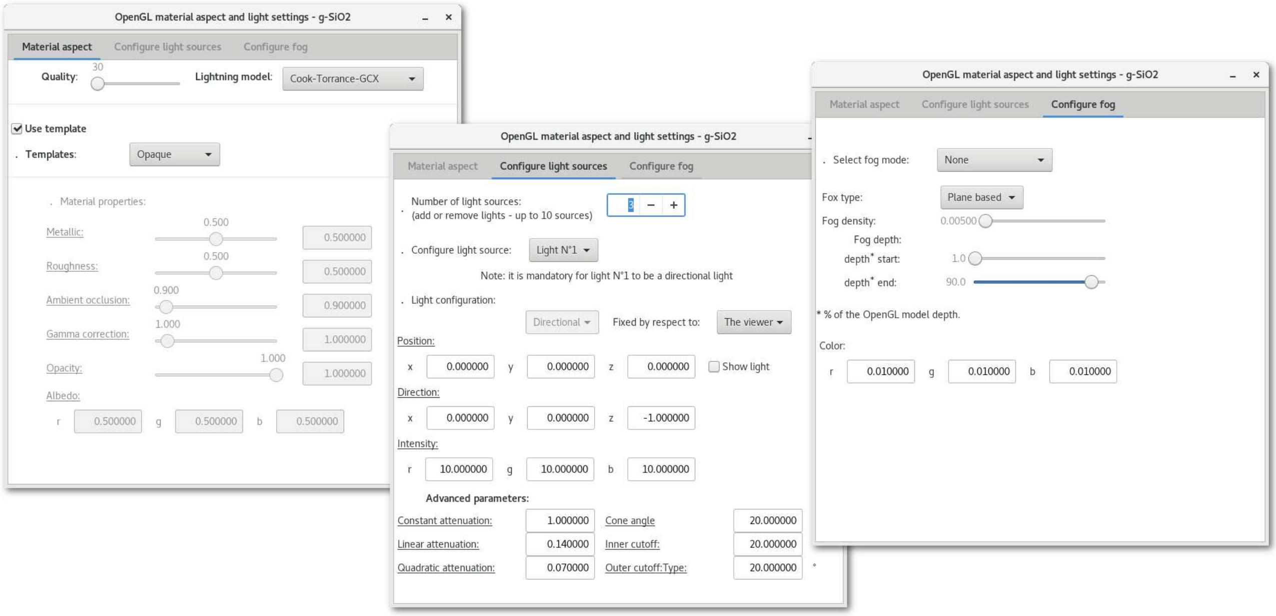
6. Finally simply apply the changes to use the new colors:



7. The "`Custom`" data and the corresponding color map are saved within the **atomes** project and workspace files (see sections 3.3.2 and 3.3.3), so that it will not be require to load a prepare the color map between work sessions.

5.1.1.3 Material and lights

The "`Material and lights`" button of the "`OpenGL`" menu opens the "`OpenGL material aspect and light settings`" dialog [Fig. 5.4]:



Quality: 30
Lightning model: Cook-Torrance-GCX
☑ Use template
. Templates: Opaque
. Material properties:
Metallic: 0.500 0.500000
Roughness: 0.500 0.500000
Ambient occlusion: 0.900 0.900000
Gamma correction: 1.000 1.000000
Opacity: 1.000 1.000000
Albedo: r 0.500000 g 0.500000 b 0.500000

. Number of light sources: (add or remove lights - up to 10 sources) 3
. Configure light source: Light N°1
Note: it is mandatory for light N°1 to be a directional light
. Light configuration: Directional Fixed by respect to: The viewer
Position: x 0.000000 y 0.000000 z 0.000000 ☐ Show light
Direction: x 0.000000 y 0.000000 z -1.000000
Intensity: r 10.000000 g 10.000000 b 10.000000
Advanced parameters:
Constant attenuation: 1.000000 Cone angle 20.000000
Linear attenuation: 0.140000 Inner cutoff: 20.000000
Quadratic attenuation: 0.070000 Outer cutoff:Type: 20.000000 °

. Select fog mode: None
Fox type: Plane based
Fog density: 0.00500
Fog depth:
depth* start: 1.0
depth* end: 90.0
* % of the OpenGL model depth.
Color: r 0.010000 g 0.010000 b 0.010000

Figure 5.4 *The "`OpenGL material aspect and light settings`" dialog in the* **atomes** *program.*

The window contains a notebook with 3 tabs:

- The first tab allows to configure/adjust:
  - The quality of the rendering, ie. the number of polygons to render a volume.
  - The lightning model, from the lowest quality (fastest to render, "`None`") to the highest quality (longer to render, "`Cook-Torrance-GCX`").
  - The material aspect, few templates being available, but all characteristics required to describe the material aspect for the light mode being available.
- The second tab allows to configure the lights sources of the model:
  - 3 type of light source being available: directional, point and spot lights.
  - With the possibility to add up to 10 light sources.
- Finally the third tab is used to adjust the fog effects

For information on OpenGL lightning models, material effects, lights, and more see:

- https://learnopengl.com/Lighting/Basic-Lighting
- https://learnopengl.com/Advanced-Lighting/Advanced-Lighting

5.1.2 The "`Model`" menu

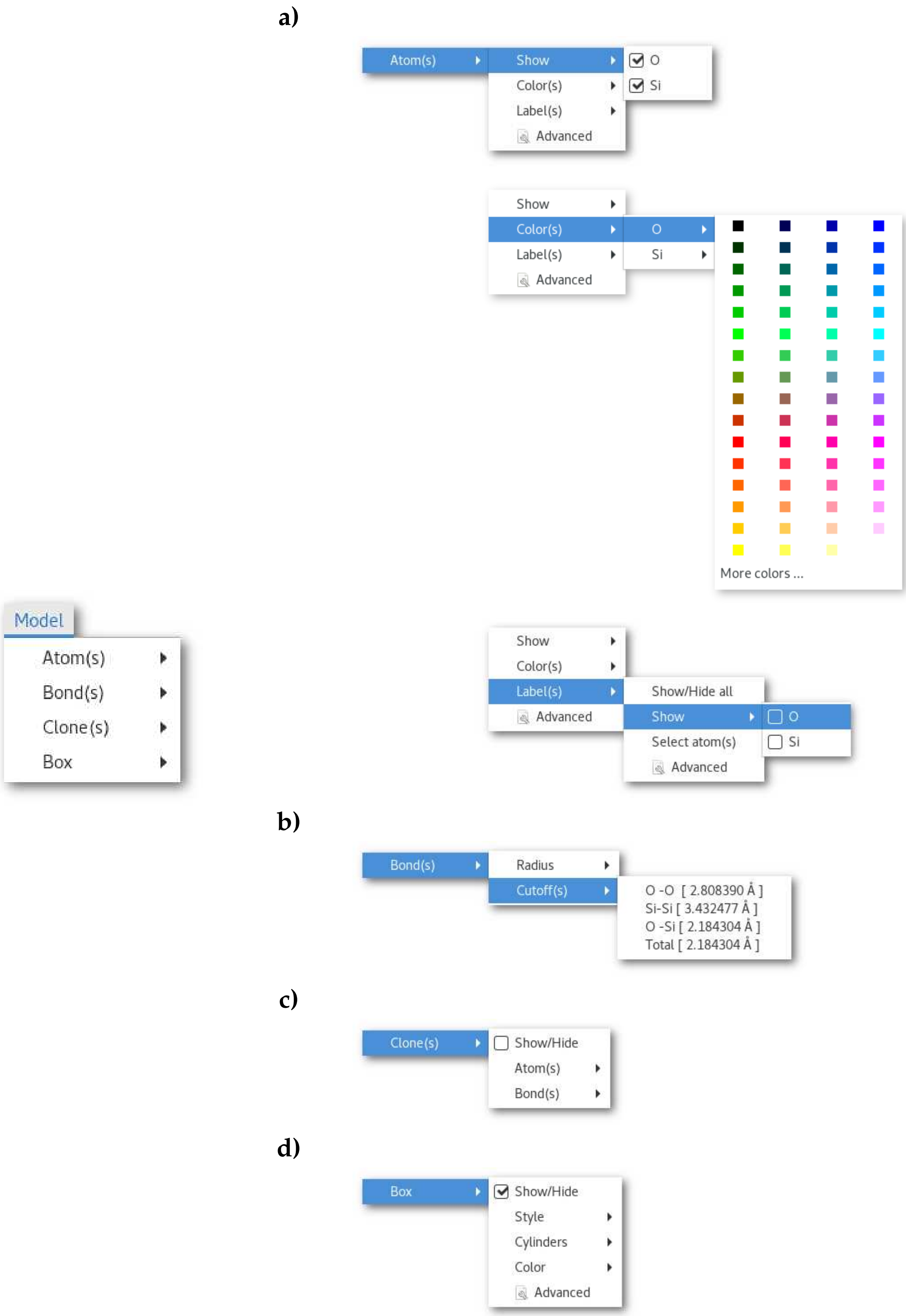
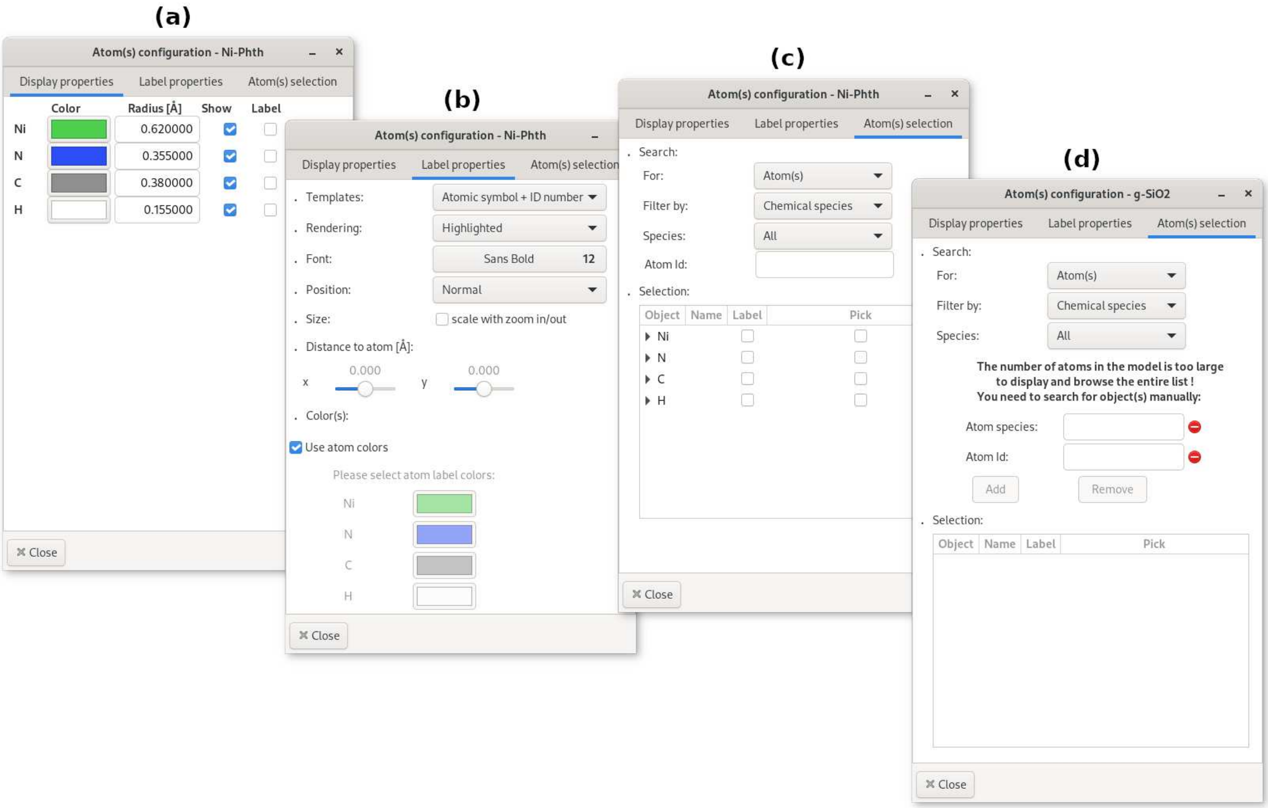


Figure 5.5 *The "`Model`" menu and the attached submenus.*

5.1.2.1 The "`Atom(s)`" menu

The "`Atom(s)`" menu [Fig. 5.5-a] offers to configure some visual features related to the chemical species in the model. This menu contains shortcuts for some the properties that can be adjusted using the more advanced "`Atom(s) configuration`" dialog, and that can be opened using any of the "`Advanced`" buttons in the menu. The "`Atom(s) configuration`" dialog is presented in figure 5.6:



(a)

	Color	Radius [Å]	Show	Label
Ni	🟩	0.620000	☑	☐
N	🟦	0.355000	☑	☐
C	⬜	0.380000	☑	☐
H	⬜	0.155000	☑	☐

(b)

Templates: Atomic symbol + ID number
Rendering: Highlighted
Font: Sans Bold 12
Position: Normal
Size: ☐ scale with zoom in/out
Distance to atom [Å]: x 0.000 y 0.000
Color(s):
☑ Use atom colors
Please select atom label colors: Ni, N, C, H

(c)

Search:
For: Atom(s)
Filter by: Chemical species
Species: All
Atom Id:
Selection:

Object	Name	Label	Pick
Ni		☐	☐
N		☐	☐
C		☐	☐
H		☐	☐

(d)

Search:
For: Atom(s)
Filter by: Chemical species
Species: All
The number of atoms in the model is too large to display and browse the entire list ! You need to search for object(s) manually:
Atom species:
Atom Id:
Selection:

Object	Name	Label	Pick

Figure 5.6 *The "`Atom(s) configuration`" dialog in the* **atomes** *program.*

The window contains a notebook with 3 tabs:

- **(a)** The "`Display properties`" tab: to adjust chemical species colors, atomic labels, and depending on the model style:
  - Ball and sticks: atomic radius
  - Wireframe or Points: point size
- **(b)** The "`Label properties`" tab: to adjust the aspect of the atomic labels.
- **(c)** or **(d)** The "`Atom(s) selection`": to search for atom(s) in the model. If the model contains less than 10 000 atoms the entire list of atoms is displayed **(c)**, otherwise it becomes too complicated to display and a search engine is proposed **(d)**.

5.1.2.2 The "`Bond(s)`" menu

Via the "`Bond(s)`" menu [Fig. 5.5-b] it is possible to adjust the bond cutoff(s), and depending on the model style:

- Ball and sticks: bonds radius(ii)
- Cylinders: bond radius
- Wireframe: line width

5.1.2.3 The "`Clone(s)`" menu

The **atomes** program uses **clones** to illustrate the presence of atomic bond(s) on the edges of the simulation box and existing because of the periodic boundary conditions (see section E.1 for more information on the PBC).
For the "`Clone(s)`" menu to be activated two conditions must be fulfilled: to use PBC, ie. the model must have a periodicity, and, for such bonds via PBC to exist. If both conditions are met, then the first button of the menu to "`Show/Hide Clones`" will be active and it becomes possible to show or hide the **clones**.
Please note that **clone** atoms/bonds are translucent to make them easily distinguishable from their atom/bond counterparts, figure 5.7 illustrates the **clones** idea using the silica glass model:

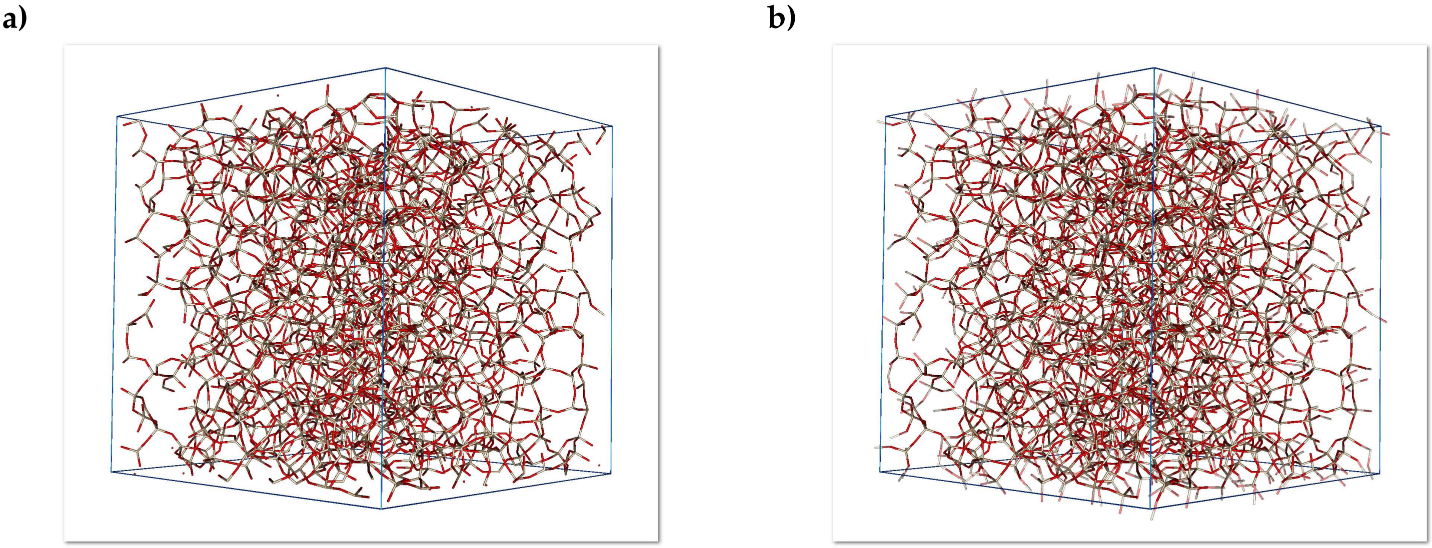


Figure 5.7 *The concept of* **clones** *in the* **atomes** *program.* **a)** *Standard representation using cylinders,* **b)** *Clones are included in the representation.*

If the **clones** are visible then the two "`Atom(s)`" and "`Bond(s)`" submenus will be activated as well. These menus are reproductions of the upper level "`Atom(s)`" and "`Bond(s)`" menus, and windows, but dedicated to the **clones**, this allows to make the **clones** even more distinguishable in the 3D representation.

5.1.3 The "`Chemistry`" menu

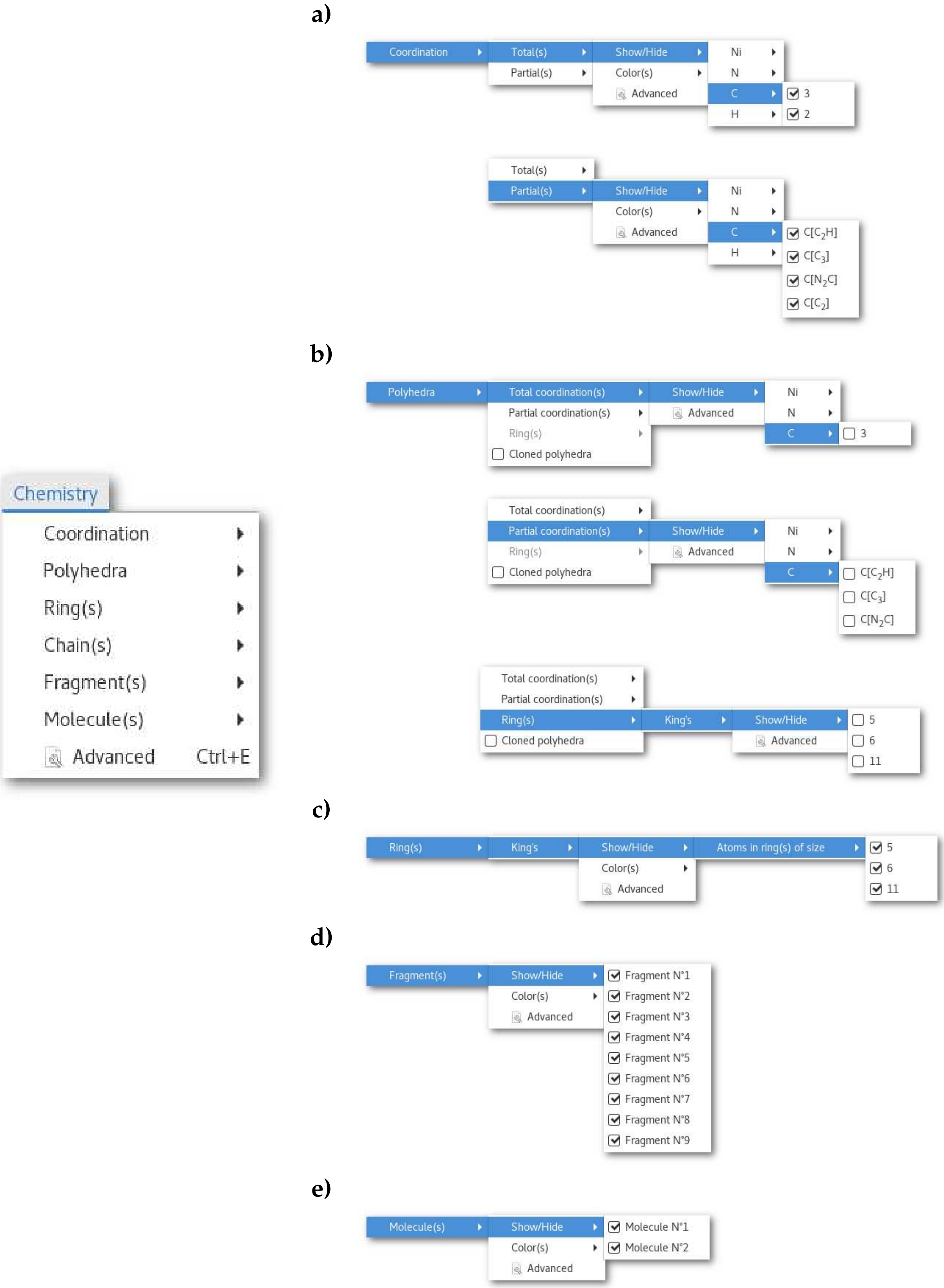


Figure 5.8 *The "`Chemistry`" menu and the attached submenus.*

The "`Chemistry`" menu [Fig. 5.8] and all the attached submenus from **a)** to **e)** are essentially composed of shortcut buttons to the options/actions that can be performed using the "`Environments configuration`" window, this section will therefore focus on the presentation of this window.

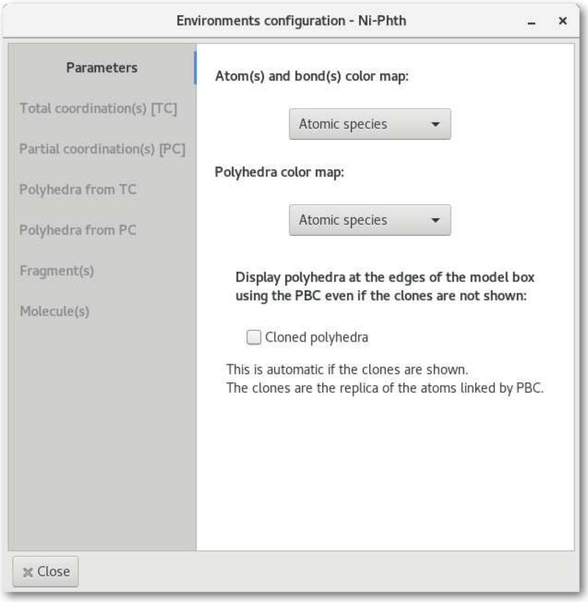
The "`Environments configuration`" window

The "`Environments configuration`" window contains a notebook with several tabs. The number of tabs depends on the calculations that were performed to analyze the model, ring statistics and chain statistics calculations will insert new tabs in the notebook. The different tabs of "`Environments configuration`" window are:

1. The "`Parameters`" tab (see 1)
2. The "`Total coordination(s) [TC]`" tab (see 2)
3. The "`Partial coordination(s) [PC]`" tab (see 2)
4. The "`Polyhedra from TC`" tab (see 3)
5. The "`Polyhedra from PC`" tab (see 3)
6. The "`Fragment(s)`" tab (see 4)
7. The "`Molecule(s)`" tab (see 4)
8. The "*`? ring(s)`* `[`*`?R`*`]`" tab (see 5 and 6)
   The "`Polyhedra from [`*`?R`*`]`" tab
   The "`Isolated ring(s) from [`*`?R`*`]`" tab
9. The "`Chain(s)`" tab (see 7)
   The "`Isolated chain(s)`" tab

Tabs 1, 2, 3, 4 and 5 are always present in the notebook, tabs 6 and 7 are present providing that the fragment(s) and the molecule(s) analysis were performed. Tabs 8 are inserted in the notebook when any of the ring statistics analysis are completed, whereas the tabs 9 are inserted when the chain statistics analysis is completed. Overall the "`Environments configuration`" window can contain up to 24 tabs.
Each tab in [1-9] is presented in detail thereafter:

1. The "`Parameters`" tab



Atom(s) and bond(s) color map: Atomic species

Polyhedra color map: Atomic species

Display polyhedra at the edges of the model box using the PBC even if the clones are not shown:

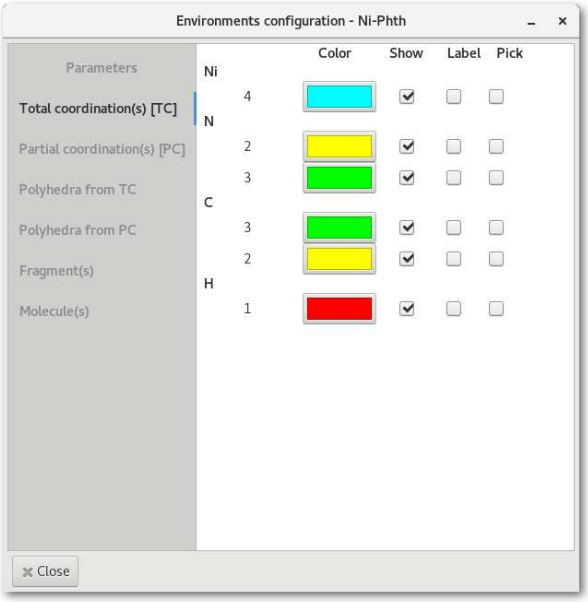
☐ Cloned polyhedra

This is automatic if the clones are shown.
The clones are the replica of the atoms linked by PBC.

This tab reproduce this available color map options from the "`Color scheme(s)`" menu (see section 5.1.1.2). Many of the following tabs allow to adjust the color of the element(s) for each color map, only for the change to be visible the corresponding color map must be used.
The "`Parameters`" tab also contains a "`Cloned polyhedra`" button, that allows to display polyhedra on the edges of the simulation box, and this even if **clones** are not shown.

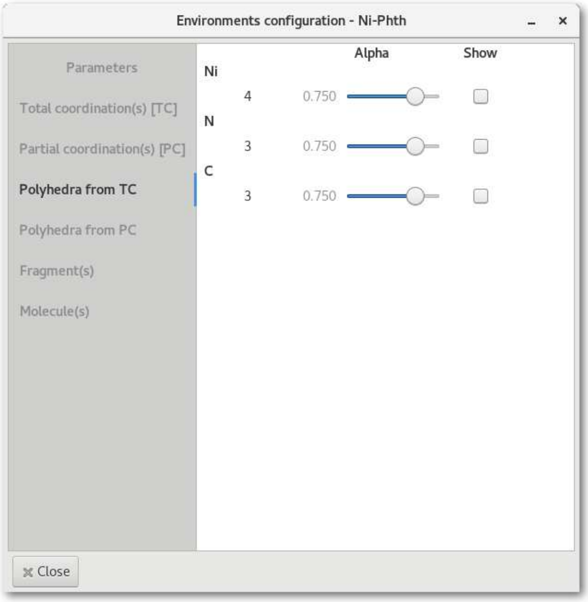
2. **The "`Total coordination(s) [TC]`" and "`Polyhedra form TC`" tabs**

a)



		Color	Show	Label	Pick
Ni	4	🟦	☑	☐	☐
N	2	🟨	☑	☐	☐
	3	🟩	☑	☐	☐
C	3	🟩	☑	☐	☐
	2	🟨	☑	☐	☐
H	1	🟥	☑	☐	☐

b)



		Alpha	Show
Ni	4	0.750	☐
N	3	0.750	☐
C	3	0.750	☐

a) The "`Total coordination(s) [TC]`" tab presents a list of options related to the total coordination sphere(s) found during the bonding analysis:

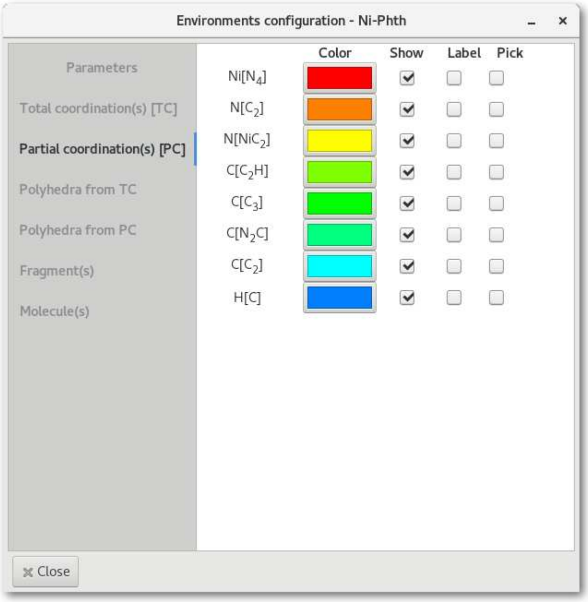
- A "`Color`" button: to adjust the color of the each element. Initially a color being assigned to each number of neighbors independently of the chemical species involved.
- A "`Show`" button: to hide/show the atom(s) matching the associated property.
- A "`Label`" button: to hide/show the atomic label of the atom(s) matching the associated property.
- A "`Pick`" button: to select/unselect the atom(s) matching the associated property (for more information on atom selection see section 5.2) .

In the "`Ni-Phth`" project example, the colors in **a** allow to obtain the representation from [Fig. 5.3-a].
b) The "`Polyhedra form TC`" tab presents a list of options related to the total coordination sphere(s) with 3 or more neighbors:

- An "`Alpha`" range: to adjust the opacity of the coordination polyhedra for the atom(s) matching the associated property.
- A "`Show`" button: to hide/show the coordination polyhedra for the atom(s) matching the associated property.

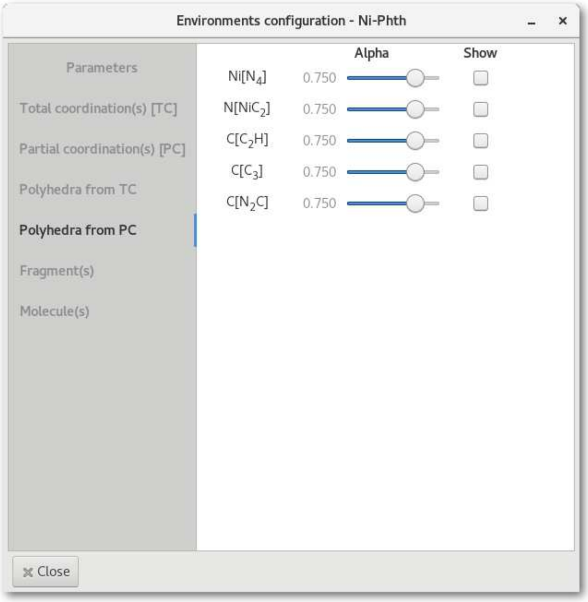
3. **The "`Partial coordination(s) [PC]`" and "`Polyhedra form PC`" tabs**

c)



	Color	Show	Label	Pick
$\mathrm{Ni[N_4]}$	🟥	☑	☐	☐
$\mathrm{N[C_2]}$	🟧	☑	☐	☐
$\mathrm{N[NiC_2]}$	🟨	☑	☐	☐
$\mathrm{C[C_2H]}$	🟩	☑	☐	☐
$\mathrm{C[C_3]}$	🟩	☑	☐	☐
$\mathrm{C[N_2C]}$	🟩	☑	☐	☐
$\mathrm{C[C_2]}$	🟦	☑	☐	☐
H[C]	🟦	☑	☐	☐

d)

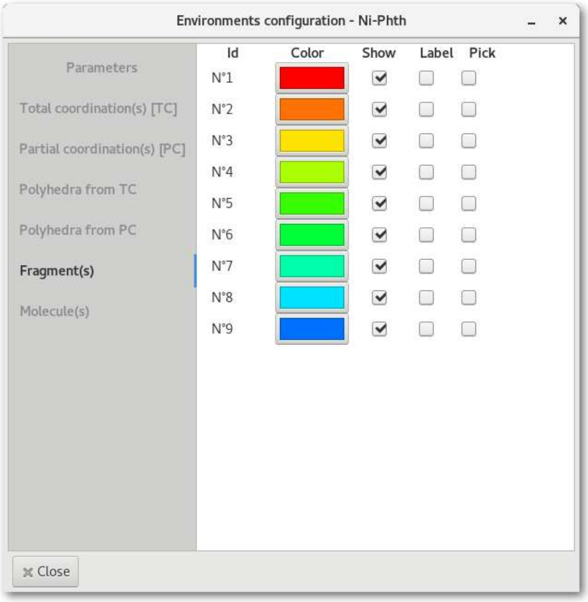


	Alpha	Show
$\mathrm{Ni[N_4]}$	0.750	☐
$\mathrm{N[NiC_2]}$	0.750	☐
$\mathrm{C[C_2H]}$	0.750	☐
$\mathrm{C[C_3]}$	0.750	☐
$\mathrm{C[N_2C]}$	0.750	☐

The "`Partial coordination(s) [PC]`" **c)** and the "`Polyhedra form PC`" **d)** tabs are similar to **a)** and **b)** respectively, coordination spheres being also separated based on the analysis of the chemistry of the bond(s). In the "`Ni-Phth`" project example, the colors in **c)** allow to obtain the representation from [Fig. 5.3-b].

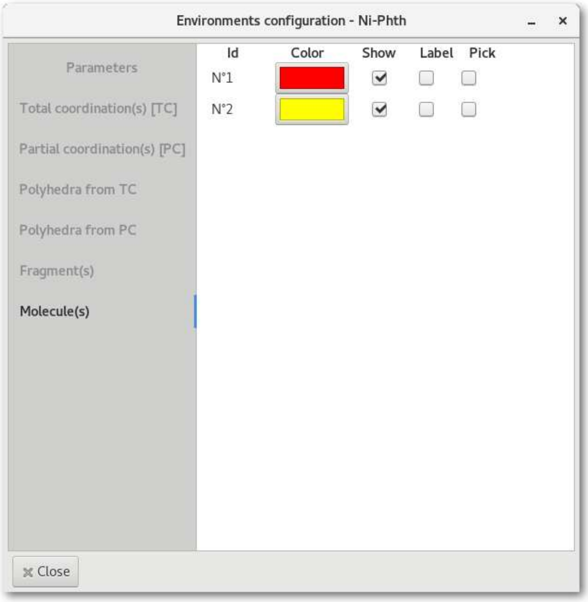
4. **The "`Fragment(s)`" and "`Molecule(s)`" tabs**

e)



Id	Color	Show	Label	Pick
N°1	🟥	☑	☐	☐
N°2	🟧	☑	☐	☐
N°3	🟨	☑	☐	☐
N°4	🟩	☑	☐	☐
N°5	🟩	☑	☐	☐
N°6	🟩	☑	☐	☐
N°7	🟩	☑	☐	☐
N°8	🟦	☑	☐	☐
N°9	🟦	☑	☐	☐

f)

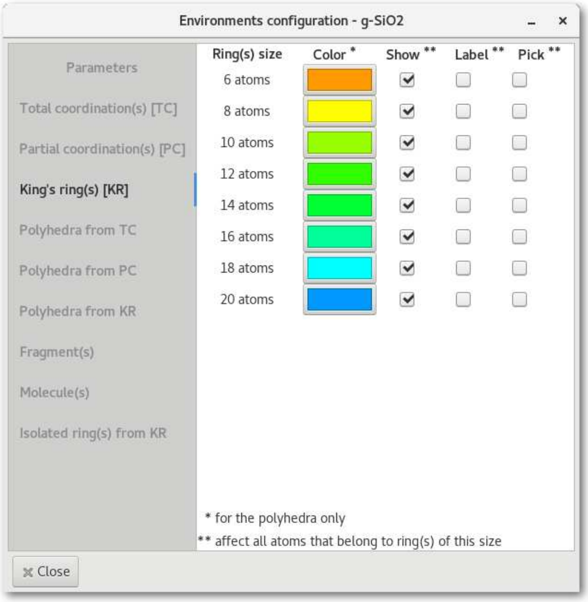


Id	Color	Show	Label	Pick
N°1	🟥	☑	☐	☐
N°2	🟨	☑	☐	☐

The "`Fragment(s)`" **e)** and "`Molecule(s)`" **f)** tabs follow similar ideas than **a)** (or **c)**) but for the **fragment(s)** and **molecule(s)** respectively. In these examples from the "`Ni-Phth`" project, the colors in **e)** and **f)** allow to obtain respectively the representations from [Fig. 5.3-c] and [Fig. 5.3-d].

5. The "`? ring(s) [?R]`", "`Polyhedra from [?R]`" tabs

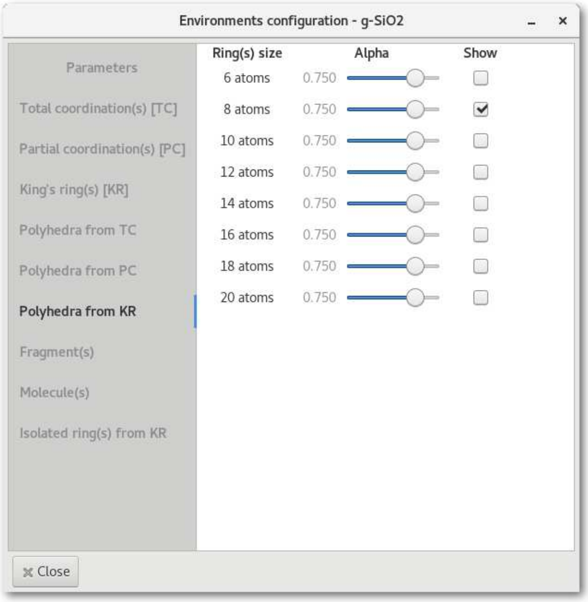
g)



Ring(s) size	Color *	Show **	Label **	Pick **
6 atoms	🟧	☑	☐	☐
8 atoms	🟨	☑	☐	☐
10 atoms	🟩	☑	☐	☐
12 atoms	🟩	☑	☐	☐
14 atoms	🟩	☑	☐	☐
16 atoms	🟩	☑	☐	☐
18 atoms	🟦	☑	☐	☐
20 atoms	🟦	☑	☐	☐

* for the polyhedra only
** affect all atoms that belong to ring(s) of this size

h)



Ring(s) size	Alpha	Show
6 atoms	0.750	☐
8 atoms	0.750	☑
10 atoms	0.750	☐
12 atoms	0.750	☐
14 atoms	0.750	☐
16 atoms	0.750	☐
18 atoms	0.750	☐
20 atoms	0.750	☐

Whenever a ring statistics calculation is performed successfully and ring(s) is/are found in the model, the "`? ring(s) [?R]`" **g)** and "`Polyhedra from [?R]`" **h)** tabs are inserted in the "`Environments configuration`" window, **g)** and **h)** are examples from the g-SiO$_2$ model for which King's rings analysis was performed. If other analyses were performed more tabs would be inserted following a similar idea, and **?** is the name of the methodology to search for rings, among: All (No rules), King's, Guttman's, Primitive and Strong (see section E.5 for more information on ring statistics).
The "`? ring(s) [?R]`" tab presents a list of options related results of the ring statistics calculation, for each size of ring:

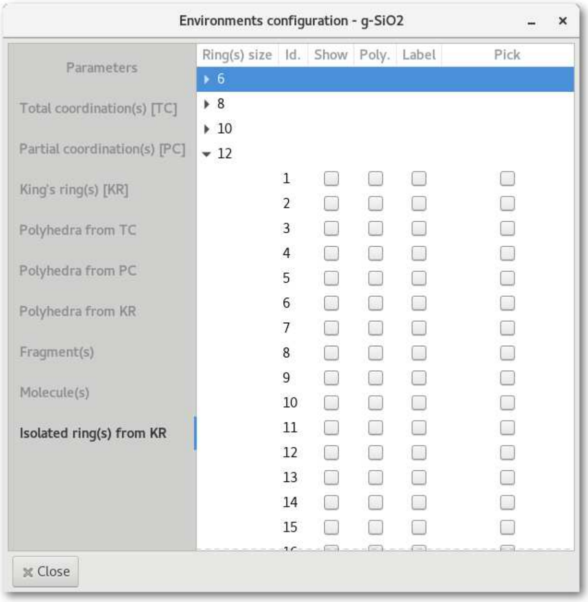
- A "`Color`" button: to adjust the color of the each element. Note that this color only concerns the polyhedra. Initially a different color is assigned to each size of ring(s).
- A "`Show`" button: to hide/show the atom(s) involved in ring(s) of that size.
- A "`Label`" button: to hide/show the atom(s) involved in ring(s) of that size.
- A "`Pick`" button: to select/unselect the atom(s) involved in ring(s) of that size.

The "`Polyhedra from [?R]`" tab present other options related results of the ring statistics calculation, for each size of ring:

- An "`Alpha`" range: to adjust the opacity of the polyhedra drawn using the atom(s) of each ring of that size as summits.
- A "`Show`" button: to hide/show the polyhedra drawn using the atom(s) of each ring of that size as summit.

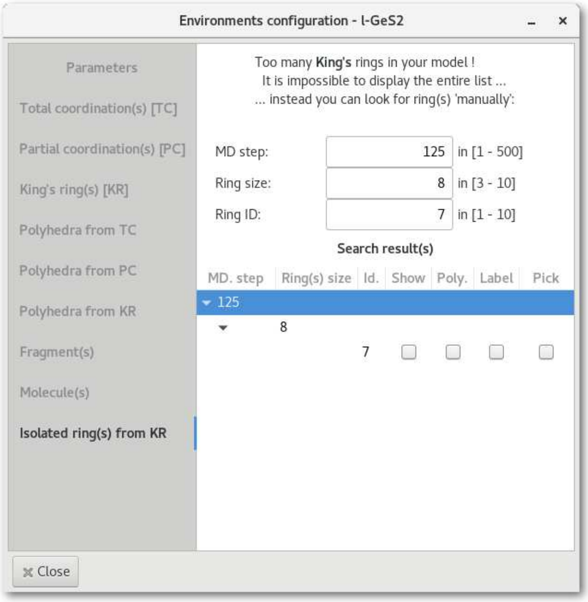
6. The "`Isolated ring(s) from [?R]`" tab

i)



Ring(s) size	Id.	Show	Poly.	Label	Pick
6					
8					
10					
12					
	1	☐	☐	☐	☐
	2	☐	☐	☐	☐
	3	☐	☐	☐	☐
	4	☐	☐	☐	☐
	5	☐	☐	☐	☐
	6	☐	☐	☐	☐
	7	☐	☐	☐	☐
	8	☐	☐	☐	☐
	9	☐	☐	☐	☐
	10	☐	☐	☐	☐
	11	☐	☐	☐	☐
	12	☐	☐	☐	☐
	13	☐	☐	☐	☐
	14	☐	☐	☐	☐
	15	☐	☐	☐	☐

j)



Too many **King's** rings in your model !
It is impossible to display the entire list ...
... instead you can look for ring(s) 'manually':

MD step: 125 in [1 - 500]
Ring size: 8 in [3 - 10]
Ring ID: 7 in [1 - 10]

Search result(s)

MD. step	Ring(s) size	Id.	Show	Poly.	Label	Pick
125						
	8					
		7	☐	☐	☐	☐

In the "`Isolated ring(s) from [?R]`" tab every single ring found can be look-up individually. Most often **i)** version of the tab is used, however if more than 10 000 rings are found it becomes too complicated to display the entire list and a search engine is proposed instead **j)**.
Among the options provided by the "`Isolated ring(s) from [?R]`" tab:

- A "`Show`" button: to hide/show the atom(s) involved in this ring.
- A "`Ploy`" button: to hide/show the polyhedra drawn using the atom(s) of this ring as summits.
- A "`Label`" button: to hide/show the atom(s) involved in this ring.
- A "`Pick`" button: to select/unselect the atom(s) involved in this ring.

7. The "`Chain(s)`" "`Isolated chain(s)`" tabs

These tabs (not shown) are dedicated to the results of the chain statistics analysis, and simply reproduces options of tabs **g)** and **i)**/**j)**, at the exception that there are no polyhedra to display.

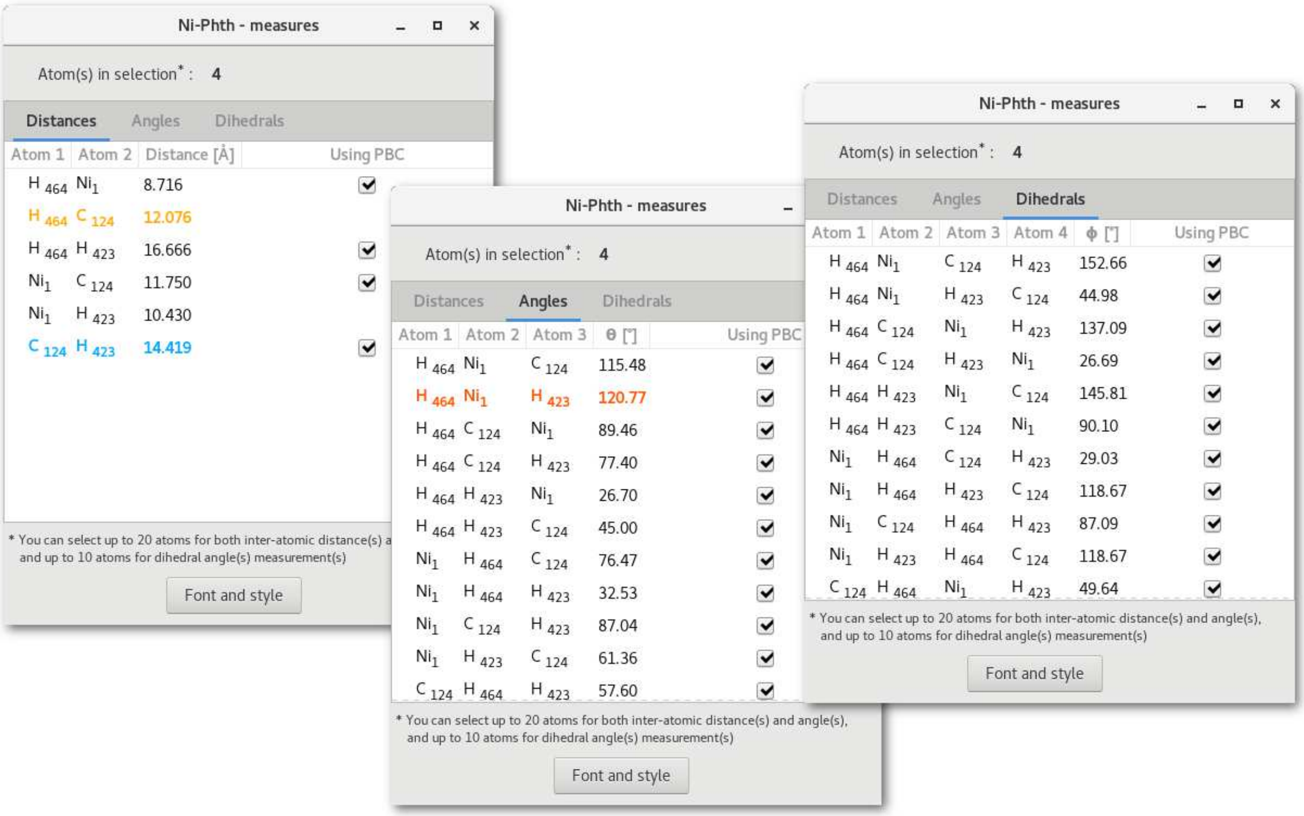
5.1.4 The "`Tools`" menu

Figure 5.9 *The "`Tools`" menu and the attached submenus in the* **atomes** *program.*

The "`Edit`" menu **a)**, that regroups the edition tools will be covered in chapter 3.7, and the "`Molecular Dynamics`" menu **d)**, regrouping the MD input assistants will be covered in chapter 7. Also the actions of the "`Invert`" menu **e)** being pretty intuitive, this section will only present the "`Measures`" button/dialog, the "`Mouse mode`" **b)**, "`Selection mode`" **c)** menus.

The "`Measures`" dialog

Pressing the "`Measures`" button will open the "`Measures`" dialog [Fig. 5.10], that contains a notebook with 3 tabs, for inter-atomic distances, angles and dihedrals, and a button labelled "`Font and style`" to configure how the measure(s) will appear on the model.



Atom(s) in selection*: 4

Atom 1	Atom 2	Distance [Å]	Using PBC
H_{464}	Ni_1	8.716	☑
H_{464}	C_{124}	12.076	
H_{464}	H_{423}	16.666	☑
Ni_1	C_{124}	11.750	☑
Ni_1	H_{423}	10.430	
C_{124}	H_{423}	14.419	☑

* You can select up to 20 atoms for both inter-atomic distance(s) a
and up to 10 atoms for dihedral angle(s) measurement(s)

Atom(s) in selection*: 4

Atom 1	Atom 2	Atom 3	θ [°]	Using PBC
H_{464}	Ni_1	C_{124}	115.48	☑
H_{464}	Ni_1	H_{423}	120.77	☑
H_{464}	C_{124}	Ni_1	89.46	☑
H_{464}	C_{124}	H_{423}	77.40	☑
H_{464}	H_{423}	Ni_1	26.70	☑
H_{464}	H_{423}	C_{124}	45.00	☑
Ni_1	H_{464}	C_{124}	76.47	☑
Ni_1	H_{464}	H_{423}	32.53	☑
Ni_1	C_{124}	H_{423}	87.04	☑
Ni_1	H_{423}	C_{124}	61.36	☑
C_{124}	H_{464}	H_{423}	57.60	☑

* You can select up to 20 atoms for both inter-atomic distance(s) and angle(s),
and up to 10 atoms for dihedral angle(s) measurement(s)

Atom(s) in selection*: 4

Atom 1	Atom 2	Atom 3	Atom 4	ϕ [°]	Using PBC
H_{464}	Ni_1	C_{124}	H_{423}	152.66	☑
H_{464}	Ni_1	H_{423}	C_{124}	44.98	☑
H_{464}	C_{124}	Ni_1	H_{423}	137.09	☑
H_{464}	C_{124}	H_{423}	Ni_1	26.69	☑
H_{464}	H_{423}	Ni_1	C_{124}	145.81	☑
H_{464}	H_{423}	C_{124}	Ni_1	90.10	☑
Ni_1	H_{464}	C_{124}	H_{423}	29.03	☑
Ni_1	H_{464}	H_{423}	C_{124}	118.67	☑
Ni_1	C_{124}	H_{464}	H_{423}	87.09	☑
Ni_1	H_{423}	H_{464}	C_{124}	118.67	☑
C_{124}	H_{464}	Ni_1	H_{423}	49.64	☑

* You can select up to 20 atoms for both inter-atomic distance(s) and angle(s),
and up to 10 atoms for dihedral angle(s) measurement(s)

Figure 5.10 *The "`Measures`" dialog in the* **atomes** *program, with the "`Distances`", "`Angles`" and "`Dihedrals`" tabs.*

Each tab contains the respective measured properties for all the atoms in selection (see section 5.2 for more information on the selection process), this means the atoms that have been selected before opening the dialog, or, while it is opened and the tabs will refresh. The tabs read as follow:

- First (2/3/4) columns the atoms id's
- Column (3/4/5): the value measured in the model
- Column (4/5/9): If PBC are used/required to measure the value (to avoid visual deception)

Behavior of the "`Measures`" dialog:

1. If too many atoms are in selection then the tabs will remain empty and the measures will not show up. To get the information about the measures back simply decrease the number of atoms selected under 20 atoms for the distances and the angles, and under 10 for the dihedrals.

2. If any line is selected by a mouse click in the tabs, then the font color of this line will change and the corresponding measure will appear in the model with the same color. In figure 5.10, 2 lines are selected in the "`Distances`" tab, and 1 line is selected in the "`Angles`" tab, the result is presented in figure 5.11.

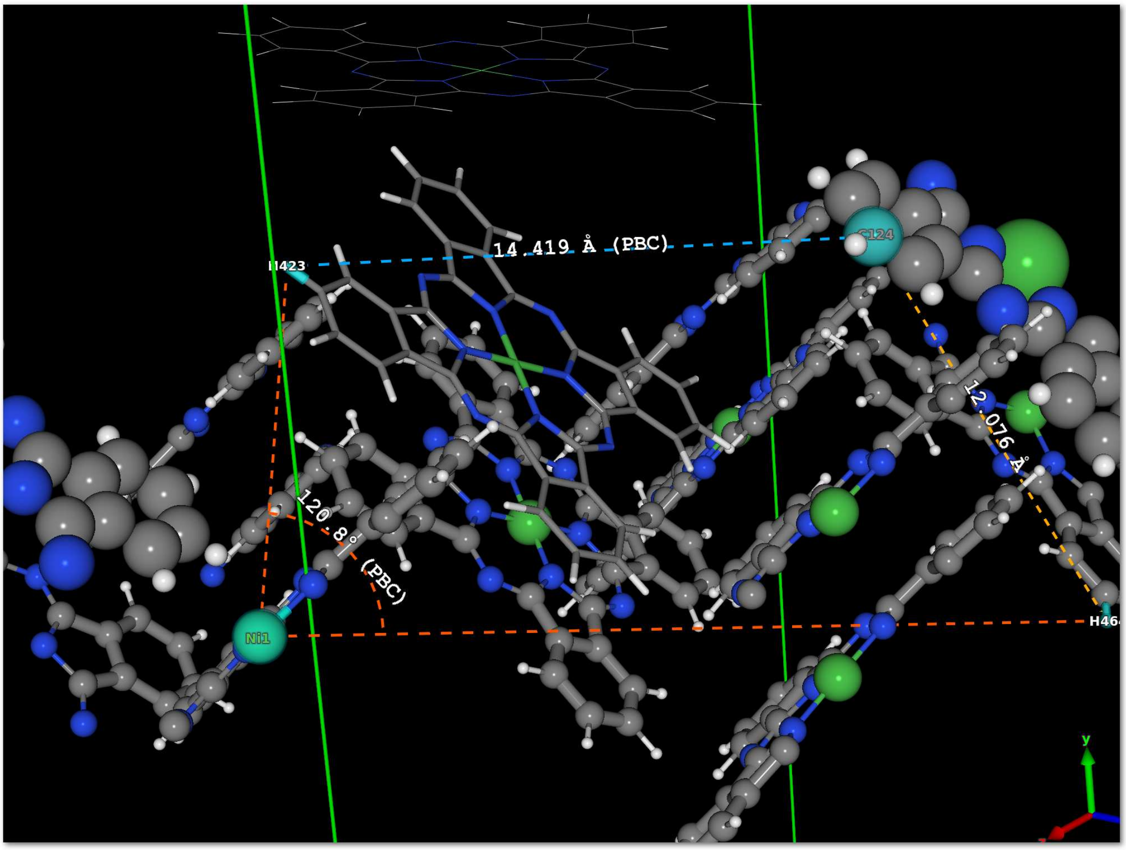
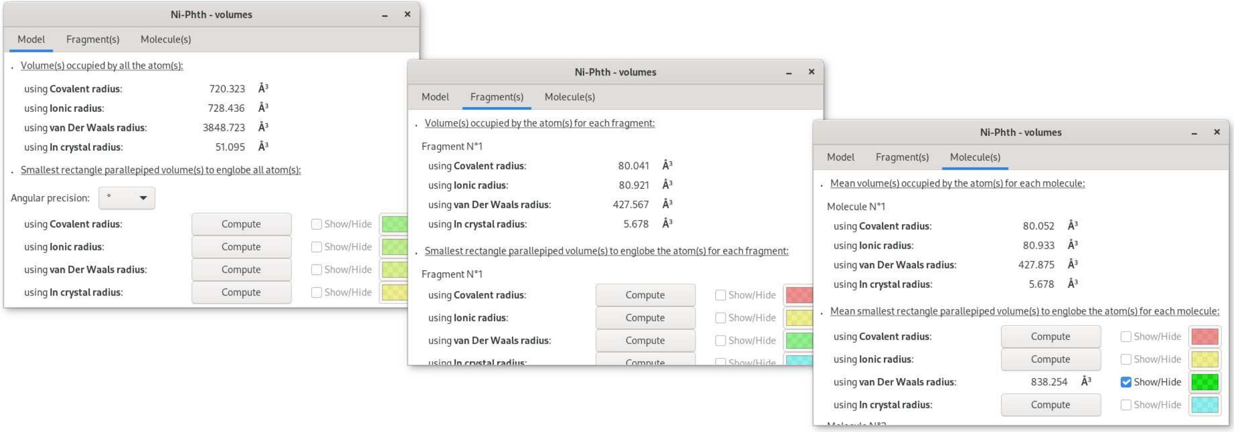


Figure 5.11 *Some examples of measurements displayed in the OpenGL window.*

3. No visual information is available for the dihedral angles and only the numerical values are provided.

The "Volumes" dialog

Pressing the "`Volumes`" button will open the "`Volumes`" dialog [Fig. 5.12], that contains a notebook with 3 tabs, for overall atomic volumes ("`Model`"), isolated fragment volumes ("`Fragment(s)`"), molecular volume ("`Molecule(s)`").



Ni-Phth - volumes
Model | Fragment(s) | Molecule(s)

. Volume(s) occupied by all the atom(s):
using **Covalent radius**: 720.323 Å³
using **Ionic radius**: 728.436 Å³
using **van Der Waals radius**: 3848.723 Å³
using **In crystal radius**: 51.095 Å³

. Smallest rectangle parallepiped volume(s) to englobe all atom(s):
Angular precision: °
using **Covalent radius**: Compute ☐ Show/Hide
using **Ionic radius**: Compute ☐ Show/Hide
using **van Der Waals radius**: Compute ☐ Show/Hide
using **In crystal radius**: Compute ☐ Show/Hide

Ni-Phth - volumes
Model | Fragment(s) | Molecule(s)

. Volume(s) occupied by the atom(s) for each fragment:
Fragment N°1
using **Covalent radius**: 80.041 Å³
using **Ionic radius**: 80.921 Å³
using **van Der Waals radius**: 427.567 Å³
using **In crystal radius**: 5.678 Å³

. Smallest rectangle parallepiped volume(s) to englobe the atom(s) for each fragment:
Fragment N°1
using **Covalent radius**: Compute ☐ Show/Hide
using **Ionic radius**: Compute ☐ Show/Hide
using **van Der Waals radius**: Compute ☐ Show/Hide
using **In crystal radius**: Compute ☐ Show/Hide

Ni-Phth - volumes
Model | Fragment(s) | Molecule(s)

. Mean volume(s) occupied by the atom(s) for each molecule:
Molecule N°1
using **Covalent radius**: 80.052 Å³
using **Ionic radius**: 80.933 Å³
using **van Der Waals radius**: 427.875 Å³
using **In crystal radius**: 5.678 Å³

. Mean smallest rectangle parallepiped volume(s) to englobe the atom(s) for each molecule:
using **Covalent radius**: Compute ☐ Show/Hide
using **Ionic radius**: Compute ☐ Show/Hide
using **van Der Waals radius**: 838.254 Å³ ☑ Show/Hide
using **In crystal radius**: Compute ☐ Show/Hide

Figure 5.12 *The "`Volumes`" dialog in the* **atomes** *program, with the "`Model`", "`Fragment(s)`" and "`Molecule(s)`" tabs.*

Tabs are divided in two parts: top for molecular volume(s) calculated for the respective target, bottom for calculations to dermine the smallest rectangle parallepiped volume for the respective target. Also volumes can be evalutated for different types of atomic radii (covalent, ionic, van Der Waals and in crystal), and on the first tab ("`Volumes`"), the angular precision (rotation of the volume) can be fine tuned for all calculations. Once a "`Compute`" button is pressed the selected calculation will be perfomed, then numerical results become available and can be visualized pressing the corresponding "`Show/Hide`" button:

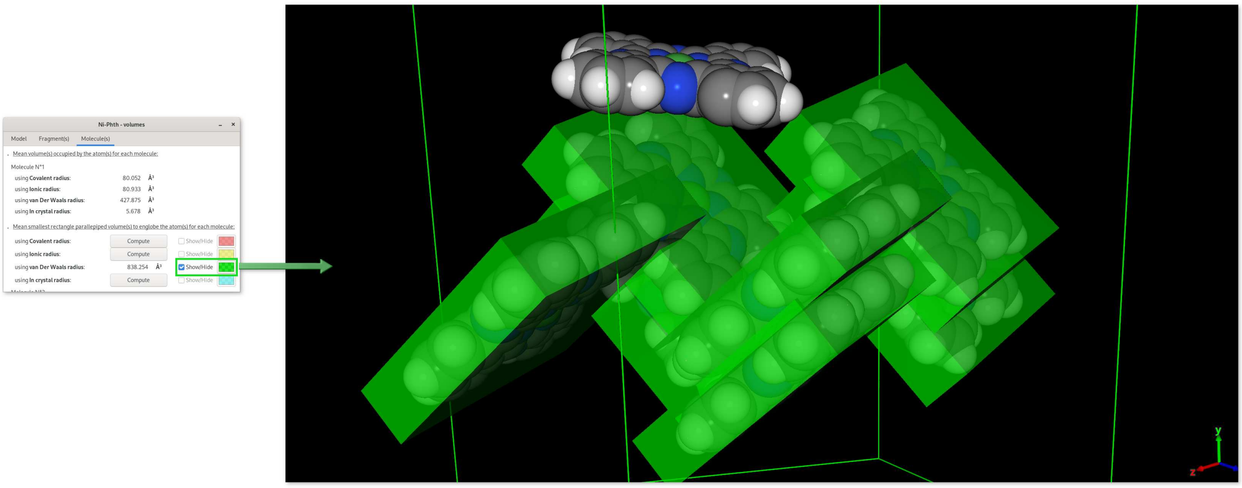


Figure 5.13 *Volumes visualization in the* **atomes** *program: smallest rectangle parallepiped volumes found for each of the isolated fragment in molecule 1.*

The "`Mouse mode`" menu

This menu allows to switch the mouse mode between "`Analysis`" (default) and "`Edition`". This menu is active, only and only if, there is a single configuration in the project (and not a molecular dynamics trajectory). Therefore when studying a MD trajectory only the "`Analysis`" mode is available.

The "`Selection mode`" menu

This menu allows to adjust the mouse selection capabilities, and switch between:

1. **Atom/bond** (default): selection atom by atom or bond by bond.
2. **Coordination sphere**: the atom and all its first neighbors.
3. **Fragment**: the atom and all other atom(s) that belong to the same **fragment**.
4. **Molecule**: the atom and all other atom(s) that belong to the same **molecule**.
5. **Single fragment**: same as 3 and unselect all other atoms in the model.
6. **Single molecule**: same as 4 and unselect all other atoms in the model.
7. **Measures (Edition mode only)**: will be covered in chapter 6.

5.1.5 The "`View`" menu

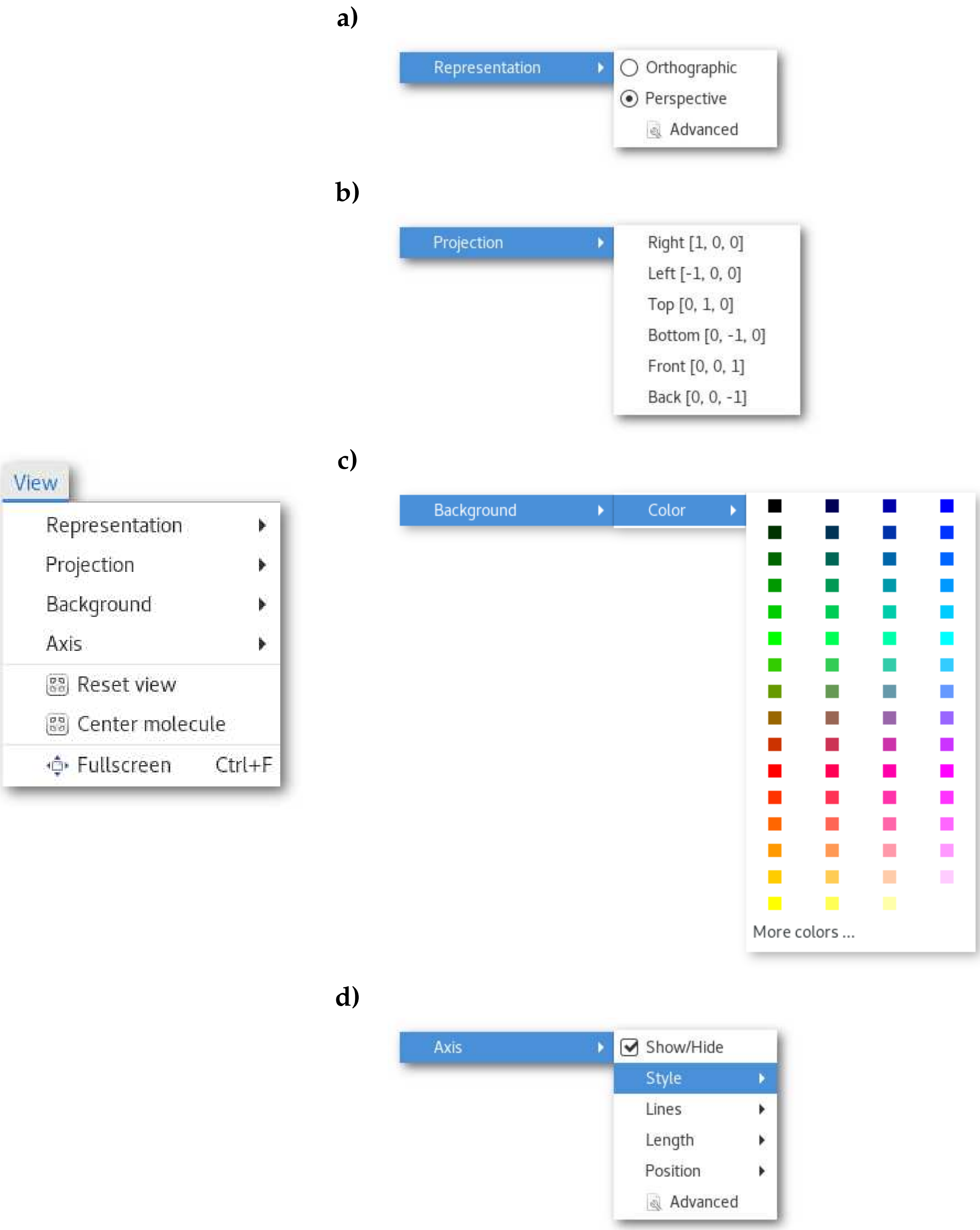


Figure 5.14 *The "`View`" menu and the attached submenus in the* **atomes** *program.*

Being very intuitive the actions of the "`View`" menu will not be discussed in this manual.

5.1.6 The "`Animate`" menu

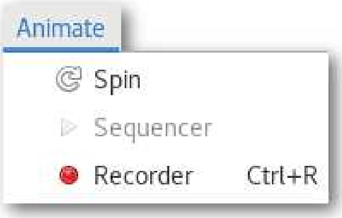


Figure 5.15 *The "`Animates`" menu of the OpenGL window in the* **atomes** *program.*

The animate menu allows to open 3 different dialog boxes:

The "`Spin`" dialog

The "`Spin`" dialog [Fig. 5.16] allows to spin the model:

Figure 5.16 *The "`Spin`" dialog of the OpenGL window in the* **atomes** *program.*

When one of the arrow (left, right, up, down) button is pressed the model will start rotating in that direction. It is possible to combine directions by pressing several buttons, also the rotation speed is determined by the number of times the button was pressed: the more it was pressed the faster the model will rotate. To decrease the rotation speed, press the arrow button(s) in the opposite direction(s) to the rotation.

The "Sequencer" dialog

The "`Sequencer`" dialog [Fig. 5.17] allows to animate and review a molecular dynamics trajectory, and is therefore only accessible if the project contains more than a single atomic configuration:

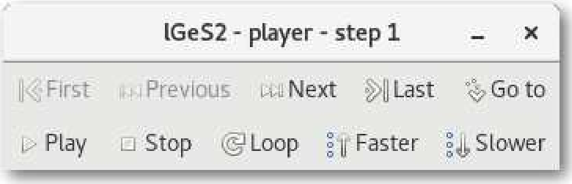


Figure 5.17 *The "`Sequencer`" dialog of the OpenGL window in the* **atomes** *program.*

The "Recorder" dialog

The "`Recorder`" dialog [Fig. 5.18] allows to record **any action** on the OpenGL window:

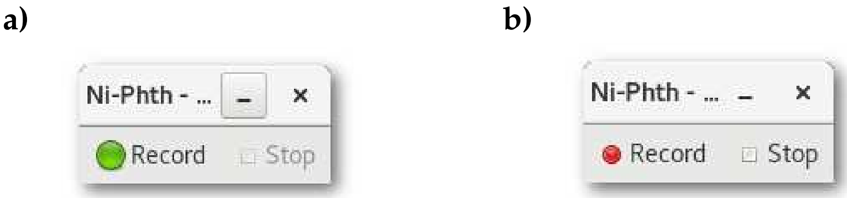
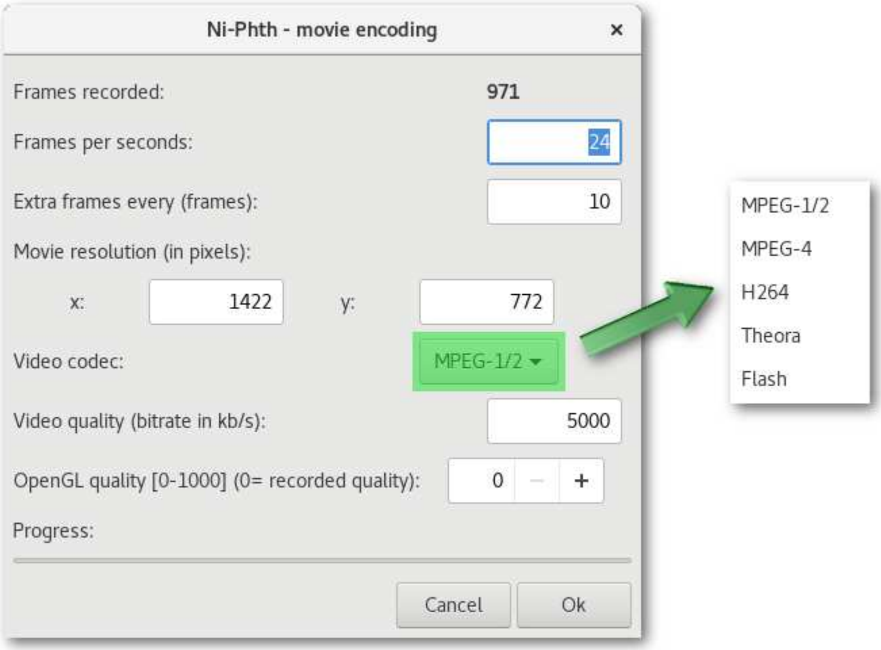


Figure 5.18 *The "`Recorder`" dialog of the OpenGL window in the* **atomes** *program.*

As soon as the green "`Record`" button [Fig. 5.18-a] is pressed, and turns to red [Fig. 5.18-b], **any action** performed on the OpenGL window will be recorded, (the "`Spin`" and the "`Sequencer`" dialogs for example can be opened and used while recording) and the recording will continue until the "`Stop`" button is pressed, then the "`Movie encoding`" dialog will pop-up [Fig. 5.19]



Ni-Phth - movie encoding

Frames recorded: 971

Frames per seconds: 24

Extra frames every (frames): 10

Movie resolution (in pixels):

x: 1422 y: 772

Video codec: MPEG-1/2

Video quality (bitrate in kb/s): 5000

OpenGL quality [0-1000] (0= recorded quality): 0

Progress:

Figure 5.19 *The "`Movie encoding`" dialog of the OpenGL window in the* **atomes** *program.*

The "`Movie encoding`" dialog allows to adjust any parameters required to encode a nice movie.
Many of the video codecs available in atoms [Fig. 5.19] are sensitive to the parameters that can be entered in this dialog. For instance the MPEG-4 and H264 video codecs seem to be very sensitive to the utilization of standard video resolutions (800x600, 1980x1024 ...). However by default **atomes** input the dimensions of the OpenGL window as Movie resolution and the codec might not like non-standard parameters as the values in figure 5.19, and the encoding could fail.
Depending on the codec this might be true for any of the parameters that can be adjusted in this dialog. Moreover error messages (from the encoding library) are not necessarily displayed, and the error might not be seen directly.
However even if the encoding fail **atomes** will not crash, and as long as the "`Cancel`" button of the dialog [Fig. 5.19] is not pressed all data required to encode the movie is perfectly safe in memory, and there is no problem in retrying to encode with a change of parameters.
Therefore before closing the "`Movie encoding`" dialog, action that will delete the data in memory it is recommended to check the result of the encoding, ie. play the movie, if the result is good enough then it is safe to close the dialog by pressing "`Cancel`".

5.2 Mouse interaction with the OpenGL window: visualization

The mouse button functions are the following:

- **Left button**
    - *Single click on object*: object selection
    - *Pressed on background + motion*: model rotation
- **Scroll button**
    - *Scrolled*: zoom in/out
    - *Pressed + motion*: model translation
- **Right button**
    - *Pressed on background*: reproduces the OpenGL window top bar menu
    - *Pressed on object*: object contextual menu

5.2.1 Object selection

The mouse left button allows to select object(s) and display atomic label(s):

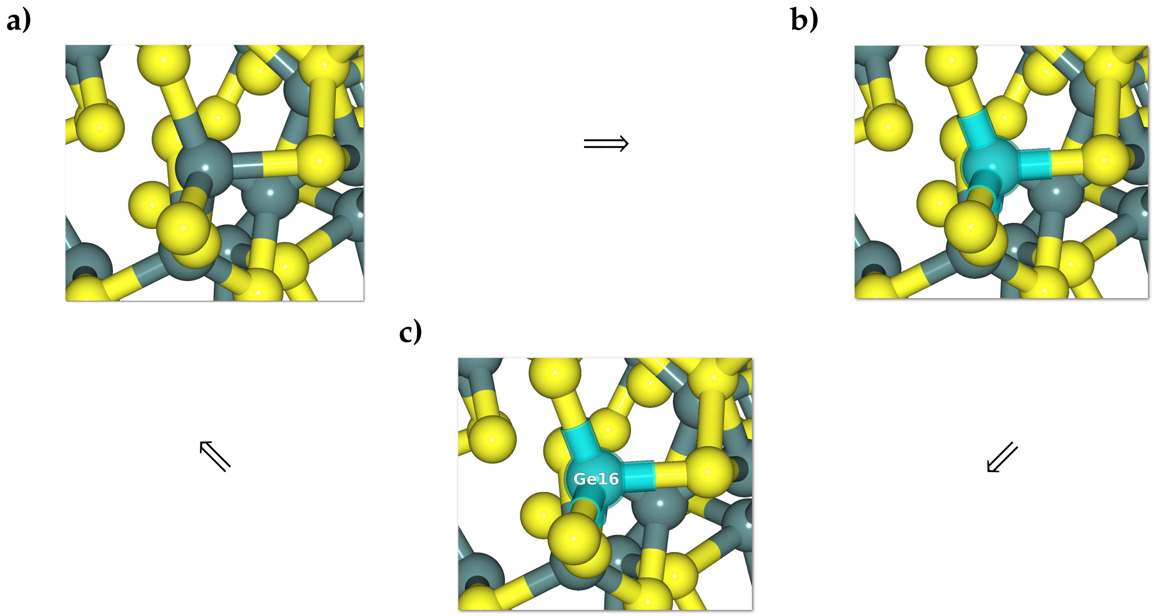
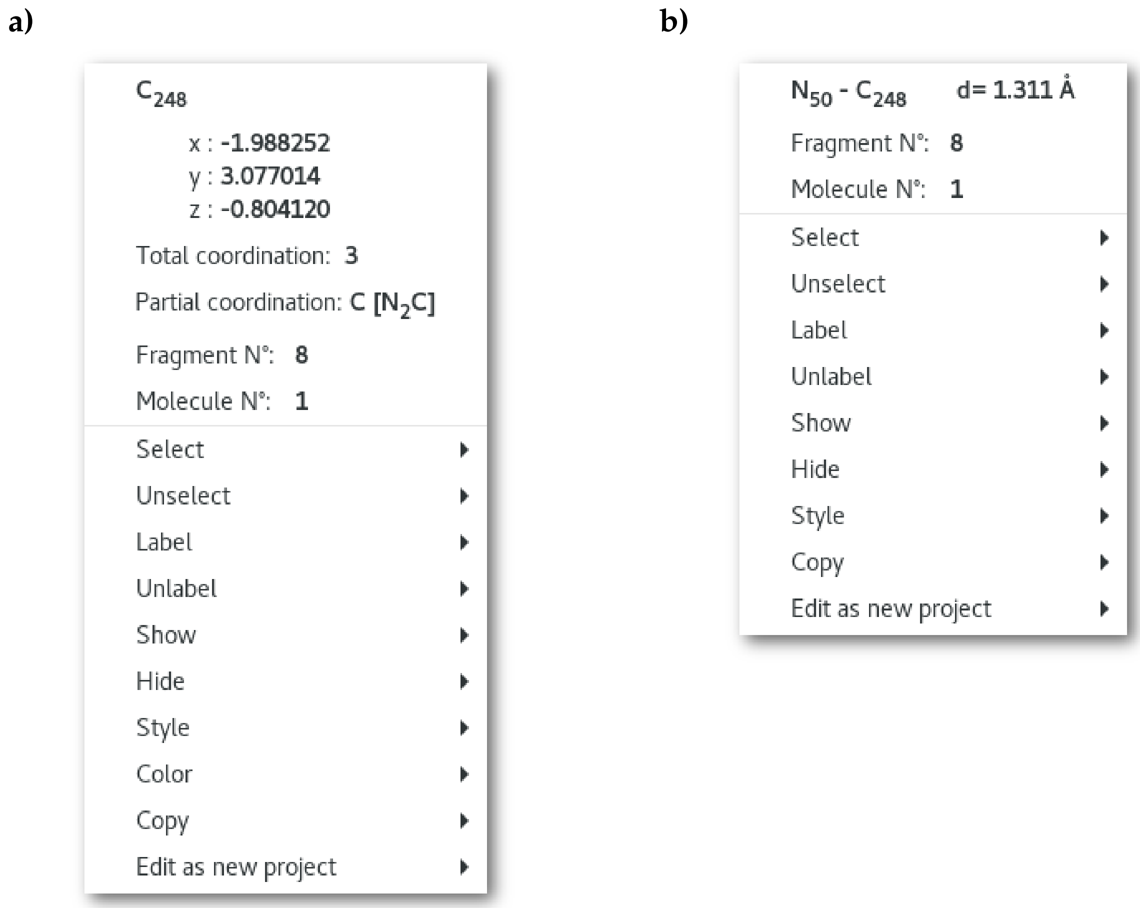


Figure 5.20 *Illustration of the selection / label process using the mouse left button.*

The first click on any atom/bond will select this atom/bond, the selection is highlighted / covered in light blue color [Fig. 5.20-b], a second click and the atom(s) label(s) will be added to the representation [Fig. 5.20-c], finally a third click will unselect the atom(s) and remove the label(s) [Fig. 5.20-a].

5.2.2 Object contextual menu

Pressed over an atom or a bond the right button opens the object contextual menu:



a)

C_{248}

x : -1.988252
y : 3.077014
z : -0.804120

Total coordination: 3

Partial coordination: C [N_2C]

Fragment N°: 8
Molecule N°: 1

b)

N_{50} - C_{248} d= 1.311 Å

Fragment N°: 8
Molecule N°: 1

Figure 5.21 *The object contextual menu:* **a)** *for an atom,* **b)** *for a chemical bond.*

- Over *An atom*: the menu in figure 5.21-a) is displayed, the top part provides several information (when available) related to the atom:
  - The atom id: chemical species and id number in the project
  - The atom coordinates
  - Total coordination of the atom
  - Partial coordination of the atom
  - Fragment and molecule id the atom belongs to
- Over *A chemical bond*: the menu in figure 5.21-b) is displayed, the top part provides several information (when available) related to the bond:
  - The atoms involved in the bond
  - The bond length
  - Fragment and molecule id the bond belongs to

The bottom parts of the object contextual menus in figure 5.21 are almost identical, and contain a list of submenus dedicated to several actions that could be performed in relation to the object, atom or chemical bond, of the contextual menu. The construction of each submenu follow a similar pattern presented bellow.

Construction of the submenus

Figure 5.22 *Construction of the submenus attached to the object contextual menu.*

If the action proposed by the submenu can be applied to this atom/bond then the first element of the menu is a line with the name of this atom/bond [Fig. 5.22-a]. The second line [Fig. 5.22-b] refers, depending on the action of the submenu and/or the status of the atom, to "`selected`" or "`non-selected`" atoms. The third line [Fig. 5.22-c] follows the same idea for the "`labelled`" or "`non-labelled`" atoms. Finally the bottom part [Fig. 5.22-c] refers to the coordinations and the chemistry of the considered object. Most of the actions provided by these submenus being very intuitive, only the "`Style`" and "`Edit as new project`" menus will be introduced in detail thereafter.

5.2.2.1 The "`Style`" submenu

The "`Style`" submenu(s) of the object contextual menu allows to change the visual style locally, ie. for an atom/bond, or any particular set of atom and bonds in the model.

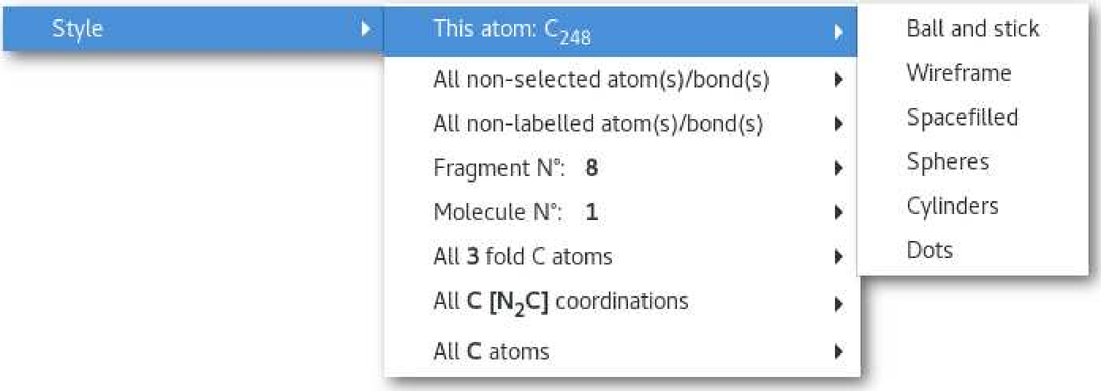


Figure 5.23 *The object contextual menu and the "`Style`" submenu(s).*

Overall using local style(s) allows to improve the visual representation and to highlights particular element(s) [Fig. 5.24].

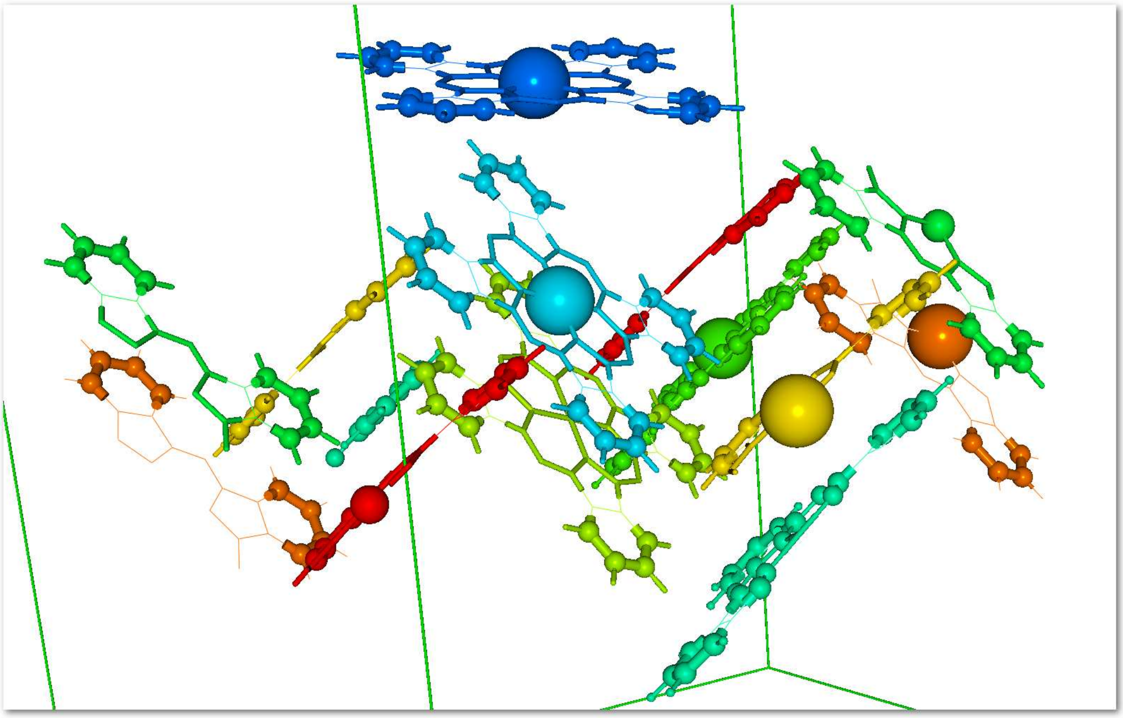


Figure 5.24 *Multiple visual styles the* **atomes** *program.*

The parameters of the local style(s), are inherited from the global style (see section 5.1.1.1). Therefore in order to modify any parameters of a particular style, ie. the sphere radius of an atom for the "`Ball and stick`" style, this style must be applied globally, and the appropriate parameters modified using the "`model`" menu (see section 5.1.2) or the "`Atom(s) configuration`" dialog (Fig. 5.6). Afterwards and when applied locally the "`Ball and stick`" style will use the new parameters. Note that the default atomic radius for the "`Spacefilled`" style, even is this style is not used, is the "`Covalent`" radius, following the local style menu's behavior and if the global "`Spacefilled`" style was not changed, then the local "`Spacefilled`" style(s) will use the same parameters.

5.2.2.2 The "`Copy`" submenu

The "`Copy`" submenu(s) of the object contextual menu allows to copy atomic coordinates, the copied data could then be re-used either using the "`Model edition`" dialog (see section 6.1.3) or the mouse "`Edition mode`" (see section 6.2).

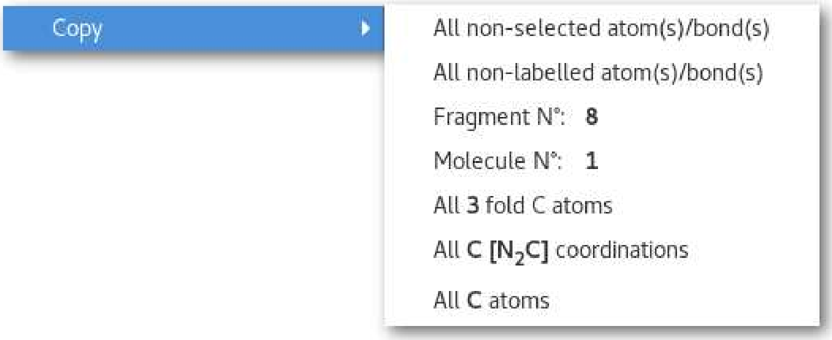


Figure 5.25 *The object contextual menu and the "`Copy`" submenu(s).*

Data can copied from any project, even from an MD trajectory however in that case only the atomic coordinates from the visible MD step will be copied, other will be ignored. Data can only be pasted in project(s) that support the "`Edition mode`" (see chapter 6).

5.2.2.3 The "`Edit as new project`" submenu

The "`Edit as new project`" submenu(s) of the object contextual menu allows to create a new project using any particular set of atom and bonds in the model.

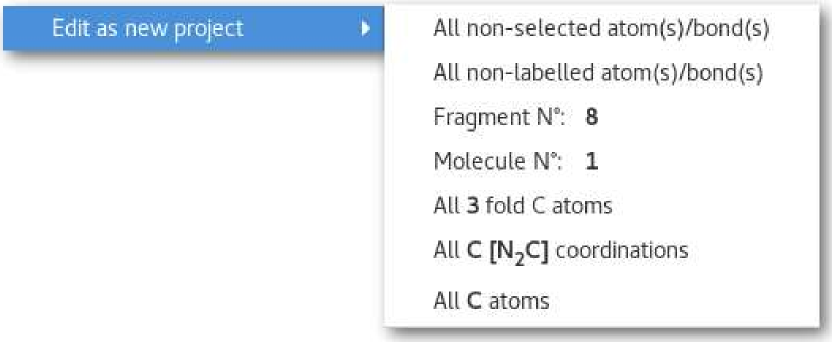
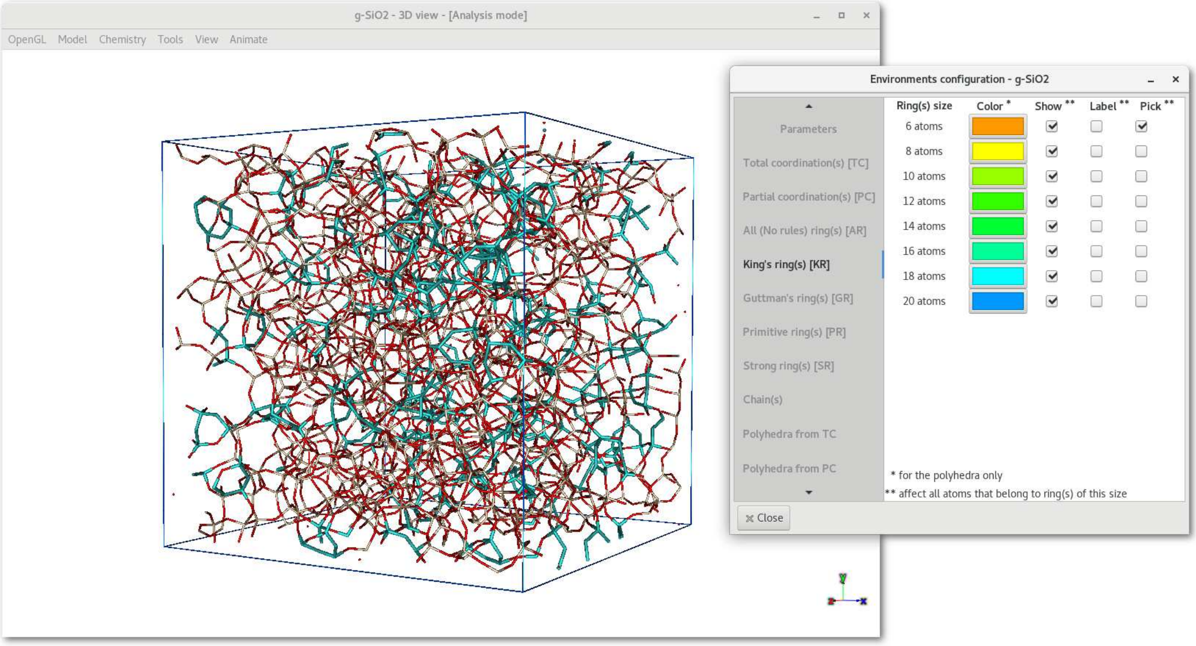


Figure 5.26 *The object contextual menu and the "`Edit as new project`" submenu(s).*

Using any button of this menu the corresponding set of atom(s)/bond(s) will be copied and exported as a new **atomes** project. This new project will immediately be inserted in the workspace tree to be available for further work and a corresponding 3D window will pop-up. Parameters of the initial project will be applied to the new one (style, colors ...), except for the periodicity, if any, that will be lost in the process.

An example is proposed thereafter:

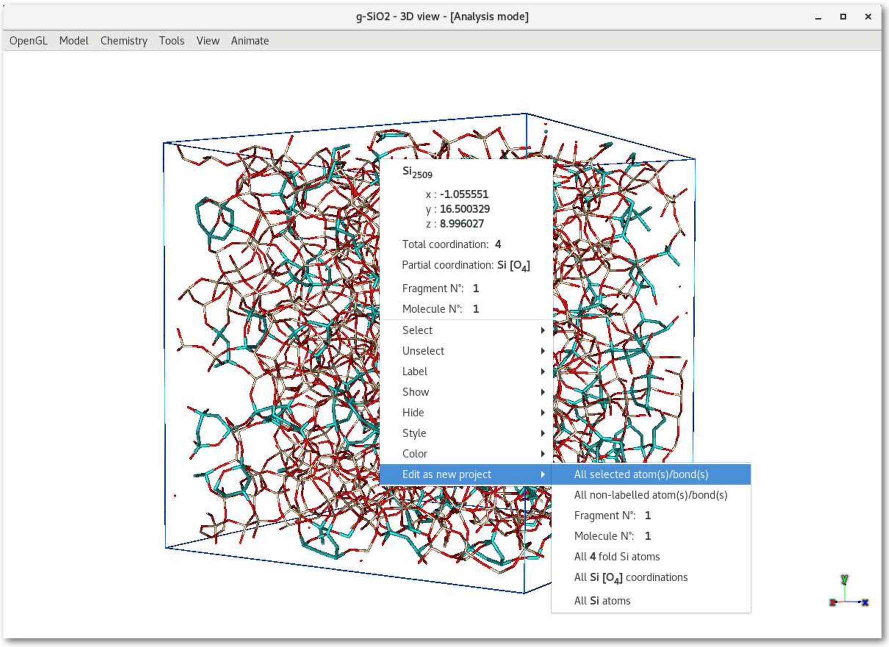
1. For this example the King's rings statistics analysis (see section E.5) was performed on SiO_2 test system, afterwards the "`Advanced environment`" dialog was opened and all atom(s) involved in ring(s) of size 6 atoms were selected (selection is highlighted in light blue):



Ring(s) size	Color *	Show **	Label **	Pick **
6 atoms	🟧	☑	☐	☑
8 atoms	🟨	☑	☐	☐
10 atoms	🟩	☑	☐	☐
12 atoms	🟩	☑	☐	☐
14 atoms	🟩	☑	☐	☐
16 atoms	🟩	☑	☐	☐
18 atoms	🟦	☑	☐	☐
20 atoms	🟦	☑	☐	☐

* for the polyhedra only
** affect all atoms that belong to ring(s) of this size

2. After the selection, the object contextual menu is used to "`Edit as new project`" the list of "`All selected atom(s)/bond(s)`":



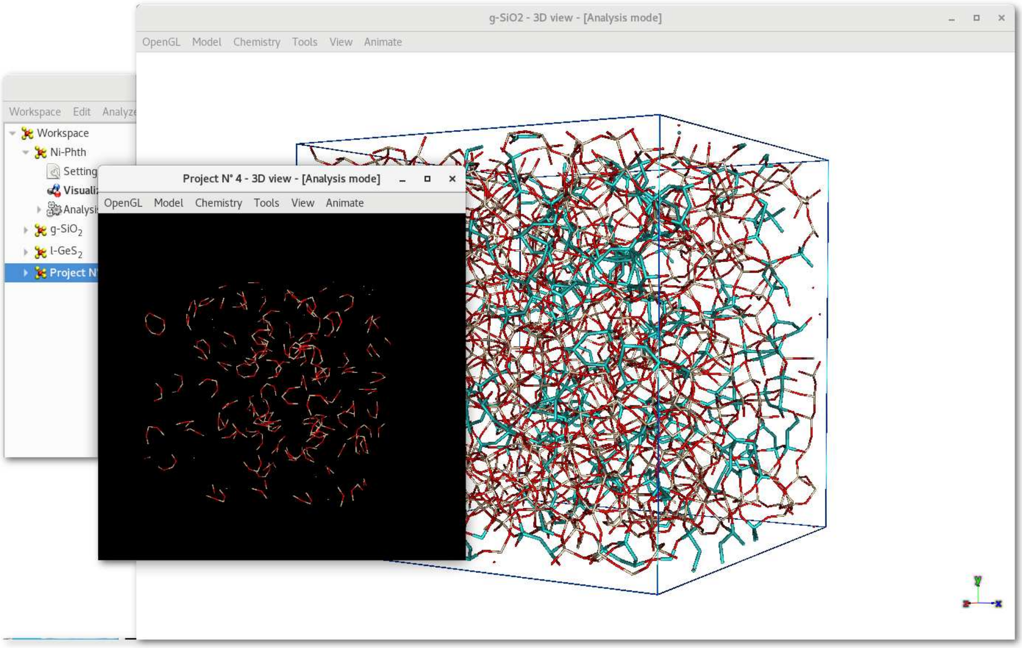
Si_{2509}

x : -1.055551
y : 16.500329
z : 8.996027

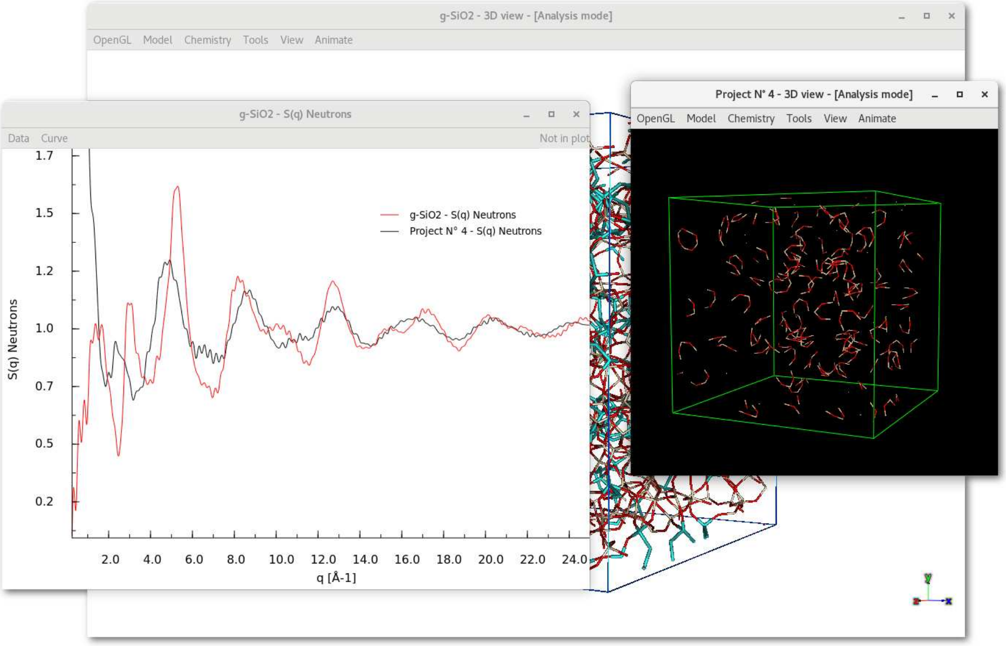
Total coordination: 4
Partial coordination: Si [O$_4$]
Fragment N°: 1
Molecule N°: 1

Fragment N°: 1
Molecule N°: 1

3. The new project "`Project N° 4`" that contains the appropriate atom(s)/bond(s) is created and inserted in the workspace tree, and the new OpenGL window pops up:



4. Finally after restoring the periodicity, it is possible to calculate any other properties for the new model, ie. the selection from the SiO_2 model, and compare the results with one for the original system:



5.3 Keyboard shortcuts

- Single key shortcuts:
  - Colors:
    a : change atom(s) colormap
    p : change polyhedra(ons) colormap
  - Styles:
    b : change default style to "`Ball and stick`"
    c : change default style to "`Cylinders`"
    d : change default style to "`Dots`"
    s : change default style to "`Spheres`"
    o : change default style to "`Covalent radius`"
    i : change default style to "`Ionic radius`"
    v : change default style to "`van Der Waals radius`"
    r : change default style to "`In cristal radius`"
    w : change default style to "`Wireframe`"
  - Measures:
    m : show all measures for the selection, if pressed:
      - once: display inter-atomic distance(s)
      - twice: display inter-atomic angles
      - a third time: hide measures
  - Model rotation:
    → : rotate right
    ← : rotate left
    ↑ : rotate up
    ↓ : rotate down
- Misc:

  Esc : exit fullscreen mode

  ␣ : pause / restart spinning

- Combined keys shortcuts:
    - Mouse mode:

      Alt + a : enter mouse "`Analysis`" mode
      Alt + e : enter mouse "`Edition`" mode

    - Selection:

      Ctrl + a : select / unselect all atoms
      Ctrl + c : copy all selected atom(s)
    - Mouse selection mode:

      Shift ⇑ + a : atom selection mode
      Shift ⇑ + c : coordination sphere selection mode
      Shift ⇑ + f : fragment selection mode
      Shift ⇑ + m : molecule selection mode

    - Camera motion:

      Ctrl + → : move camera right
      Ctrl + ← : move camera left
      Ctrl + ↑ : move camera up
      Ctrl + ↓ : move camera down
      Shift ⇑ + ↑ : zoom out
      Shift ⇑ + ↓ : zoom in

    - Spinning:

      Ctrl + Shift ⇑ + → : spin right / increase speed right or reduce speed left
      Ctrl + Shift ⇑ + → : spin left / increase speed left or reduce speed right
      Ctrl + Shift ⇑ + ↑ : spin up / increase speed up or reduce speed down
      Ctrl + Shift ⇑ + ↓ : spin down / increase speed down or reduce speed up
      Ctrl + s : stop spinning

    - Misc:

      Ctrl + l : label / unlabel all atoms
      Ctrl + e : open the "`Environments configuration`" window [Sec. 5.1.3]
      Ctrl + m : open the "`Measures`" dialog [Sec. 5.1.4]
      Ctrl + r : open the "`Recorder`" dialog [Sec. 5.1.6]
      Ctrl + f : enter / exit fullscreen mode

Visual edition in atomes

In this chapter the examples will be illustrated using the same workspace used to illustrate the visual analysis capabilities of **atomes** in the previous chapter and presented in figure 5.1.
Edition tools are available via the "`Tools`" menu, and using either the "`Edit`" submenu [Fig. 6.1-a] or the mouse "`Edition`" from in the "`Mouse mode`" submenu [Fig. 6.1-b]:

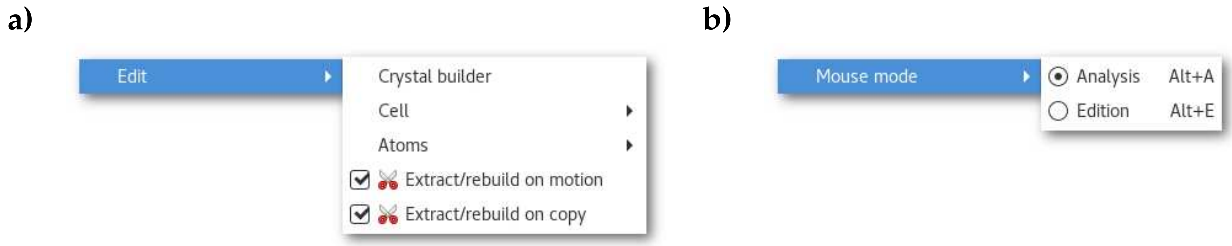


Figure 6.1 *Accessing the edition tools in the* **atomes** *program.*

6.1 The "`Edit`" submenu

6.1.1 The "`Crystal builder`" window

The "`Crystal builder`" button [Fig. 6.2] allows to open the corresponding window.

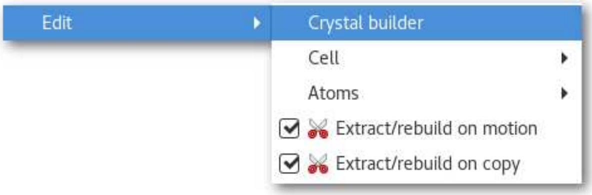
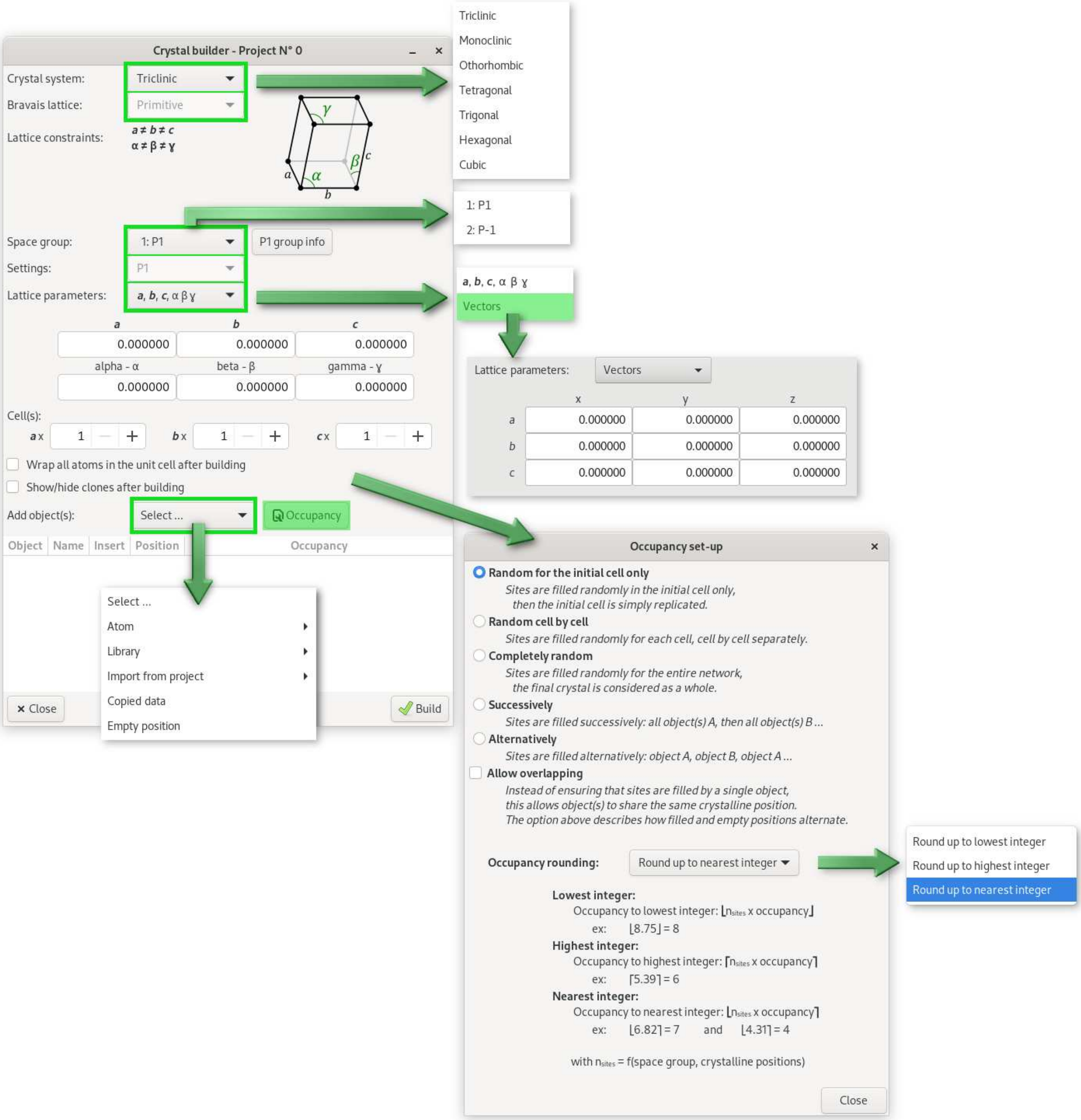


Figure 6.2 *Accessing the "*`Crystal builder`*" window in the* **atomes** *program.*



● **Random for the initial cell only**
Sites are filled randomly in the initial cell only, then the initial cell is simply replicated.

○ **Random cell by cell**
Sites are filled randomly for each cell, cell by cell separately.

○ **Completely random**
Sites are filled randomly for the entire network, the final crystal is considered as a whole.

○ **Successively**
Sites are filled successively: all object(s) A, then all object(s) B ...

○ **Alternatively**
Sites are filled alternatively: object A, object B, object A ...

☐ **Allow overlapping**
Instead of ensuring that sites are filled by a single object, this allows object(s) to share the same crystalline position. The option above describes how filled and empty positions alternate.

Occupancy rounding: Round up to nearest integer

Lowest integer:
Occupancy to lowest integer: $\lfloor n_{sites} \times occupancy \rfloor$
ex: $\lfloor 8.75 \rfloor = 8$
Highest integer:
Occupancy to highest integer: $\lceil n_{sites} \times occupancy \rceil$
ex: $\lceil 5.39 \rceil = 6$
Nearest integer:
Occupancy to nearest integer: $\lfloor n_{sites} \times occupancy \rceil$
ex: $\lfloor 6.82 \rceil = 7$ and $\lfloor 4.31 \rceil = 4$

with n_{sites} = f(space group, crystalline positions)

Figure 6.3 *The "`Crystal builder`" window in the* **atomes** *program.*

The "`Crystal builder`" window [Fig. 6.3] allows the creation of crystalline structure(s) and super-structure(s). Thus not only atom(s) but also molecules can be inserted to the crystalline positions defined by the space group.
The "`Select ...`" menu allows to insert objects: atoms, molecules, and atom selections from any other project opened in the **atomes** workspace. It will be presented in details in section 6.1.3, at the exception of the "`Empty site`" button unique to the "`Crystal builder`" and that will be introduced in the next pages related to the occupancy.

Each object will be inserted at a position specified using the fractional coordinates, in the proportion of the occupancy, and following the rules of the selected space group. The following parameters can be adjusted:

1. The crystal system:
    - Triclinic
    - Monoclinic
    - Orthorhombic
    - Tetragonal
    - Trigonal
    - Hexagonal
    - Cubic
2. The type of Bravais lattice, depending on 1, in:
    - Primitive
    - Base-centered
    - Body-centered
    - Face-centered
    - Hexagonal axes
    - Rhombohedral axes
3. The space group, from 230 groups of the International tables for Crystallography Vol. A, [29] and filtered using 1 and 2
4. The space group setting, if more than one is available.
5. The format of the lattice parameters:
    - $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ and α, β, γ
    - Vector components: a(x,y,z), b(x,y,z), c(x,y,z)
6. The number of cell(s) to replicate on $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ to create the final supercell.
7. If atomic coordinates are to be wrapped in the crystalline unit after building it.
8. If clones are to be shown afer building the crytal.
9. The object to insert to build the crystal using information specified at steps 1, 2, 3, 4 and 5, including the following options:
    - The type of object (atom, molecule ...)
    - The fractional coordinates of the object
    - The occupancy of the crystallographic site (between 0.0 and 1.0)
    - How to handle occupancy (if < 1.0), object(s) and/or empty position(s):
        - "`Random for the initial cell only`": sites are filled randomly in the initial cell only, then the initial cell is simply replicated.
        - "`Random cell by cell`": sites are filled randomly for each cell, cell by cell separately.
        - "`Completely random`": sites are filled randomly for the entire network, the final crystal is considered as whole.
        - "`Successively`": sites are filled successively, all object(s) A are inserted (for the first $n(A)$ positions), then all object(s) B are inserted (for the next $n(B)$ positions) ...
        - "`Alternatively`": sites are filled alternatively: object A is inserted on the first position, object B is inserted on the second position, object A on the third position, object B on the fourth position ... and so on.

In any case the number $n(A)$ of object(s) A to be inserted in calculated using:

$$n(A) = NP \times occ(A)$$

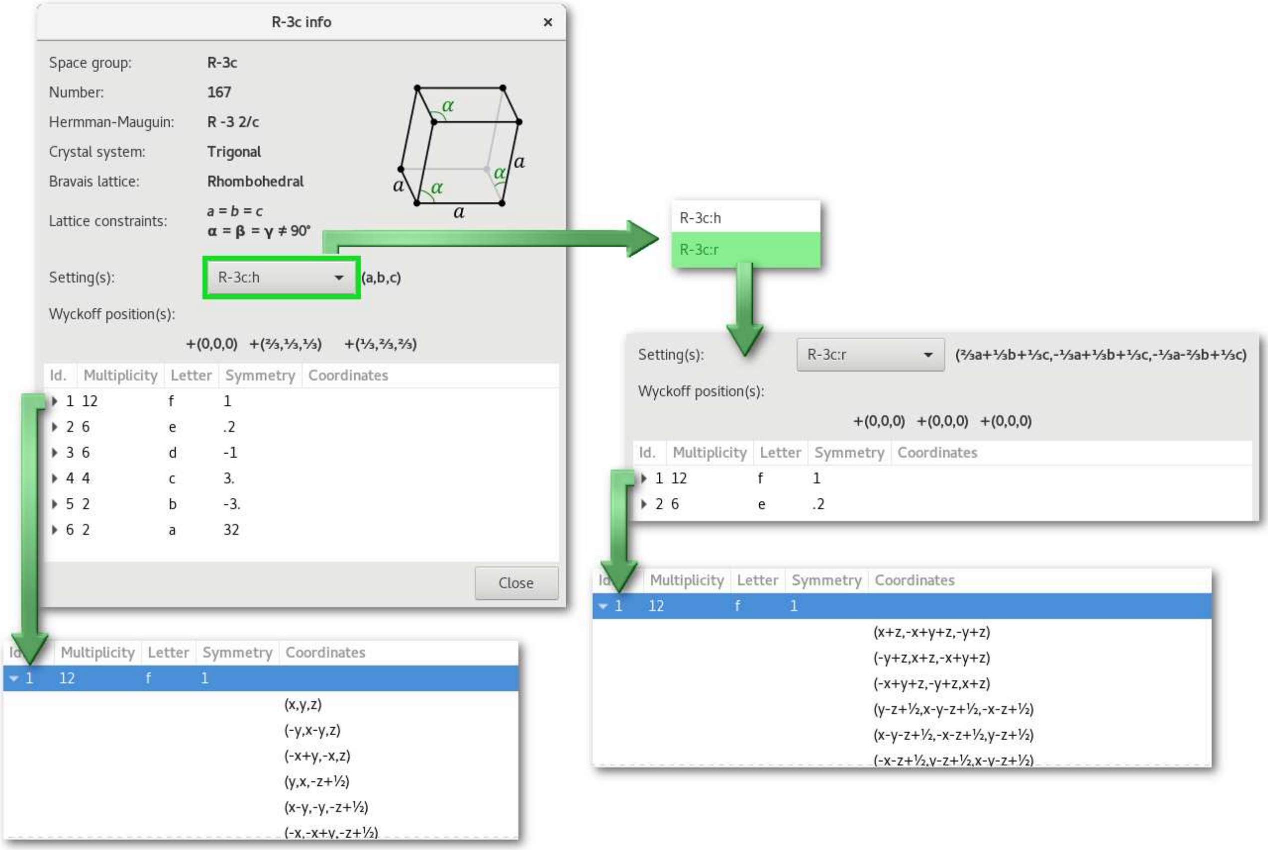
NP is the number of position(s) to fill, $occ(A)$ is the occupancy for object A. Note that it is possible to adjust how the rounding is performed to determine occupancy:

- Lowest integer: $\lfloor NP \times occ(A) \rfloor$
- Highest integer: $\lceil NP \times occ(A) \rceil$
- Nearest integer: $\lfloor NP \times occ(A) \rceil$

Overlapping, object(s) on the same position, can also be allowed, the concept will be illustrated in the following examples.

Using the crystal builder: space group information

Once a space group has been selected it is possible to access the "`Space group info`" dialog using the "`group info`" button:



R-3c info

Space group: R-3c
Number: 167
Hermman-Mauguin: R -3 2/c
Crystal system: Trigonal
Bravais lattice: Rhombohedral
Lattice constraints: a = b = c
α = β = γ ≠ 90°

Setting(s): R-3c:h (a,b,c)

Wyckoff position(s):

+(0,0,0) +(⅔,⅓,⅓) +(⅓,⅔,⅔)

Id.	Multiplicity	Letter	Symmetry	Coordinates
1	12	f	1	
2	6	e	.2	
3	6	d	-1	
4	4	c	3.	
5	2	b	-3.	
6	2	a	32	

Id.	Multiplicity	Letter	Symmetry	Coordinates
1	12	f	1	
				(x,y,z)
				(-y,x-y,z)
				(-x+y,-x,z)
				(y,x,-z+½)
				(x-y,-y,-z+½)
				(-x,-x+y,-z+½)

Setting(s): R-3c:r (⅔a+⅓b+⅓c,-⅓a+⅓b+⅓c,-⅓a-⅔b+⅓c)

Wyckoff position(s):

+(0,0,0) +(0,0,0) +(0,0,0)

Id.	Multiplicity	Letter	Symmetry	Coordinates
1	12	f	1	
2	6	e	.2	

Id.	Multiplicity	Letter	Symmetry	Coordinates
1	12	f	1	
				(x+z,-x+y+z,-y+z)
				(-y+z,x+z,-x+y+z)
				(-x+y+z,-y+z,x+z)
				(y-z+½,x-y-z+½,-x-z+½)
				(x-y-z+½,-x-z+½,y-z+½)
				(-x-z+½,y-z+½,x-y-z+½)

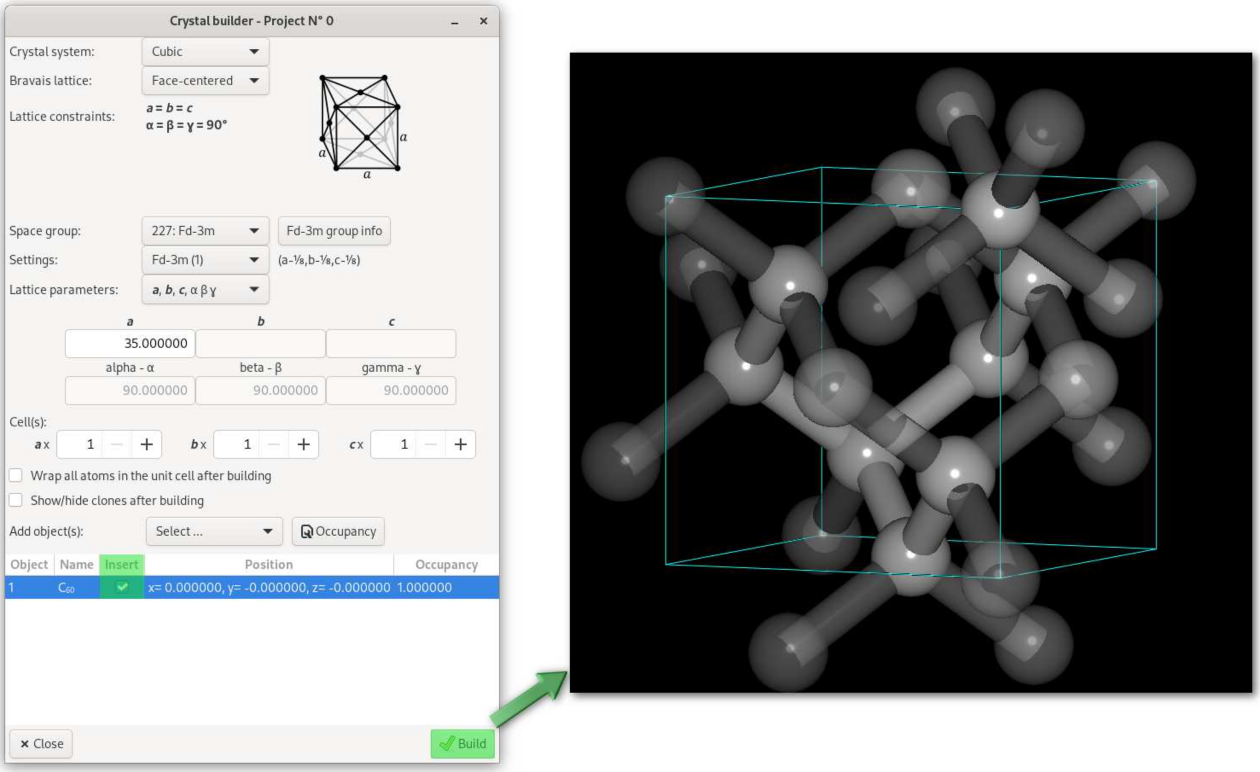
Figure 6.4 *The "`space group info`" dialog for the* **R$\bar{3}$c** *group in the* **atomes** *program.*

The main information available is presented in the "`space group info`" dialog [Fig. 6.4], including the different setting(s), and the corresponding initial coordinates and Wyckoff positions.

Using the crystal builder: building crystal(s)

The following pages will present crystal building examples using the **Fd$\bar{3}$m** (origin 1 setting) space group (diamond-like structure):

1. ***The C-diamond structure***:



Crystal builder - Project N° 0

Crystal system: Cubic

Bravais lattice: Face-centered

Lattice constraints: $a = b = c$, $\alpha = \beta = \gamma = 90°$

Space group: 227: Fd-3m

Settings: Fd-3m (1) (a-⅛,b-⅛,c-⅛)

Lattice parameters: a, b, c, α β γ

a	b	c
35.000000		
alpha - α	beta - β	gamma - γ
90.000000	90.000000	90.000000

Cell(s): a x 1, b x 1, c x 1

☐ Wrap all atoms in the unit cell after building

☐ Show/hide clones after building

Add object(s): Select ...

Object	Name	Insert	Position	Occupancy
1	C_{60}	✓	x= 0.000000, y= -0.000000, z= -0.000000	1.000000

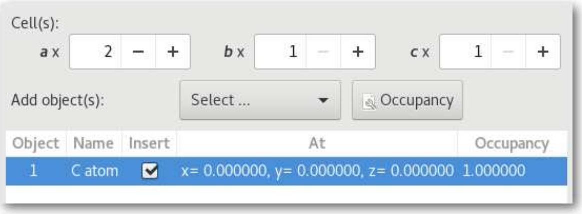
Figure 6.5 *Building a C-diamond crystal in the* **atomes** *program.*

The following steps are required to build the C-diamond crystalline structure (see figure 6.5-left):

- Select the **Fd$\bar{3}$m** space group ("`Cubic -> Face-centered -> 227: Fd-3m`")
- Set the value for the lattice parameter: ≃ 3.5 Å
- Insert a C atom at (0.0, 0.0, 0.0) with occupancy to 1.0, you can edit both coordinates and occupancy by double-clicking on the corresponding line.
- Select the "`Insert check button`" to use the atom to build the crystal, or alternatively click to top of the "Insert" column to insert all elements.
- Finally simply click on the "`Build / Build (new project)`" button.

The crystal is then displayed (see figure 6.5-right), also clones (atoms linked using the PBC see section 5.1.2.3) are immediately shown. The existence of a chemical bond depending on the cutoff(s), determined automatically when creating the crystal, you might need to adjust the values to define properly the bonding of the system.

2. ***The C-diamond structure, playing with occupancy***:
   In these examples the parameters to build the crystal remain exactly similar to 1, only the total number of cells will be increased to 2 on ***a***:

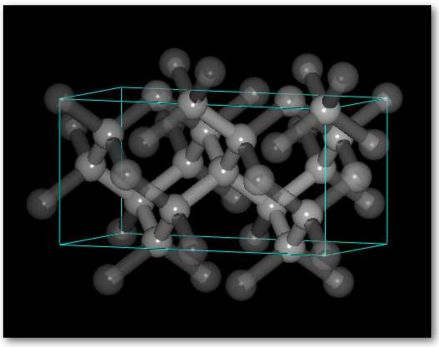


Cell(s):
a x 2
b x 1
c x 1

Add object(s): Select ...

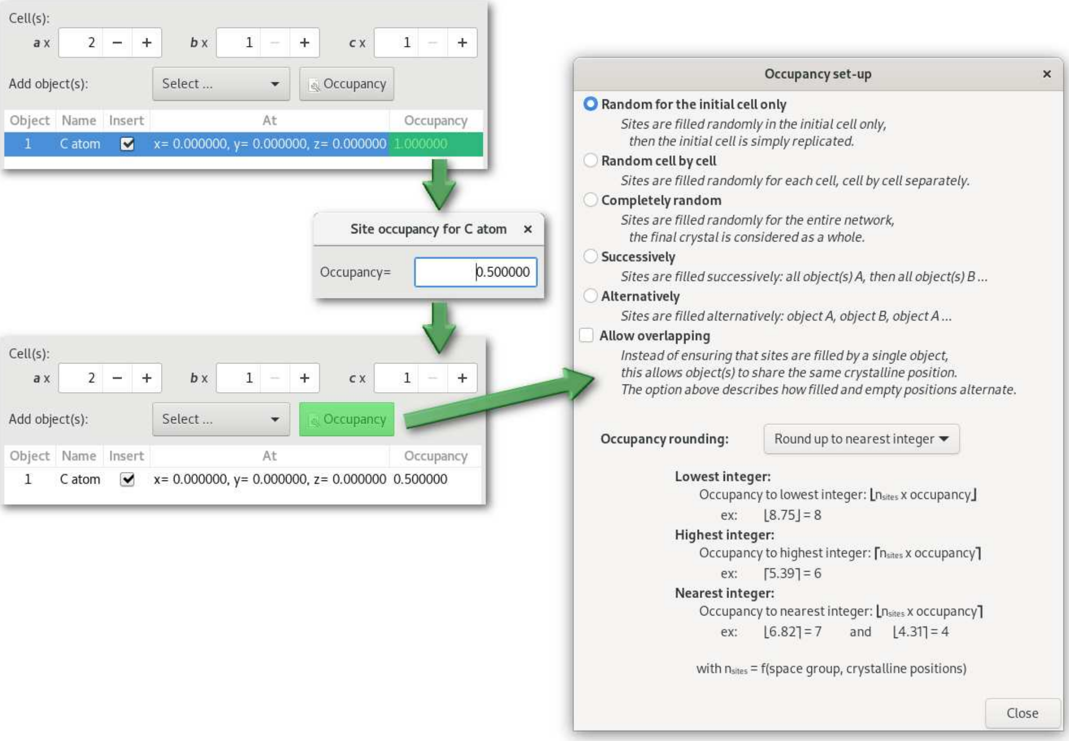
Object	Name	Insert	At	Occupancy
1	C atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	1.000000

- Occupancy = 1.0:



With 8 atoms per cell, the total number of atoms in the system is equal to 16.

- Occupancy = 0.5:



Cell(s):
a x 2
b x 1
c x 1

Add object(s): Select ...

Object	Name	Insert	At	Occupancy
1	C atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	1.000000

Site occupancy for C atom

Occupancy= 0.500000

Cell(s):
a x 2
b x 1
c x 1

Add object(s): Select ...

Object	Name	Insert	At	Occupancy
1	C atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.500000

Occupancy set-up

● **Random for the initial cell only**
Sites are filled randomly in the initial cell only, then the initial cell is simply replicated.
○ **Random cell by cell**
Sites are filled randomly for each cell, cell by cell separately.
○ **Completely random**
Sites are filled randomly for the entire network, the final crystal is considered as a whole.
○ **Successively**
Sites are filled successively: all object(s) A, then all object(s) B ...
○ **Alternatively**
Sites are filled alternatively: object A, object B, object A ...
☐ **Allow overlapping**
Instead of ensuring that sites are filled by a single object, this allows object(s) to share the same crystalline position. The option above describes how filled and empty positions alternate.

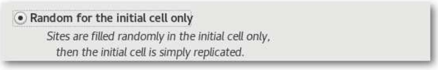
Occupancy rounding: Round up to nearest integer

Lowest integer:
Occupancy to lowest integer: $\lfloor n_{sites} \times occupancy \rfloor$
ex: $\lfloor 8.75 \rfloor = 8$
Highest integer:
Occupancy to highest integer: $\lceil n_{sites} \times occupancy \rceil$
ex: $\lceil 5.39 \rceil = 6$
Nearest integer:
Occupancy to nearest integer: $\lfloor n_{sites} \times occupancy \rceil$
ex: $\lfloor 6.82 \rceil = 7$ and $\lfloor 4.31 \rceil = 4$

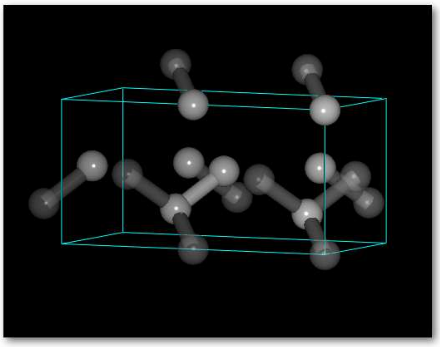
with n_{sites} = f(space group, crystalline positions)

With an occupancy of 0.5 the number of atoms per cell will be reduced to 4, and the total number of atoms in the system to 8.

(1)

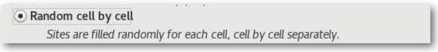

● Random for the initial cell only
Sites are filled randomly in the initial cell only,
then the initial cell is simply replicated.

⟹

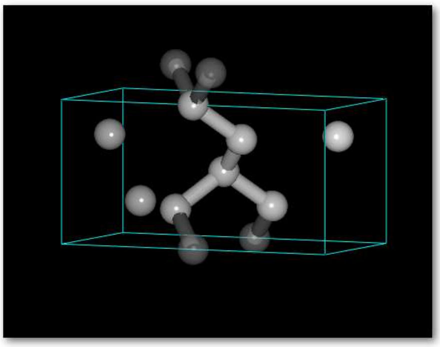


"`Random for the initial cell only`":
The same treatment is applied to each cell, inducing an overall symmetry.
The system is not disordered with 4 atoms per cell at the exact same positions.

(2)

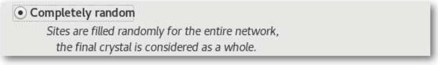

● Random cell by cell
Sites are filled randomly for each cell, cell by cell separately.

⟹

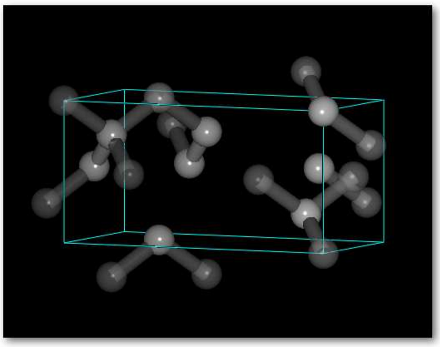


"`Random cell by cell`":
A random treatment is applied to each cell independently.
The system is disordered, but the number of atoms per cell remains equal to 4.

(3)


● Completely random
Sites are filled randomly for the entire network,
the final crystal is considered as a whole.

⟹

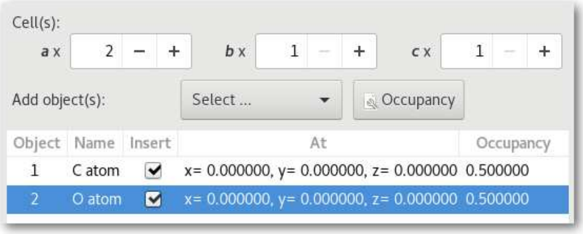


"`Completely random`":
The system is entirely disordered.
The average value 0.5 C atoms per site is respected for the entire structure,
but the number of atom(s) per cell can change.
This option if particularly useful when the occupancy for a particular site is very low,
see the section remarks afterwards for more information.

To illustrate (4) "`Successively`" and (5) "`Alternatively`" it is interesting to use more than one chemical species:

Adding O atoms:
For all chemical species:
- The occupancy is equal to 0.5
- The site is the same (0.0, 0.0, 0.0)

⇓

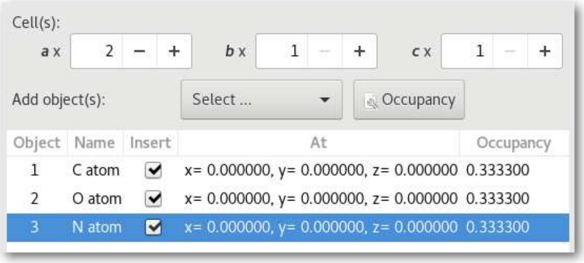

Cell(s):
a x 2
b x 1
c x 1
Add object(s):

Object	Name	Insert	At	Occupancy
1	C atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.500000
2	O atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.500000

⇓

Adding O and N atoms:
For all chemical species:
- The occupancy is equal 0.333
- The site is the same (0.0, 0.0, 0.0)

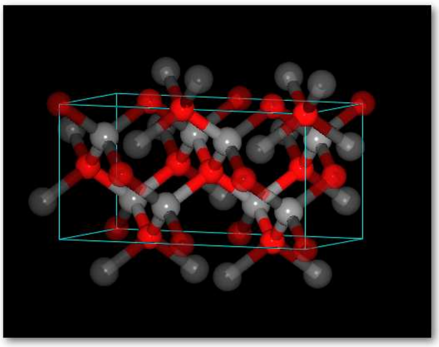
⇓

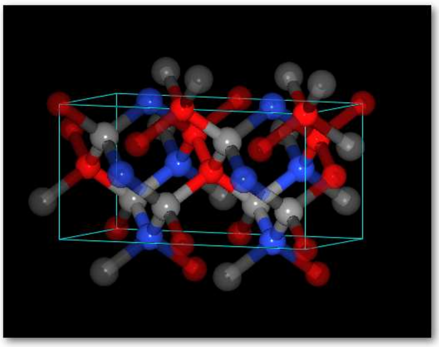

Cell(s):
a x 2
b x 1
c x 1
Add object(s):

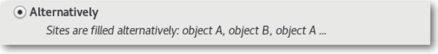
Object	Name	Insert	At	Occupancy
1	C atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.333300
2	O atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.333300
3	N atom	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.333300

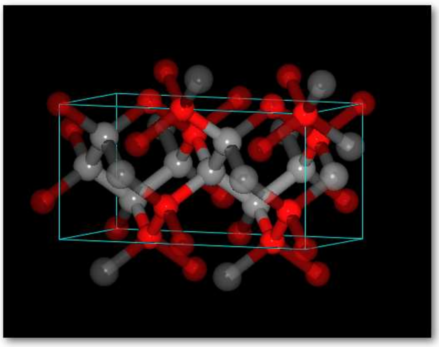
⇓

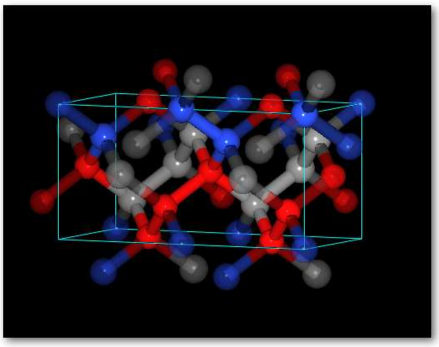

● Successively
Sites are filled successively: all object(s) A, then all object(s) B ...






● Alternatively
Sites are filled alternatively: object A, object B, object A ...

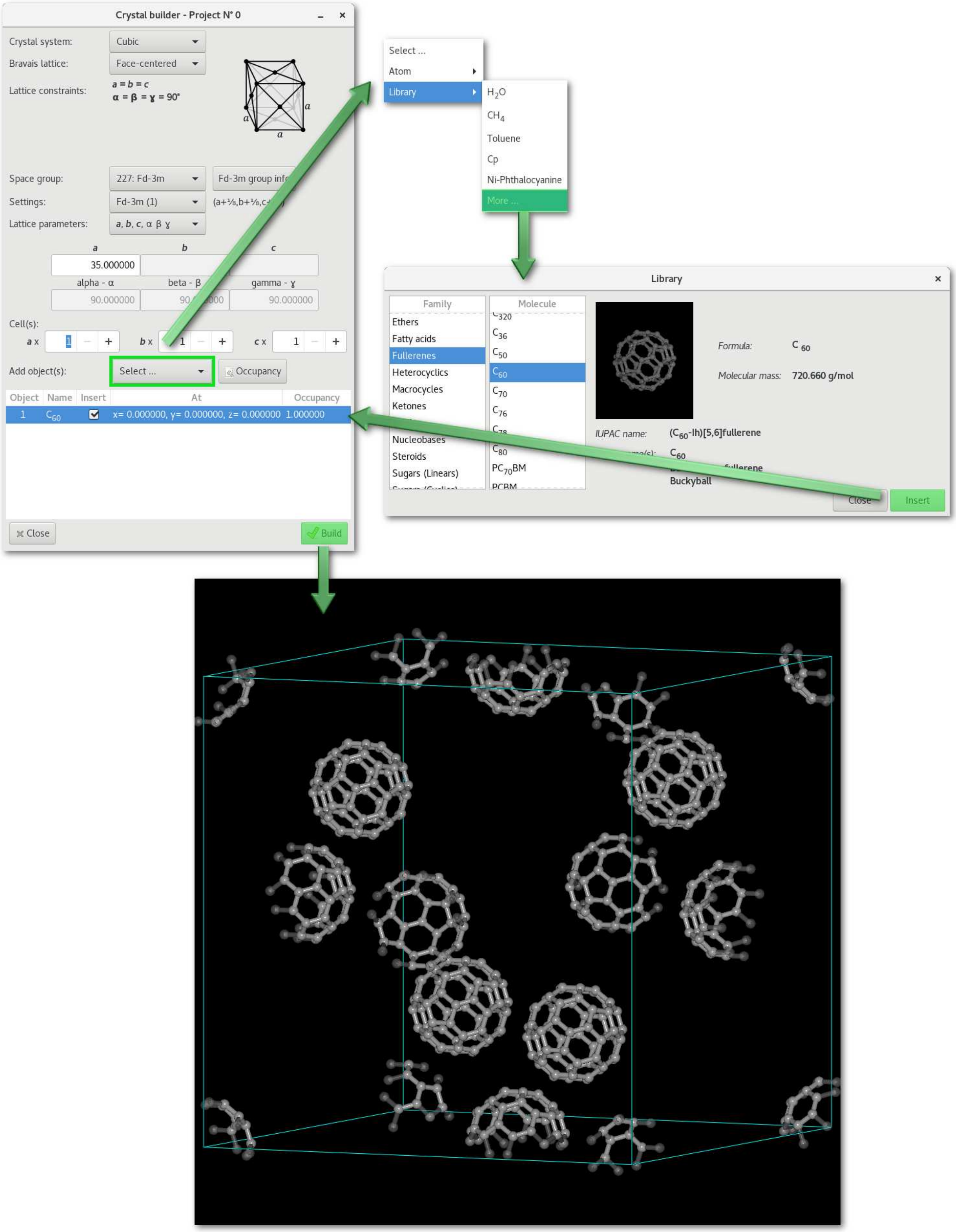




In both cases (4) "`Successively`" and (5) "`Alternatively`":

The system is ordered.
The average values of the occupancy per site are respected for the entire structure.

- ***The C-diamond structure, playing with molecules***:
  As already mentioned **atomes** does not only allow to build atomic crystalline structures but also molecular crystalline super-structures.



Crystal builder - Project N° 0

Crystal system: Cubic
Bravais lattice: Face-centered
Lattice constraints: $a = b = c$, $\alpha = \beta = \gamma = 90°$
Space group: 227: Fd-3m
Settings: Fd-3m (1)
Lattice parameters: a, b, c, α β γ
a: 35.000000
alpha - α: 90.000000
gamma - γ: 90.000000
Cell(s): a x 1, b x 1, c x 1
Add object(s): Select ...

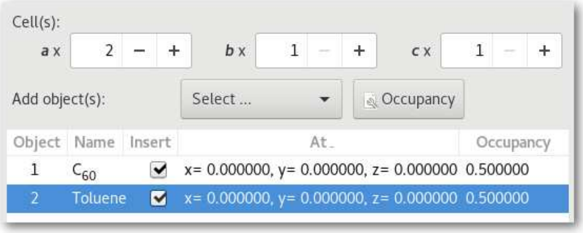
Object	Name	Insert	At	Occupancy
1	C_{60}	☑	x= 0.000000, y= 0.000000, z= 0.000000	1.000000

Library

Formula: C_{60}
Molecular mass: 720.660 g/mol
IUPAC name: $(C_{60}$-Ih)[5,6]fullerene
Buckyball

Figure 6.6 *Building a C-diamond like C_{60} crystalline super-structure.*

The "`Insert...`" menu allows indeed to insert fragments from the library or from any project opened in the workspace.
Using C_{60} fullerene molecules instead of carbon atoms (and increasing the lattice parameter appropriately) allows to obtain the structure illustrated in figure 6.6.
As for the atom(s) tweaking the occupancy can be useful with molecules:



Cell(s):

a x 2 − + b x 1 − + c x 1 − +

Add object(s): Select ... Occupancy

Object	Name	Insert	At.	Occupancy
1	C_{60}	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.500000
2	Toluene	☑	x= 0.000000, y= 0.000000, z= 0.000000	0.500000

Using the (4) "`Successively`" occupancy set-up, you build:

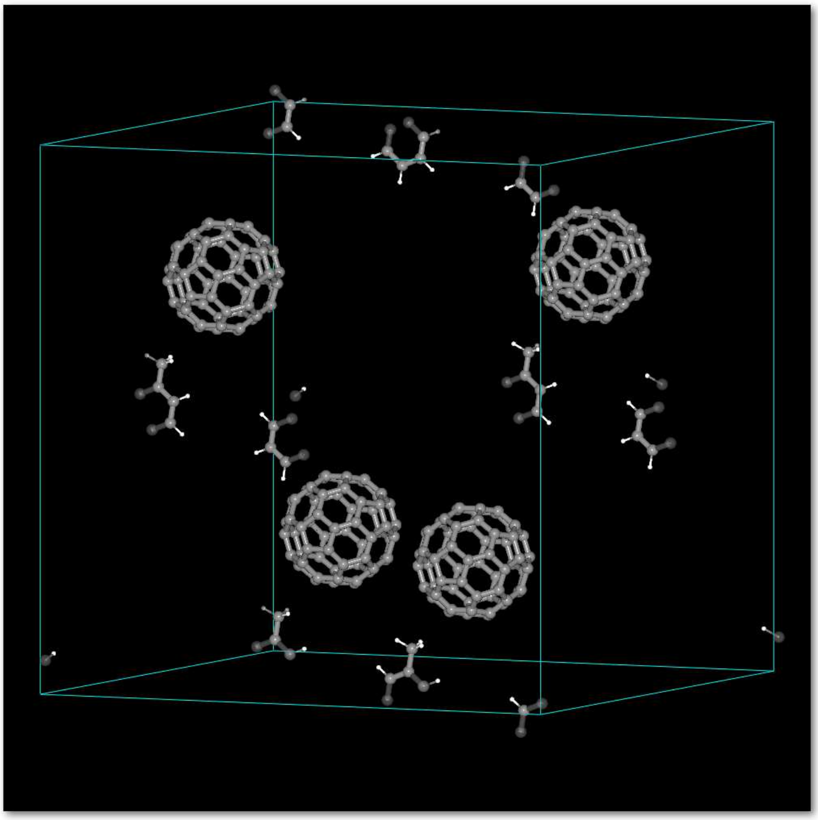
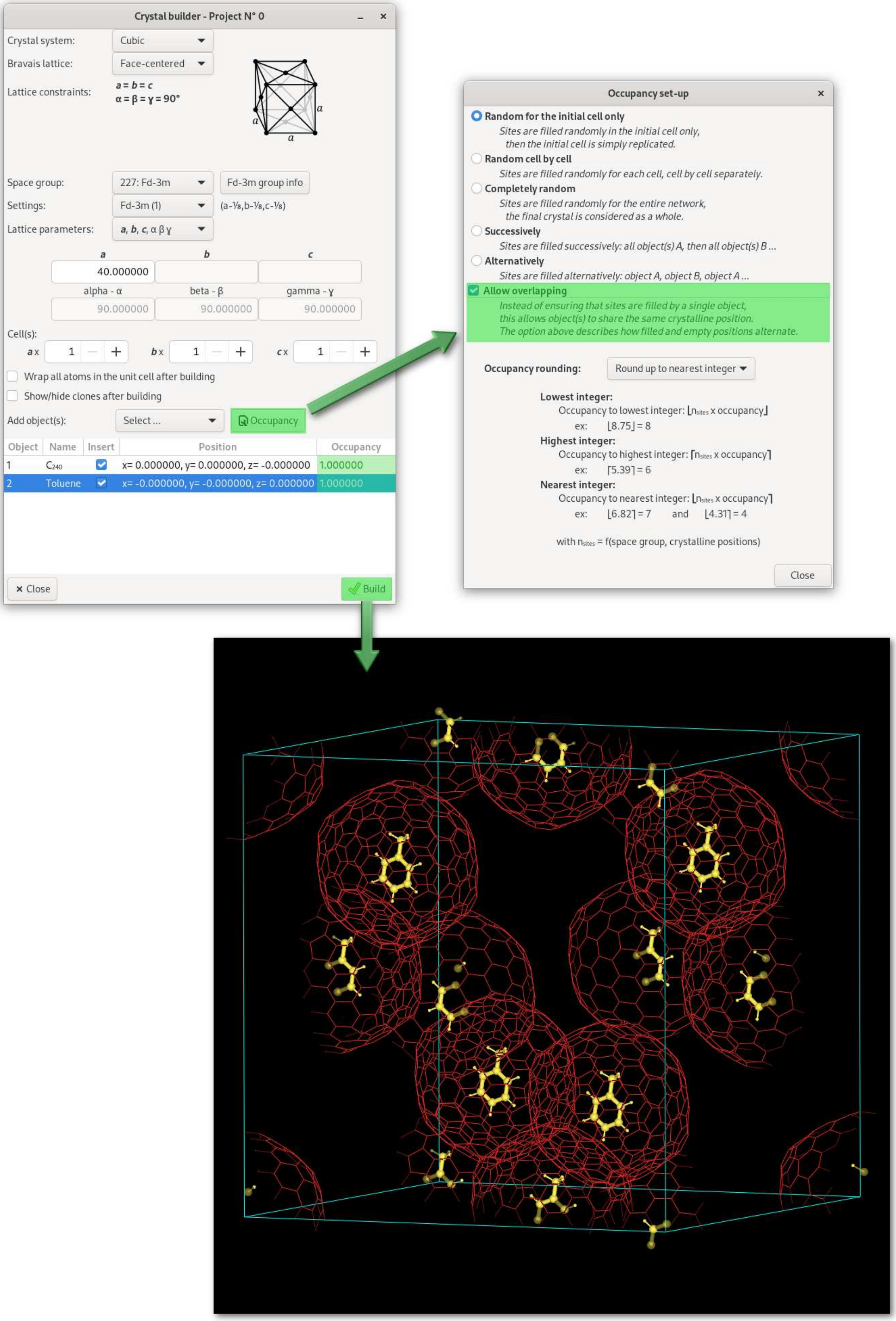


Figure 6.7 *Building a C-diamond like, alternating C_{60} and toluene molecules, crystalline super-structure.*

- ***The C-diamond structure, molecules and overlapping***:
  As mentioned using the "`Allow overlapping`" option allows to insert at the same crystalline positions. The interest is limited to molecules-molecules overlapping or molecules-atoms overlapping, there is no point in getting two atoms at the same position. The idea behind this concept is to allows the encapsulation of an object by another one:



Crystal system: Cubic

Bravais lattice: Face-centered

Lattice constraints: $a = b = c$ $\alpha = \beta = \gamma = 90°$

Space group: 227: Fd-3m — Fd-3m group info

Settings: Fd-3m (1) — (a-⅛,b-⅛,c-⅛)

Lattice parameters: a, b, c, α β γ

a	b	c
40.000000		
alpha - α	beta - β	gamma - γ
90.000000	90.000000	90.000000

Cell(s): a x 1 — b x 1 — c x 1

☐ Wrap all atoms in the unit cell after building

☐ Show/hide clones after building

Add object(s): Select ... — Occupancy

Object	Name	Insert	Position	Occupancy
1	C_{240}	☑	x= 0.000000, y= 0.000000, z= -0.000000	1.000000
2	Toluene	☑	x= -0.000000, y= -0.000000, z= 0.000000	1.000000

● **Random for the initial cell only**
Sites are filled randomly in the initial cell only, then the initial cell is simply replicated.

○ **Random cell by cell**
Sites are filled randomly for each cell, cell by cell separately.

○ **Completely random**
Sites are filled randomly for the entire network, the final crystal is considered as a whole.

○ **Successively**
Sites are filled successively: all object(s) A, then all object(s) B ...

○ **Alternatively**
Sites are filled alternatively: object A, object B, object A ...

☑ **Allow overlapping**
Instead of ensuring that sites are filled by a single object, this allows object(s) to share the same crystalline position. The option above describes how filled and empty positions alternate.

Occupancy rounding: Round up to nearest integer

Lowest integer:
Occupancy to lowest integer: $\lfloor n_{sites} \times occupancy \rfloor$
ex: $\lfloor 8.75 \rfloor = 8$

Highest integer:
Occupancy to highest integer: $\lceil n_{sites} \times occupancy \rceil$
ex: $\lceil 5.39 \rceil = 6$

Nearest integer:
Occupancy to nearest integer: $\lfloor n_{sites} \times occupancy \rceil$
ex: $\lfloor 6.82 \rceil = 7$ and $\lfloor 4.31 \rceil = 4$

with n_{sites} = f(space group, crystalline positions)

Figure 6.8 *Building a C-diamond like, toluene encapsulated C_{240}, crystalline super-structure. The "`Molecules`" color-map (see sec. 5.1.1.2) for atoms and bonds is used for clarity purposes.*

Notes:

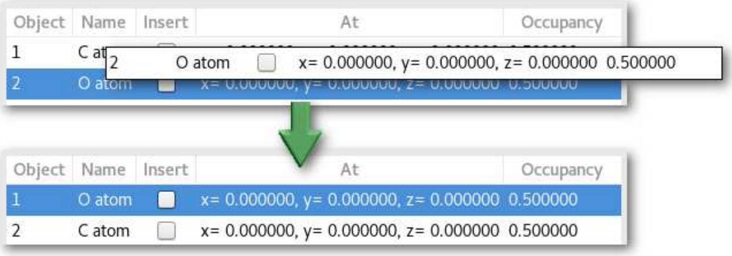
- Crystal building: for more on the crystal building process see appendix D.

  Here are some important things happening when building a crystal in **atomes**:

  - At the beginning of the process the size of the object(s) to insert is compared to the lattice parameters, if the lattice parameters are considered too small a warning message will pop-up:
    - For an atom, the size is set to 1.0 Å.
    - For a molecule, the size is the maximum interatomic distance within the molecule.

    The process is not fail-safe, and without being careful it is possible to build a crystal with an improper bonding.
    The distance matrix calculation to determine bonding information is performed on the fly at the end of the building process, if the crystal bonding is too bad, this calculation could fail and no bond will be display. If the crystalline structure is good, then simply correct the bond cutoff to perform the calculation again, and get the correct bonding information.
  - At the end of the process all the atoms are wrapped back in the unit cell.
  - The bond cutoff are determined automatically, therefore the visual aspect of the final structure might be misleading, with too much of too few bonds compared to what was expected.
  - When inserting a molecule remember that there is not way to determine its orientation, with water molecules for instance it might be required to rotate the molecule(s) afterwards, see section 6.1.3 for more information.

- Occupancy: as illustrated previously the order the object(s) is(are) inserted on the crystalline positions might have an importance on the final structure. This is true when the occupancy is < 1.0 and / or when object can share the same site when using the "`Allow overlapping`" option.
  To ensure that the desired crystal will be built, either insert the object in the proper order or re-order them using the mouse drag an drop:



Object	Name	Insert	At	Occupancy
1	C at			
2	O atom	☐	x= 0.000000, y= 0.000000, z= 0.000000	0.500000

2 O atom ☐ x= 0.000000, y= 0.000000, z= 0.000000 0.500000

Object	Name	Insert	At	Occupancy
1	O atom	☐	x= 0.000000, y= 0.000000, z= 0.000000	0.500000
2	C atom	☐	x= 0.000000, y= 0.000000, z= 0.000000	0.500000

  The occupancy $occ(s)$ for a site $\boldsymbol{s}$ (x_s, y_s, z_s) is defined as:

$$occ(s) = \sum_{i=1}^{N} occ(i) \tag{6.1}$$

  for the N object(s) on the same site (x_s, y_s, z_s)

- Empty position: the "`Empty position`" button of the "`Select ...`" menu is used to force the insertion of empty position(s).
  The empty site(s) are always treated before any object insertion(s), even if the position in the insertion tree is not on top.
  In the case of "`Overlapping`"+"`Empty position`" the rules for occupancy are modified as follow:

$$occ(s) = \max_{i=1}^{N} occ(i) + \sum_{j=1}^{E} occ(j) \tag{6.2}$$

  for the N object(s) and E empty positions on the same site (x_s, y_s, z_s).

6.1.2 The "`Cell edition`" window

The "`Cell edition`" window allows to adjust many parameters related to the periodicity of the material, and is accessible using any of the buttons of the "`Cell`" submenu [Fig. 6.9].

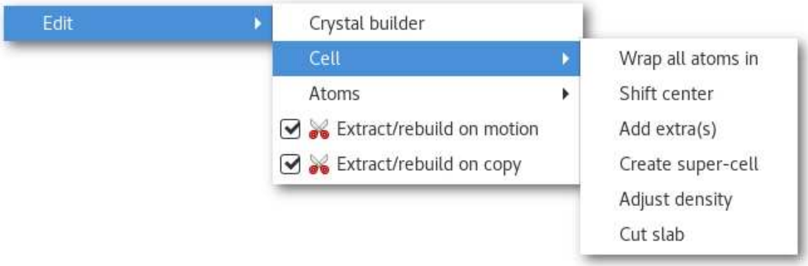


Figure 6.9 *Accessing the "`Cell edition`" window in the* **atomes** *program.*

Each of the buttons in the "`Cell`" menu [Fig. 6.9] allows to open the corresponding tab in the "`Cell edition`" window.
Each of these tabs and the action they provide will be introduced in the following:

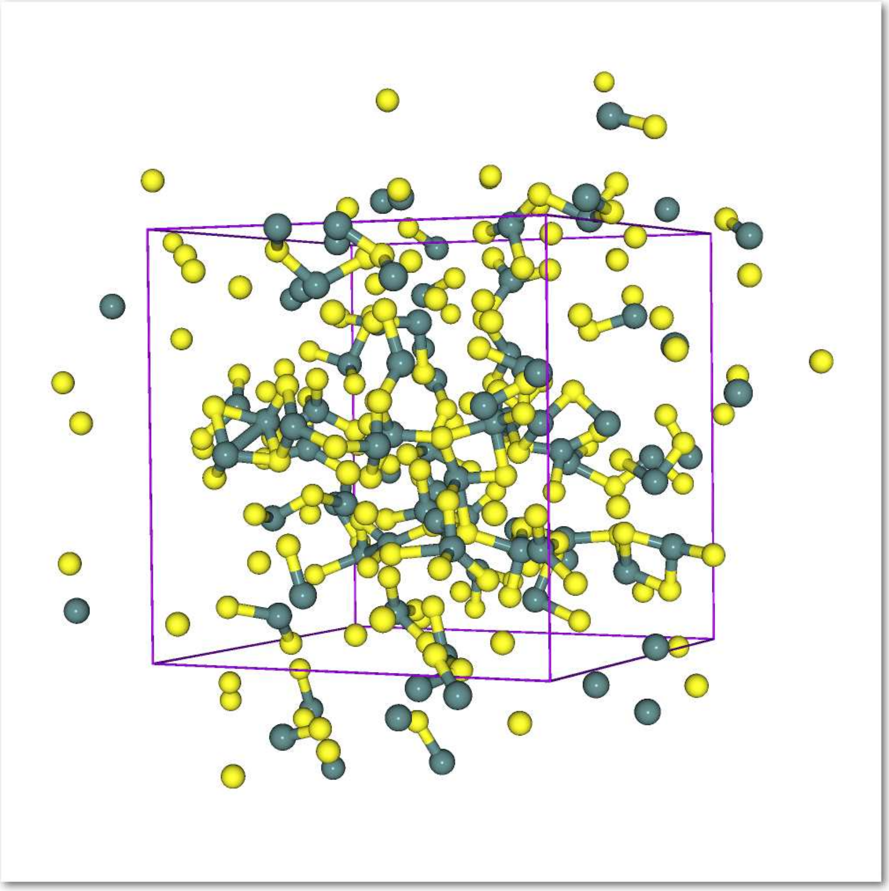
- The actions of the "`Cell edition`" window are accessible if and only if there is a model box.

- The actions "`Create super-cell`", "`Adjust density`" and "`Cut slab`" are not available in the case of MD trajectory.

Wrap all atoms in

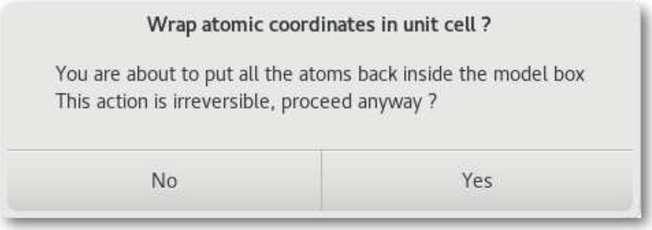
The "`Wrap all atoms in`" button allows to wrap all atomic coordinates in the original unit cell.

1. As illustrated bellow MD codes sometimes output MD trajectory / atomic coordinates in real coordinates, the visual assessment of such trajectory / atomic coordinates becomes complicated:



2. To simplify the visual analysis **atomes** can put back all atoms back in the unit cell using the periodicity and the box parameters as described in the "`Box and periodicity`" dialog [Fig. 3.5].
   Simply select the "`Wrap atomic coordinates in unit cell`" menu item from [Fig. 6.9]:

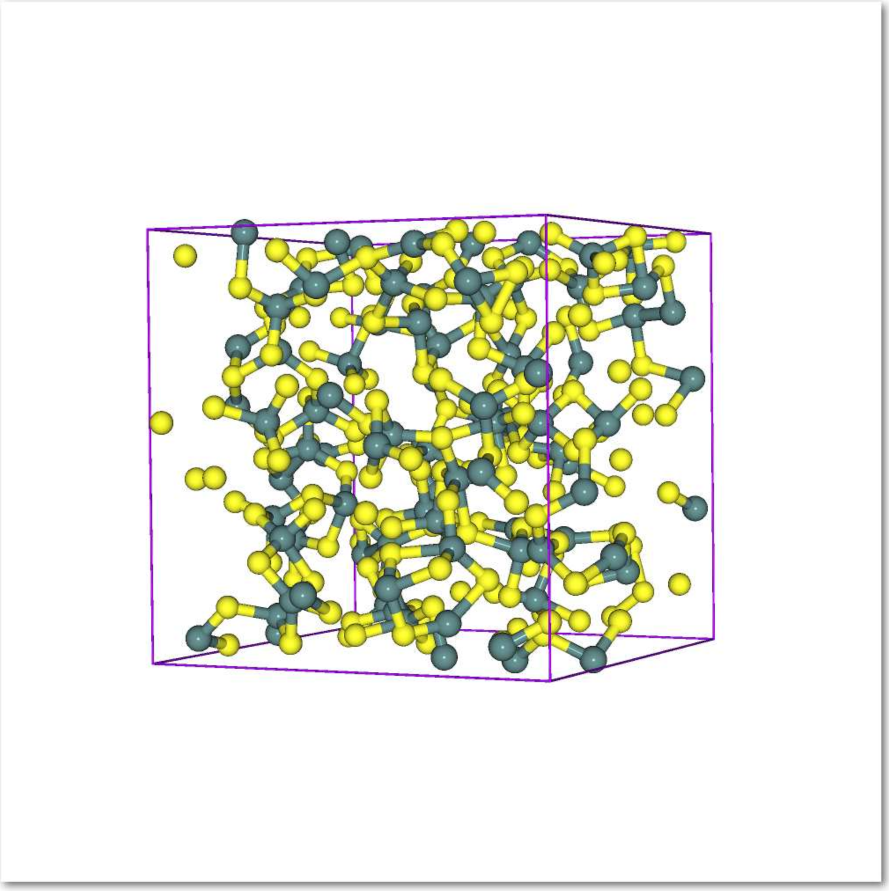
   The action being irreversible it is required to confirm it:



Wrap atomic coordinates in unit cell ?

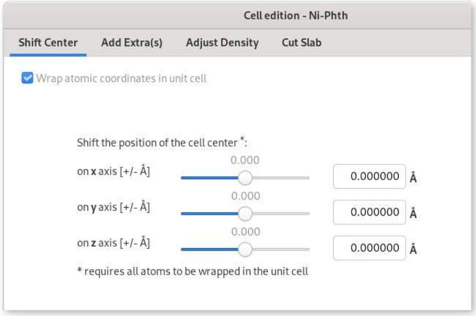
You are about to put all the atoms back inside the model box
This action is irreversible, proceed anyway ?

3. After confirmation the operation is performed and the OpenGL window updated:



Shift center

The "`Shift center`" tab allows to shift the atomic coordinates within the unit cell:



Cell edition - Ni-Phth

Shift Center | Add Extra(s) | Adjust Density | Cut Slab

☑ Wrap atomic coordinates in unit cell

Shift the position of the cell center *:

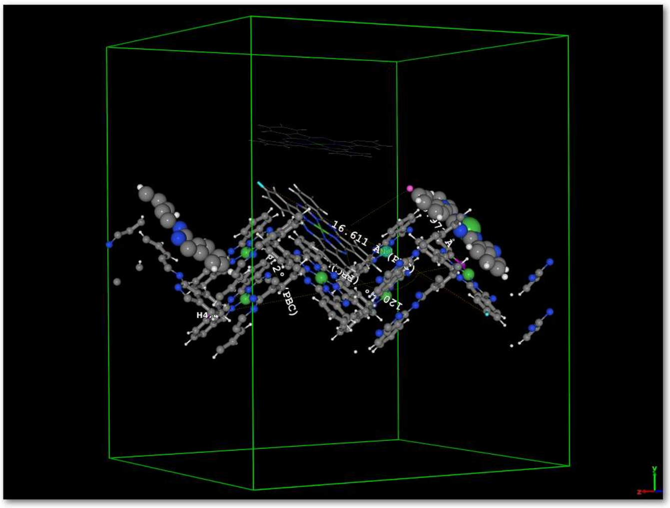
on **x** axis [+/- Å] 0.000 0.000000 Å

on **y** axis [+/- Å] 0.000 0.000000 Å

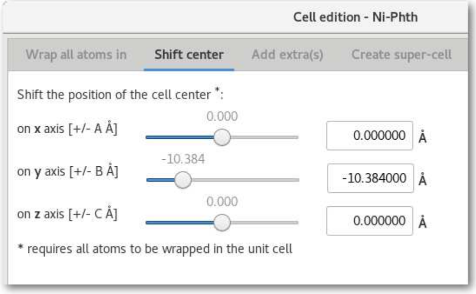
on **z** axis [+/- Å] 0.000 0.000000 Å

* requires all atoms to be wrapped in the unit cell

⟹



⇙



Cell edition - Ni-Phth

Wrap all atoms in | Shift center | Add extra(s) | Create super-cell

Shift the position of the cell center *:

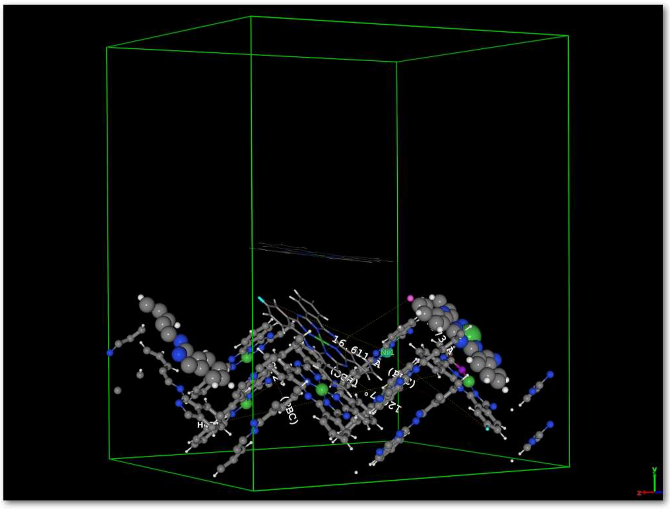
on **x** axis [+/- A Å] 0.000 0.000000 Å

on **y** axis [+/- B Å] -10.384 -10.384000 Å

on **z** axis [+/- C Å] 0.000 0.000000 Å

* requires all atoms to be wrapped in the unit cell

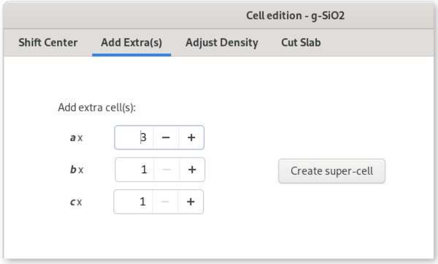
⟹



It is possible to shift atomic coordinates along the x, y and/or z model axis. The periodicity is preserved and if needed bonding properties are re-evaluated on the fly during this operation.

Note that it this required to wrap the atomic coordinates in the unit cell before being able to shift them.

Add extra(s)



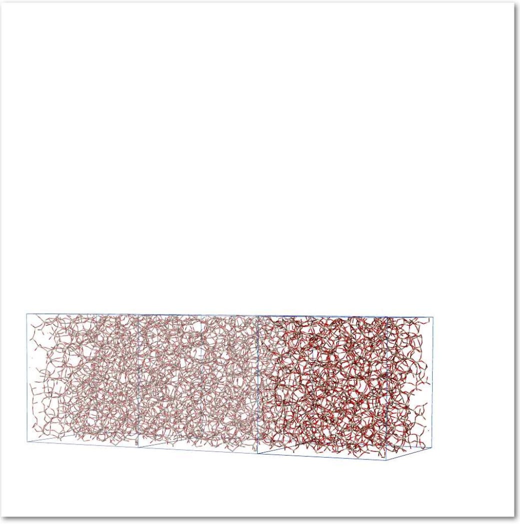
Add extra cell(s):

a x 3

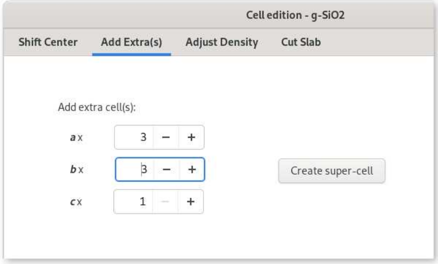
b x 1

c x 1

⟹



⇙



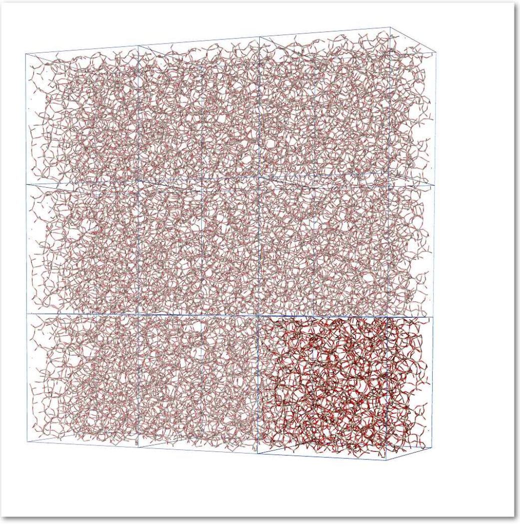
Add extra cell(s):

a x 3

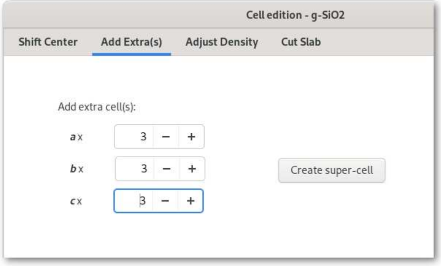
b x 3

c x 1

⟹



⇙



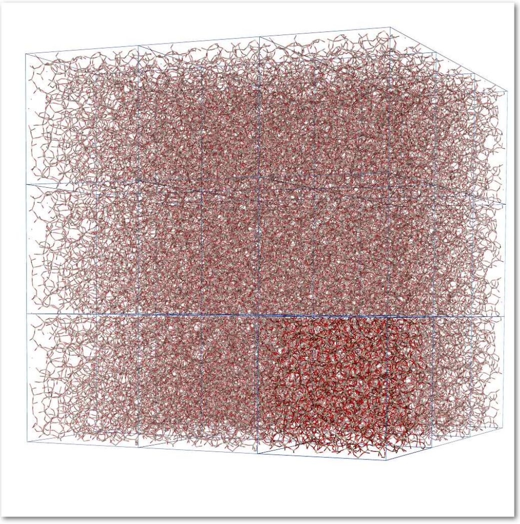
Add extra cell(s):

a x 3

b x 3

c x 3

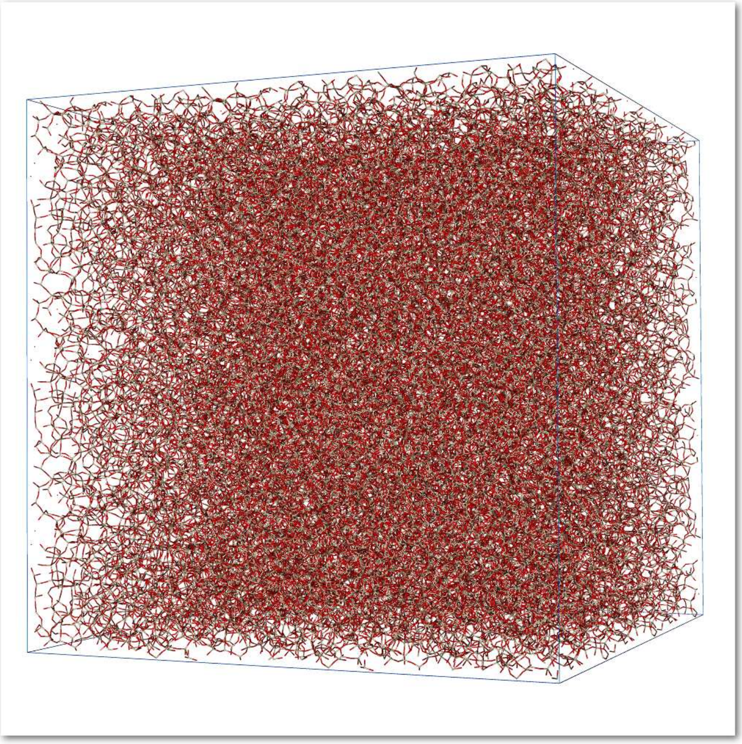
⟹



The "`Add extra(s)`" tab allows to add extra unit-cell(s) to the model, any object visible within the original unit cell will be duplicated (atom, bond, polyhedra, measure, label ...) as well. The duplicates cells are slightly translucent compared to the initial unit cell.

Create super-cell

The "`Create super-cell`" button allows to change the periodicity of the system and transform the unit cell to the extended structure created after using the "`Add extra(s)`" tab.

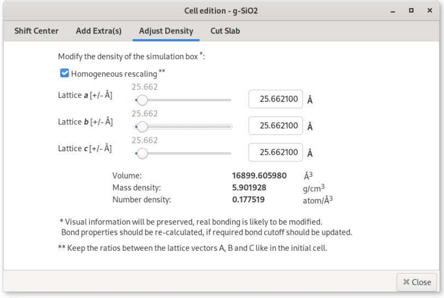


Adjust density

The "`Adjust density`" tab allows to modify the density of the material using homothetic rescaling that can be:

- Homogeneous: the $\frac{a}{b}$ and $\frac{a}{c}$ ratio of the initial unit cell are preserved
- Heterogeneous: a, b, and c are adjust individually

Note that to perform this operation any bonding information will be lost, and only the visual information will not be immediately erased. Therefore it is strongly recommended to recompute the bonding proprieties afterwards, this can not be done on the fly because changing the density is likely to require to change the bond cutoffs as well.



Modify the density of the simulation box *:

☑ Homogeneous rescaling **

Lattice *a* [+/- Å] 25.662 25.662100 Å

Lattice *b* [+/- Å] 25.662 25.662100 Å

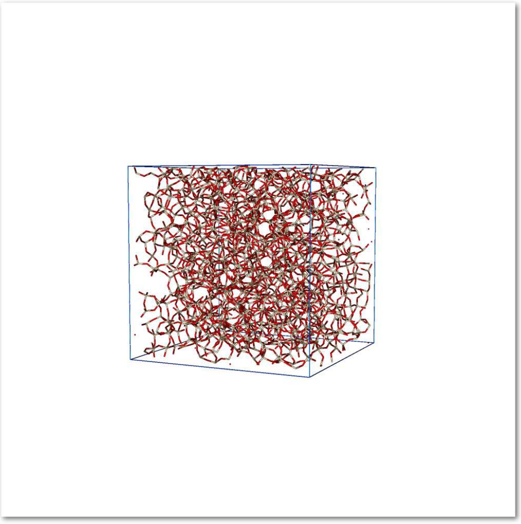
Lattice *c* [+/- Å] 25.662 25.662100 Å

Volume: **16899.605980** $Å^3$
Mass density: **5.901928** g/cm^3
Number density: **0.177519** $atom/Å^3$

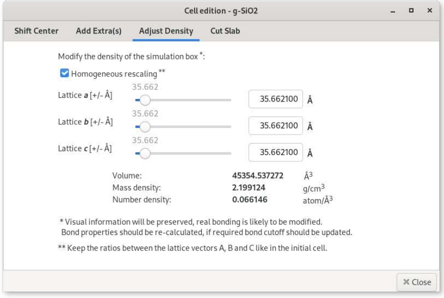
* Visual information will be preserved, real bonding is likely to be modified.
Bond properties should be re-calculated, if required bond cutoff should be updated.

** Keep the ratios between the lattice vectors A, B and C like in the initial cell.

⟹



⇑



Modify the density of the simulation box *:

☑ Homogeneous rescaling **

Lattice *a* [+/- Å] 35.662 35.662100 Å

Lattice *b* [+/- Å] 35.662 35.662100 Å

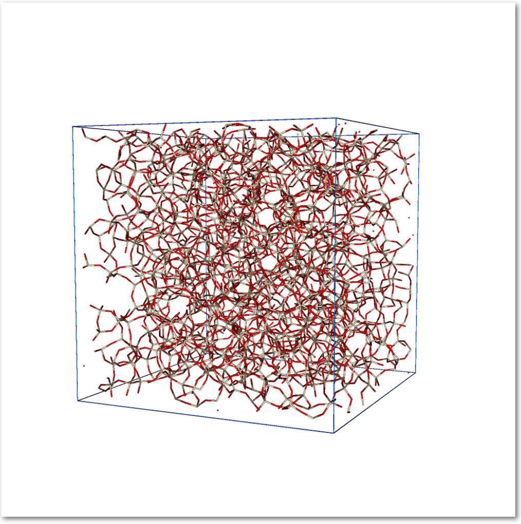
Lattice *c* [+/- Å] 35.662 35.662100 Å

Volume: **45354.537272** $Å^3$
Mass density: **2.199124** g/cm^3
Number density: **0.066146** $atom/Å^3$

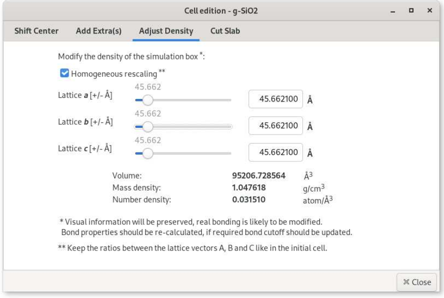
* Visual information will be preserved, real bonding is likely to be modified.
Bond properties should be re-calculated, if required bond cutoff should be updated.

** Keep the ratios between the lattice vectors A, B and C like in the initial cell.

⟹



⇓



Modify the density of the simulation box *:

☑ Homogeneous rescaling **

Lattice *a* [+/- Å] 45.662 45.662100 Å

Lattice *b* [+/- Å] 45.662 45.662100 Å

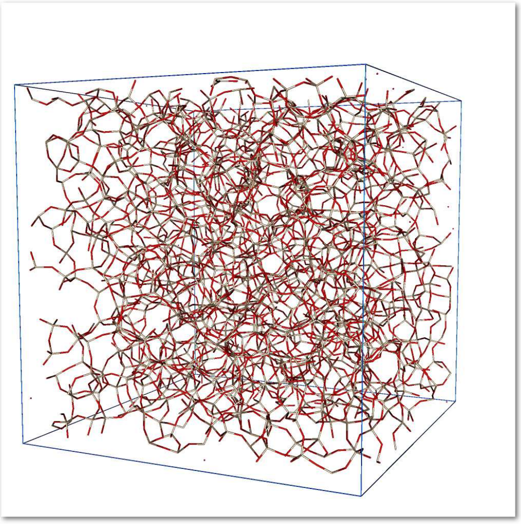
Lattice *c* [+/- Å] 45.662 45.662100 Å

Volume: **95206.728564** $Å^3$
Mass density: **1.047618** g/cm^3
Number density: **0.031510** $atom/Å^3$

* Visual information will be preserved, real bonding is likely to be modified.
Bond properties should be re-calculated, if required bond cutoff should be updated.

** Keep the ratios between the lattice vectors A, B and C like in the initial cell.

⟹



Cut slab

The "`Cut slab`" tab allows in the model using geometric patterns: parallelpiped, cylindrical and spherical. The "`Cut slab`" tab displays slab information, including slab volume and the number of atom of each chemical species inside it. The values are refreshed each time the shape, position size, and/or rotation of the slab is modified. Examples are presented in figure. 6.10.

6.1.3 The "`Model edition`" window

The "`Model edition`" window offers several tools dedicated to the edition of the atomic coordinates and is accessible using any of the buttons of the "`Atom`" submenu [Fig. 6.11].

It is not possible to access the "`Model edition`", and therefore to move / replace / remove and insert atom(s) in the case of MD trajectory.

Selection process

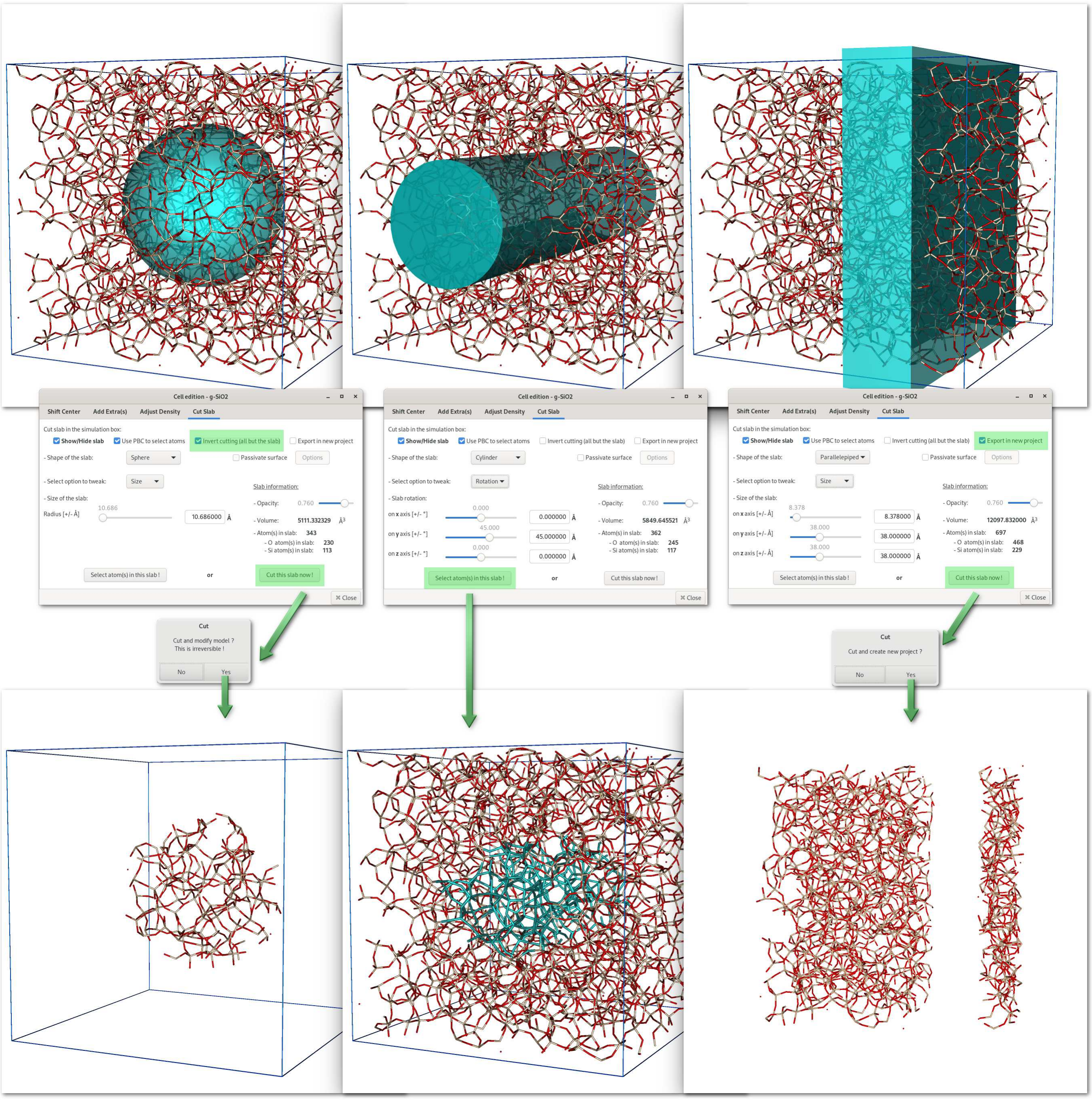
When the "`Atom edition`" window is opened the main OpenGL window remains active, and it is still possible to work in it. However having the "`Model edition`" window opened will modify the results of the atom selection process, whether is it performed using any dialog window or using with the mouse describe in section 5.2.1 and 5.2.2. The newly extra-selected atom(s) will be covered in pink (instead of light blue), see [Fig. 6.12], and even already selected atoms (in light blue) can be re-selected. As long as the "`Model edition`" window remains open, the "`Measures`" dialog [Fig. 5.10] will only presented measurement(s) related to the new pink atoms.
The utilization and purpose of this extra selection feature will be illustrated when presenting the action tabs of the "`Model edition`" window.

General behavior

Before browsing each and every tab of the "`Model edition`" window it is required to introduce the "`atom search`" tool [Fig. 6.13] common to almost every tab (in the top part) in the window. Each tab being dedicated to a particular action the search tool will help to find and selected the atom(s) you want the action to be performed upon:

1. Search for atom(s) among [Fig. 6.13-1]:
    (a) non-selected atom(s) only: search only in "`All non-selected atoms`" [Fig. 6.13-1]
    (b) selected atom(s) only: search only in "`All selected atoms`" [Fig. 6.13-1]
    (c) or all atoms: search in all "`All atom(s)`" [Fig. 6.13-1]

   1b is the default value for menu [Fig. 6.13-1] if some atoms are selected, and 1c is the default value otherwise.



Cell edition - g-SiO2

Cut slab in the simulation box:

☑ Show/Hide slab ☑ Use PBC to select atoms ☑ Invert cutting (all but the slab) ☐ Export in new project

- Shape of the slab: Sphere ☐ Passivate surface

- Select option to tweak: Size

- Size of the slab:

Radius [+/- Å] 10.686 10.686000 Å

Slab information:

- Opacity: 0.760
- Volume: 5111.332329 Å3
- Atom(s) in slab: 343
  - O atom(s) in slab: 230
  - Si atom(s) in slab: 113

Select atom(s) in this slab ! or Cut this slab now !

Cut

Cut and modify model ?
This is irreversible !

No Yes

Cell edition - g-SiO2

Cut slab in the simulation box:

☑ Show/Hide slab ☑ Use PBC to select atoms ☐ Invert cutting (all but the slab) ☐ Export in new project

- Shape of the slab: Cylinder ☐ Passivate surface

- Select option to tweak: Rotation

- Slab rotation:

on x axis [+/- °] 0.000 0.000000 Å
on y axis [+/- °] 45.000 45.000000 Å
on z axis [+/- °] 0.000 0.000000 Å

Slab information:

- Opacity: 0.760
- Volume: 5849.645521 Å3
- Atom(s) in slab: 362
  - O atom(s) in slab: 245
  - Si atom(s) in slab: 117

Select atom(s) in this slab ! or Cut this slab now !

Cell edition - g-SiO2

Cut slab in the simulation box:

☑ Show/Hide slab ☑ Use PBC to select atoms ☐ Invert cutting (all but the slab) ☑ Export in new project

- Shape of the slab: Parallelepiped ☐ Passivate surface

- Select option to tweak: Size

- Size of the slab:

on x axis [+/- Å] 8.378 8.378000 Å
on y axis [+/- Å] 38.000 38.000000 Å
on z axis [+/- Å] 38.000 38.000000 Å

Slab information:

- Opacity: 0.760
- Volume: 12097.832000 Å3
- Atom(s) in slab: 697
  - O atom(s) in slab: 468
  - Si atom(s) in slab: 229

Select atom(s) in this slab ! or Cut this slab now !

Cut

Cut and create new project ?

No Yes

Figure 6.10 *Model edition using the "`Cut slab`" tab, from left to right: 1) all atoms outside the sphere are deleted, 2) atoms inside the cylinder are selected, 3) all atoms in the parallelpiped slab are deleted and the results is exported in a new project.*

2. Apply the action to [Fig. 6.13-2]:
   (a) The atoms as single object(s): pick "`Atom(s)`" [Fig. 6.13-2]
   (b) Group of atom(s): pick "`Group of atoms`" [Fig. 6.13-2]

In case 2a the action will be performed on the atom(s) that will be selected and

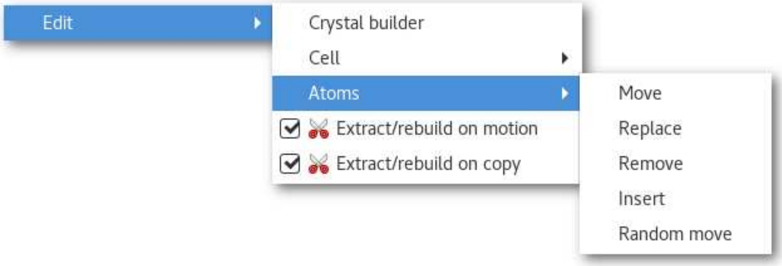


Figure 6.11 *Accessing the "`Model edition`" window in the* **atomes** *program.*

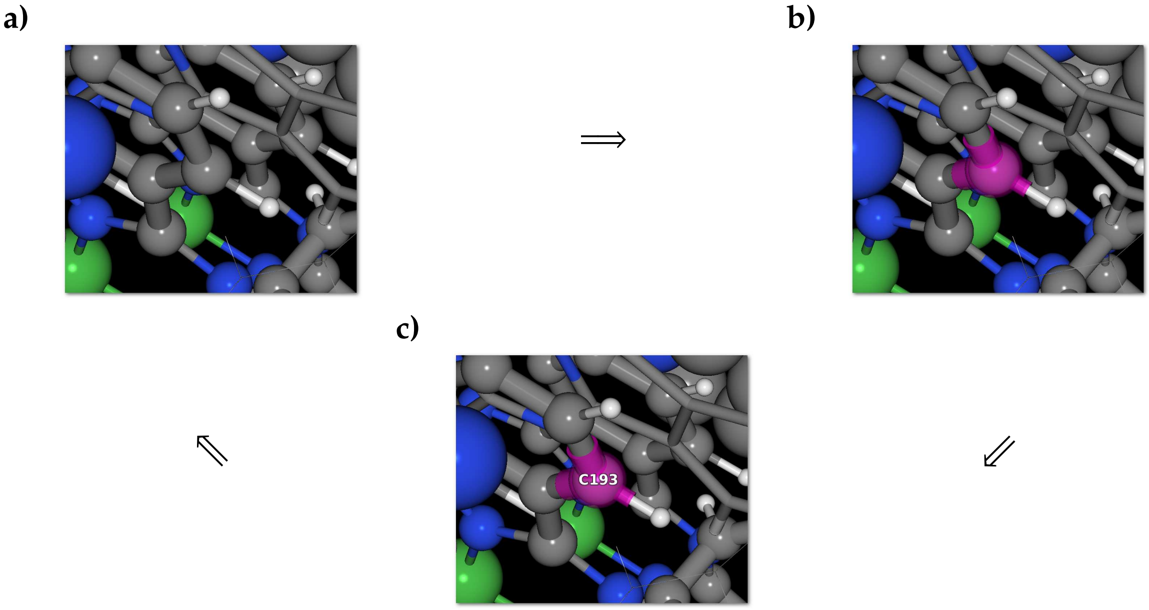


Figure 6.12 *Modified selection process when the "`Model edition`" window is opened.*

each of these atoms will be treated as an isolated object. In case 2b the action will be performed on the group(s) of atoms, the atom(s) that will be selected afterwards belong to: entire coordination sphere(s), fragment(s) or molecule(s).

3. Filter the result of the search depending on the type of object you are interested in figure 6.13-3:
   (a) Chemical species (Available only if 2a is selected for [Fig. 6.13-2])
   (b) Total coordination
   (c) Partial coordination
   (d) Fragment
   (e) Molecule

   Pick the appropriate value in figure 6.13-3 and the selection tree bellow will be updated accordingly.

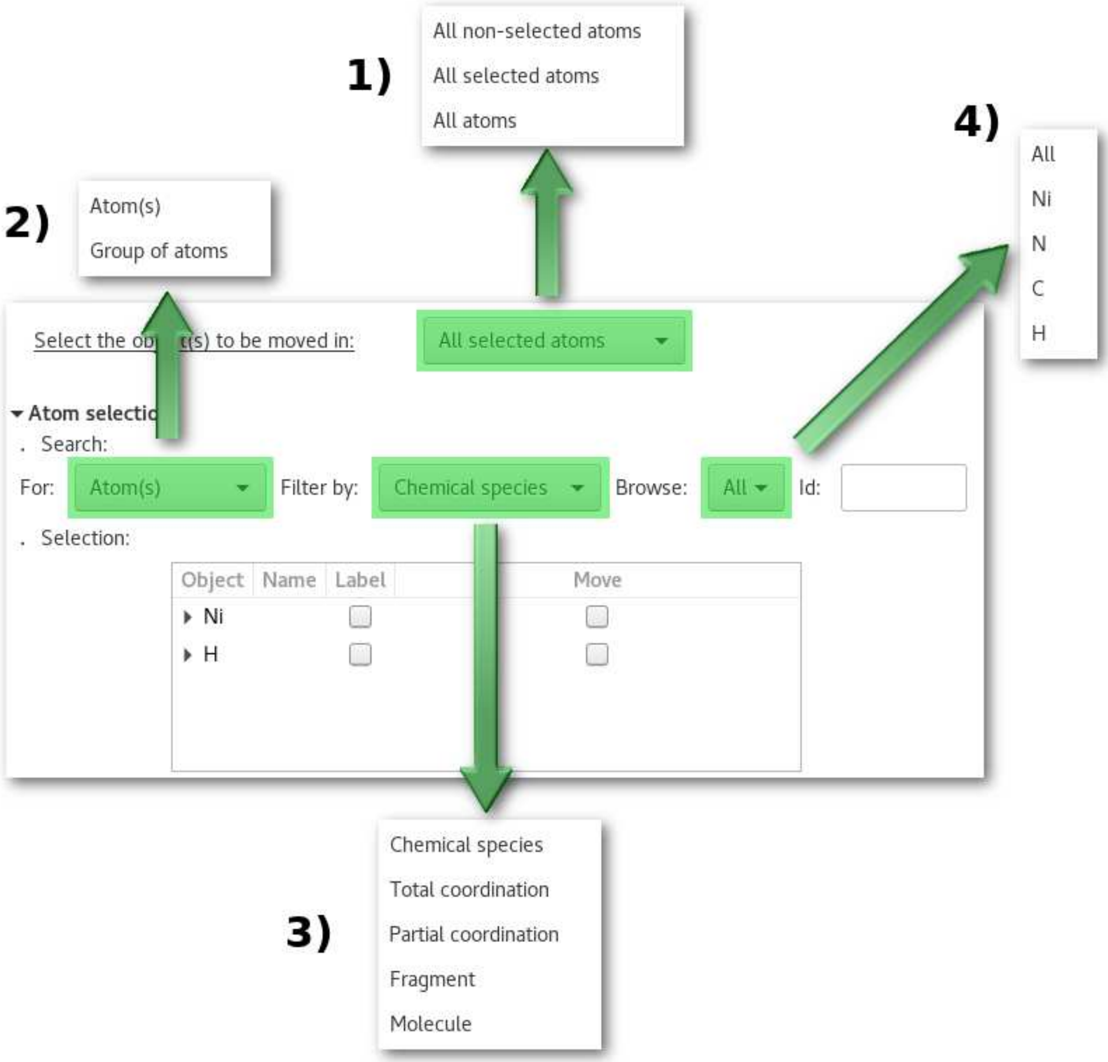


Figure 6.13 *The atom(s) search tool.*

4. Refine the search to present only the atom(s) of that particular chemical species (if 2a was selected in figure 6.13-2) or the group of atoms that contains such chemical species (if 2b was selected in figure 6.13-2)

Notes:

- Clickable : some of the column headers in the search tree are clickable, in the top part if you click on the "`Label`" or "`Move`" the corresponding action will be applied / unapplied to the entire data set available in the search tree.

- Update : whenever the values for the menus 2 [Fig. 6.13-2] and 3 [Fig. 6.13-3] are modified the tree is not only refreshed but also cleaned, and so is the corresponding data thus previous selection sets would be lost in the process.

Examples of the utilization of the "`atom search`" tool [Fig. 6.13] will be presented along with each actions available in the "`Model edition`" window.

The "`Move`" tab

The "`Move`" tab allows to move atom(s) (translation only) or group of atoms (translation and rotation around the groups barycenter). In the following example one of the fragment in the model is selected, the fragment appears to be split because of the periodic boundary conditions:

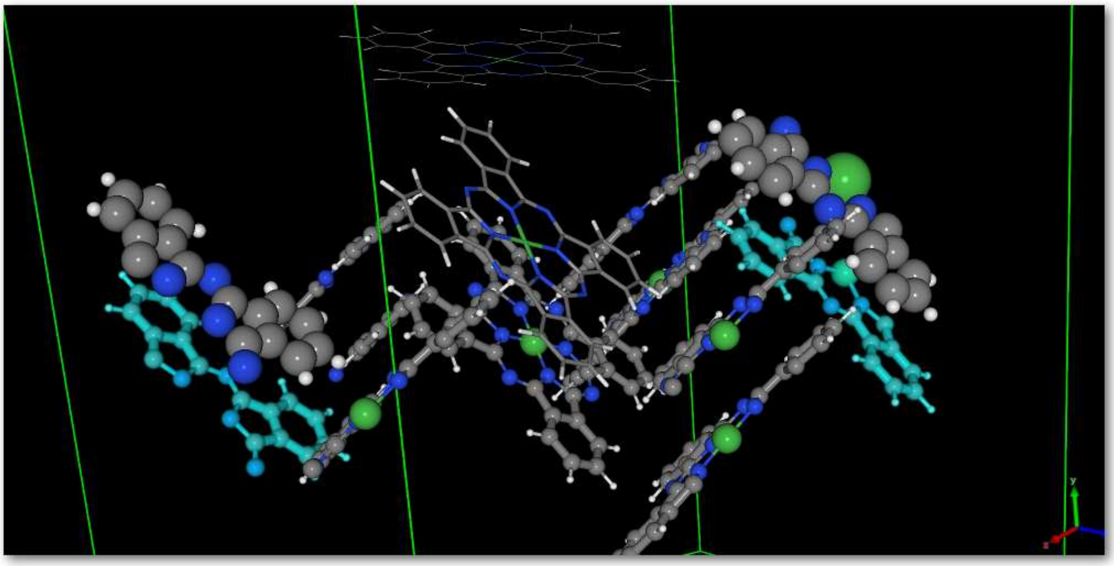
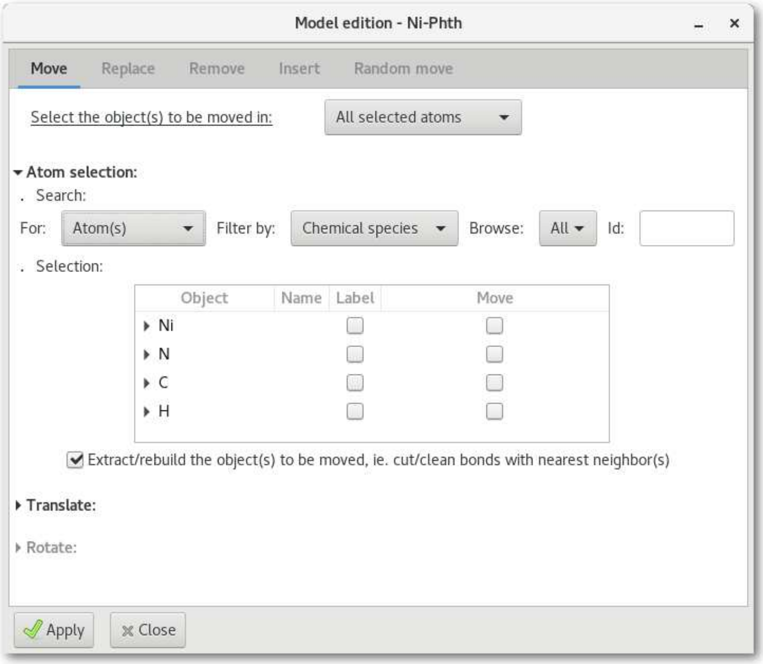


Figure 6.14 *Initial position with an isolated fragment selected in the model.*

To move the selected fragment:

1. Open the "`Move`" atom(s) tab:



Model edition - Ni-Phth

Select the object(s) to be moved in: All selected atoms

Atom selection:

. Search:

For: Atom(s) Filter by: Chemical species Browse: All Id:

. Selection:

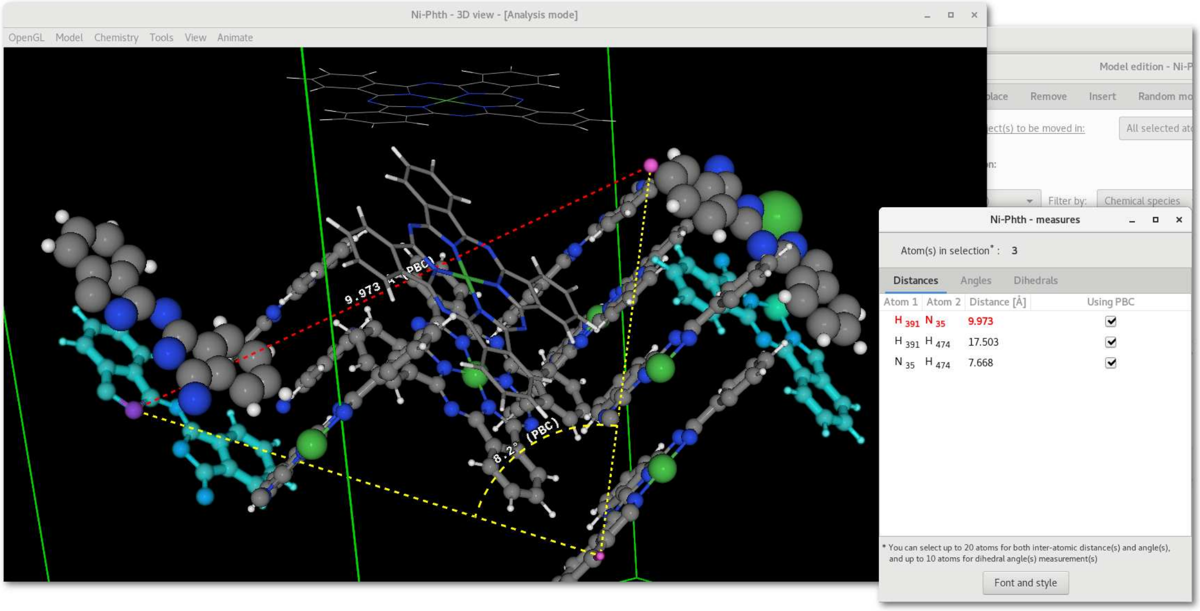
Object	Name	Label	Move
Ni		☐	☐
N		☐	☐
C		☐	☐
H		☐	☐

☑ Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)

Translate:

Rotate:

2. Go back to the main OpenGL window, keeping the "`Model edition`" window opened, and select few atoms, that will appear in pink color. Then open the "`Measures`" dialog [Fig. 5.10] to select a bunch of measurements to be displayed:



Ni-Phth - measures

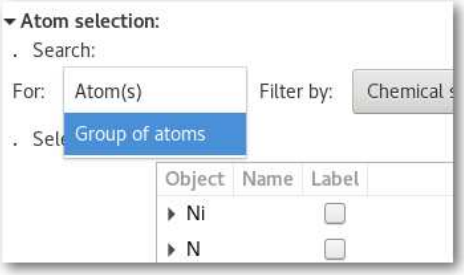
Atom(s) in selection* : 3

Distances | Angles | Dihedrals

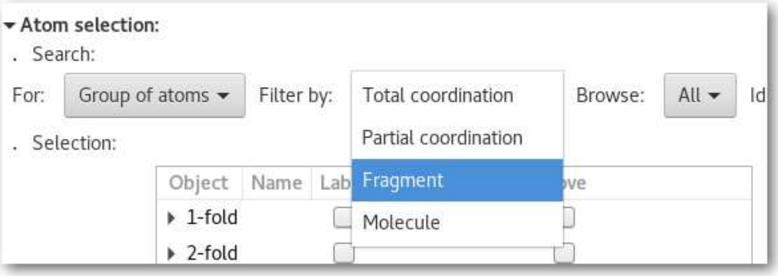
Atom 1	Atom 2	Distance [Å]	Using PBC
H_{391}	N_{35}	9.973	☑
H_{391}	H_{474}	17.503	☑
N_{35}	H_{474}	7.668	☑

* You can select up to 20 atoms for both inter-atomic distance(s) and angle(s), and up to 10 atoms for dihedral angle(s) measurement(s)

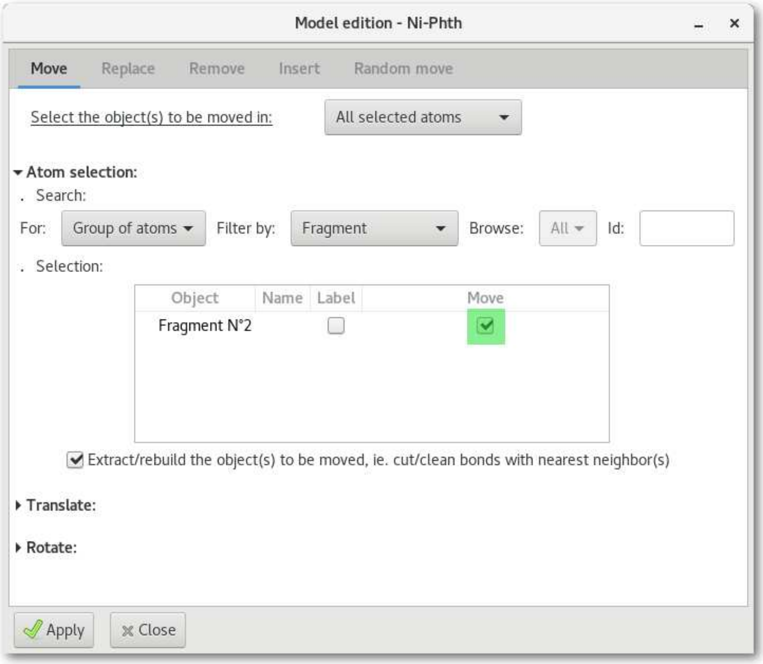
3. Go back to the "`Model edition`" window and adjust the search "`For`" option and select "`Group of atom(s)`":



4. Adjust the search "`Filter by`" option and select "`Fragment`":



5. Then select the fragment in the selection tree:



Select the object(s) to be moved in: All selected atoms

Atom selection:

Search:

For: Group of atoms Filter by: Fragment Browse: All Id:

Selection:

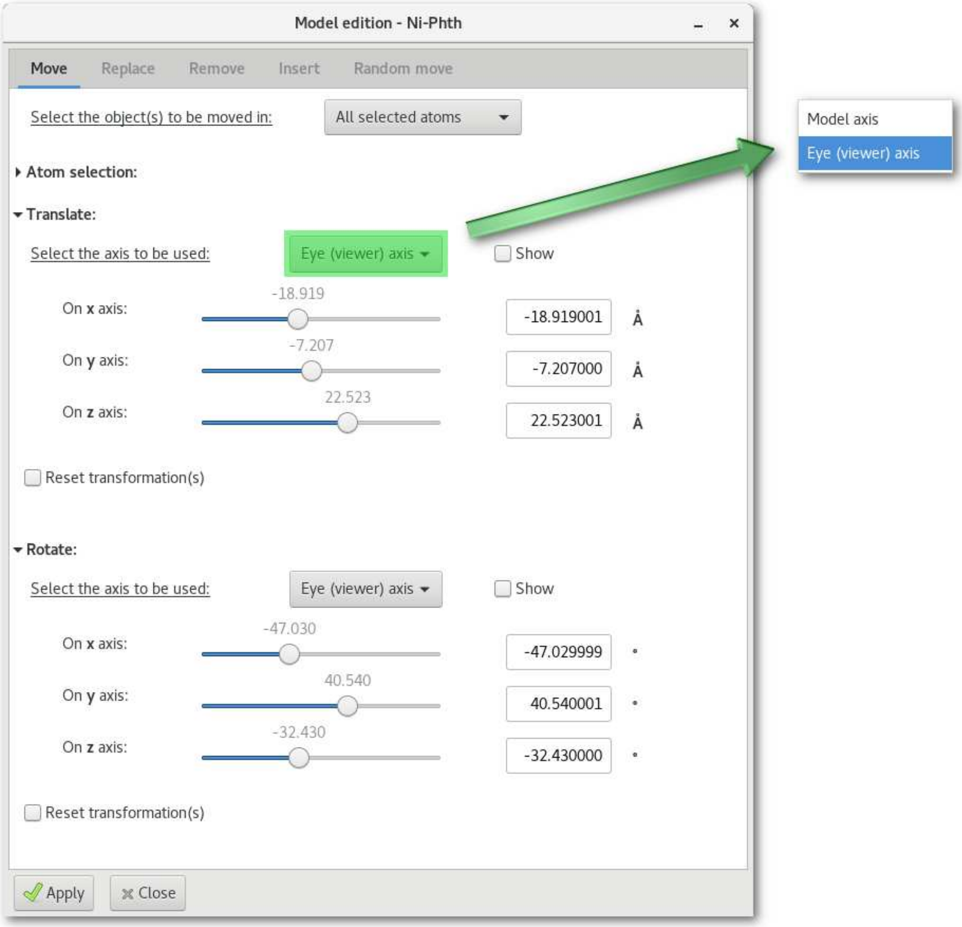
Object	Name	Label	Move
Fragment N°2		☐	☑

☑ Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)

Translate:

Rotate:

6. Open the lower part(s) to move the fragment:



Select the object(s) to be moved in: All selected atoms

Atom selection:

Translate:

Select the axis to be used: Eye (viewer) axis ☐ Show

On x axis: -18.919 -18.919001 Å

On y axis: -7.207 -7.207000 Å

On z axis: 22.523 22.523001 Å

☐ Reset transformation(s)

Rotate:

Select the axis to be used: Eye (viewer) axis ☐ Show

On x axis: -47.030 -47.029999 °

On y axis: 40.540 40.540001 °

On z axis: -32.430 -32.430000 °

☐ Reset transformation(s)

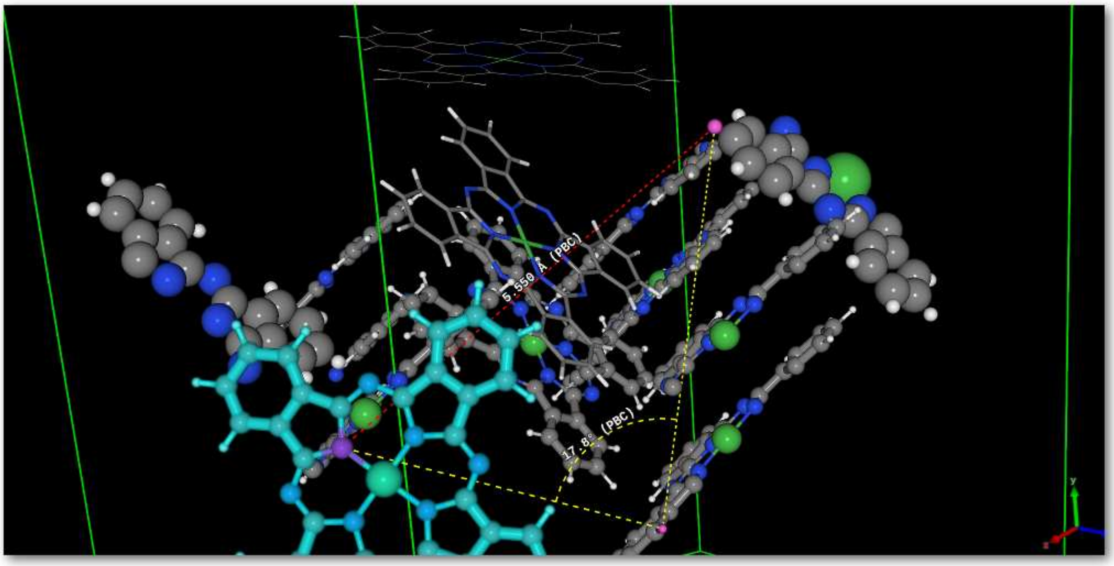


Figure 6.15 *Final position of the fragment, after translation and rotation in the model.*

Notes:

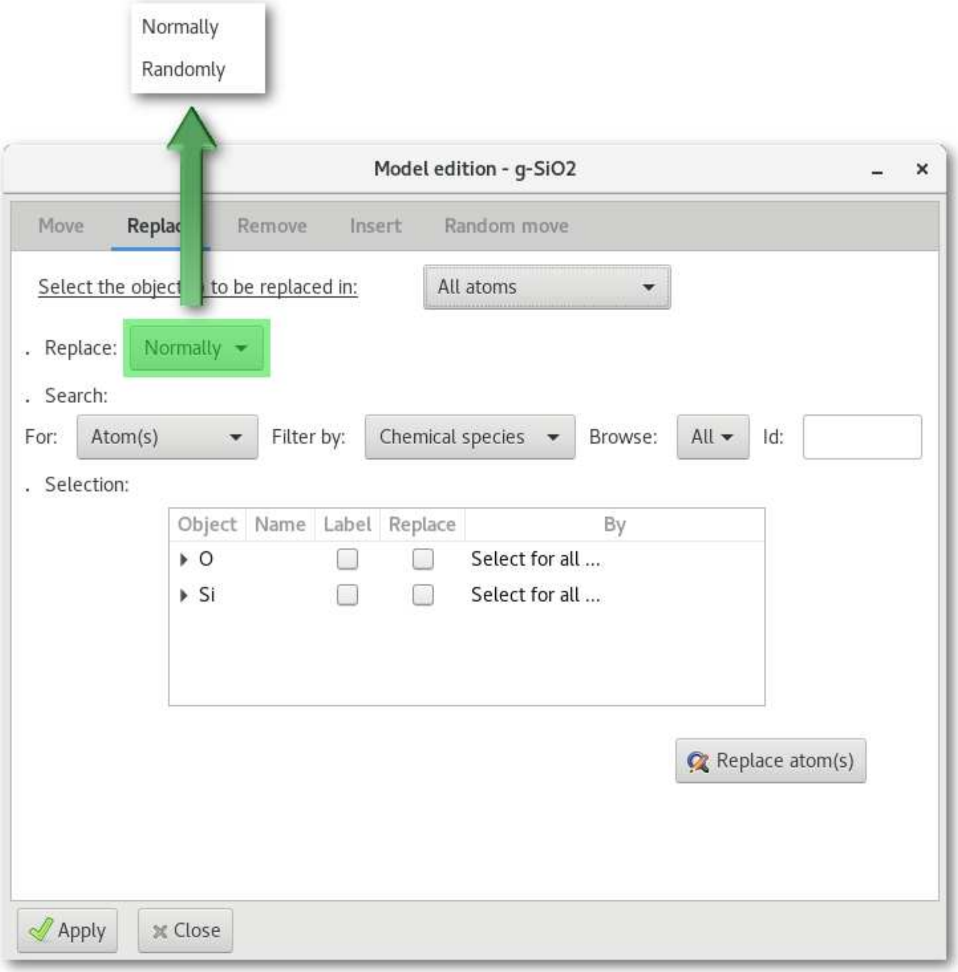
- Motion axis: it is possible to select (and visualize) the motion axis and choose between the "`Eye (viewer) axis`" and the "`Model axis`" (real x, y and z of the atoms).
- Motion actions: the motion interactors (ranges and input entries) allow to adjust motion very precisely, slightly more approximate motion is also available using the mouse (see Sec. 6.2)
- Measurements: if already present in the OpenGL window, measurement(s) are updated on the fly, allowing to adjust perfectly position and orientation of the object in the model, see [Fig. 6.15].
- Motions: translation is always available, however rotation is only available for "`Group of atom(s)`" and is performed around the barycenter(s) of the object(s) to be rotated.
- Reconstruction: the check button labelled "`Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)`" offers the following option:
  - For "`Atom(s)`": if activated the object(s) to be moved will be extracted from the model and translated independently, otherwise chemical bond(s) will simply be stretched.
  - For "`Group of atom(s)`": if activated the atomic positions of the object(s) will be corrected to get only single piece object(s).

As illustrated in figure 6.14 the fragment visually appears in 2 pieces, and as illustrated by the example as a single piece object after motion [Fig. 6.15].
If the object(s) to be moved are coordination spheres and if the spheres that are being moved share atom(s), then the positions of these atoms might be affected twice by this procedure, leading to an awkward, yet correct, 3D representation.

- Bonding: During motion, the coordination information is modified, all related menus and corresponding dialogs are updated accordingly, however detailed bonding information is lost. It is therefore strongly recommended to recompute bonding properties afterwards.

The "`Replace`" tab

The "`Replace`" tab allows to replace object(s), atom(s) or group of atoms, by either: atom(s), molecules imported from the internal library or atom(s) imported from any project opened within the same instance of the **atomes** program:



Model edition - g-SiO2

Select the object(s) to be replaced in: All atoms

Replace: Normally

Search: For: Atom(s) Filter by: Chemical species Browse: All Id:

Object	Name	Label	Replace	By
O		☐	☐	Select for all ...
Si		☐	☐	Select for all ...

Figure 6.16 *The "`Replace`" tab, with the option of replace objects "`Normally`", ie. object by object, or "`Randomly`", in the model.*

As illustrated in figure 6.16 it is possible to replace object(s) one by one ("`Normally`") or by random pick ("`Randomly`"). The difference between the normal and the random search trees are illustrated in top part of figure 6.17.

For normal substitution(s) [Fig. 6.17-a] it is possible to select the replacement object(s) either at once for all objects, using the "`Select for all ...`" menu, or alternatively one by one when browsing the tree and using the "`Select ...`" menu(s).

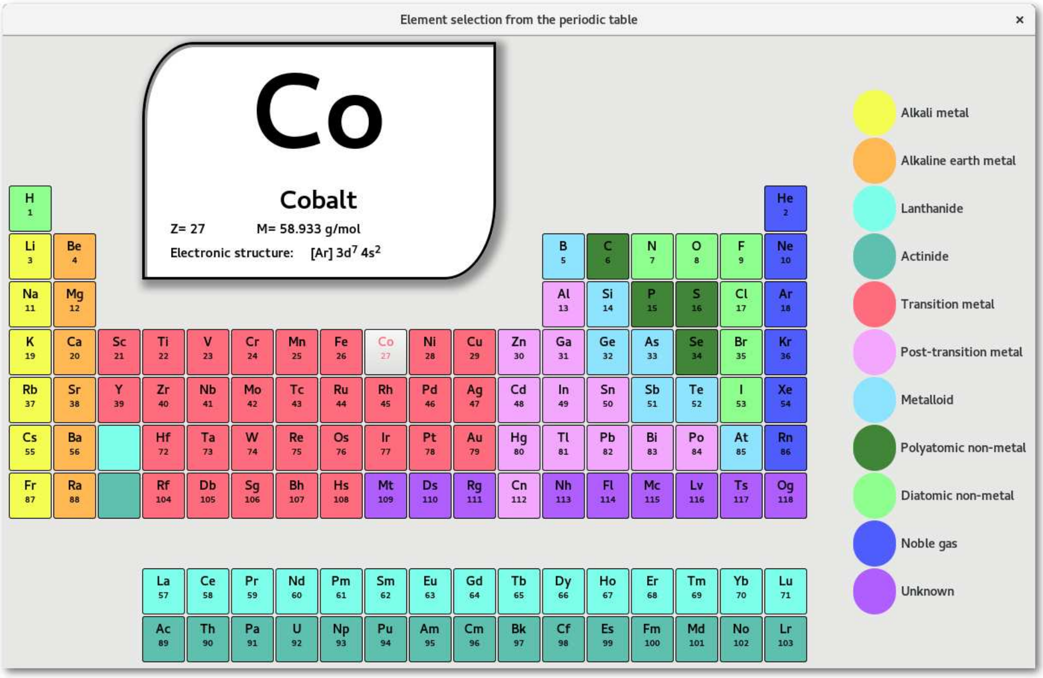
For random substitution(s) [Fig. 6.17-b] only a single replacement is selected for each type of object, and it is require to enter the number of substitution(s) to be performed.

The substitution options accessible using the "`Select ...`" menu are illustrated in the bottom part in figure 6.17 with the different "`atoms`" c), "`Library`" d) and "`Import from project`" e) submenus.

Figure 6.17 *Top: search trees* **a)** *replacing object(s) one by one,* **b)** *replacing object(s) randomly. Bottom: the "*`Select for ...`*" replacement menu and the attached* **c)** *"*`Atom`*",* **d)** *"*`Library`*",* **e)** *"*`Import from project`*" and* **f)** *"*`Copied data`*" submenus.*

Substitution options

- The "`Atom`" submenu [Fig. 6.17-c], to insert a new atom in place of the object(s) to be removed. Some shortcuts are proposed, if required the "`Other ...`" button allows to open a periodic table to pick any appropriate atom:

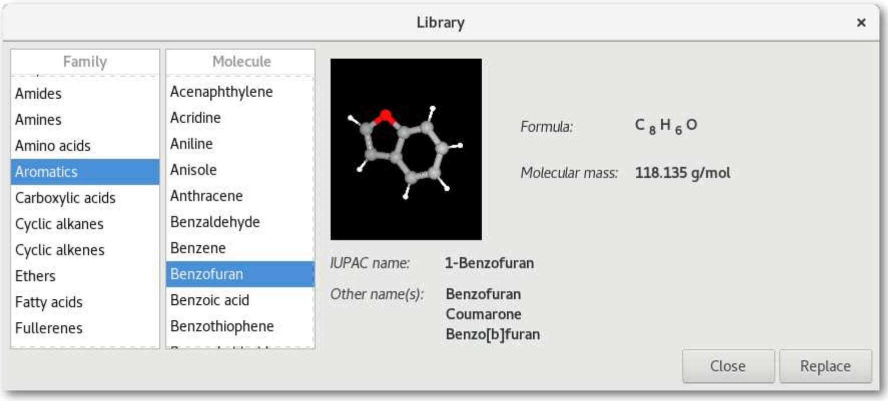


Cobalt

Z= 27 M= 58.933 g/mol

Electronic structure: [Ar] $3d^7\ 4s^2$

- The "`Library`" submenu [Fig. 6.17-d], to insert an new molecule in place of the object(s) to be removed. Some shortcuts are proposed as well, and the "`More ...`" button allows to open the "`Library`" dialog:



Formula: C_8H_6O

Molecular mass: 118.135 g/mol

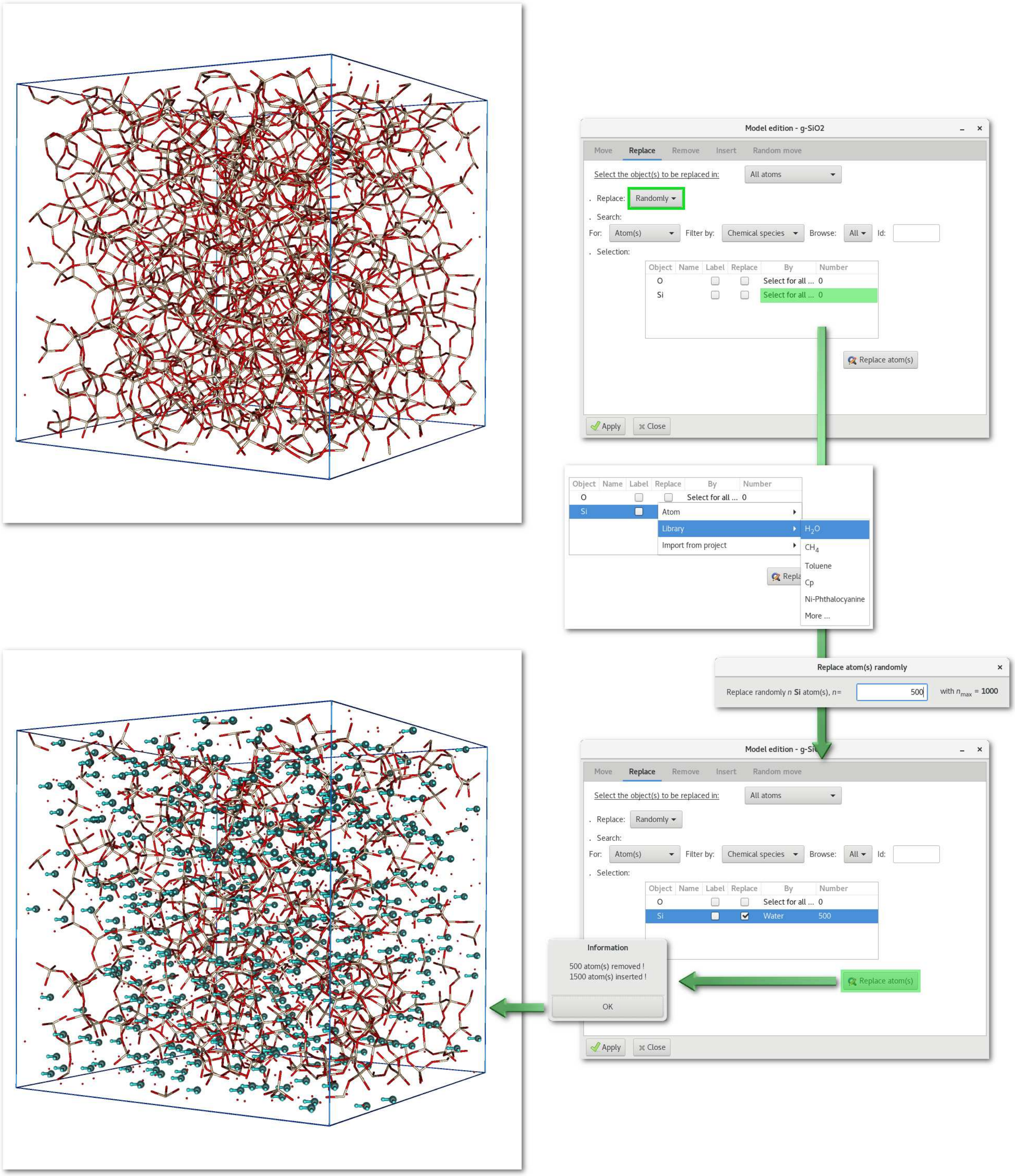
IUPAC name: 1-Benzofuran

Other name(s): Benzofuran
Coumarone
Benzo[b]furan

The "`Library`" dialog provides a bunch of sample molecules roughly sorted by chemical properties (see appendix C for more details).

- The "`Import from project`" submenu [Fig. 6.17-e], to insert atom(s) from any **atomes** project opened in the workspace.
- The "`Copied data`" button [Fig. 6.17-f], to copied data selection from any workspace in **atomes**.

An example is provided in figure 6.18 with the random substitution of 500 "`Si`" atoms from the "$\texttt{SiO}_2$" project by "`water`" molecules.



Model edition - g-SiO2

Select the object(s) to be replaced in: All atoms

Replace: Randomly

For: Atom(s) Filter by: Chemical species Browse: All Id:

Replace atom(s) randomly

Replace randomly *n* **Si** atom(s), *n*= 500 with n_{max} = 1000

Information

500 atom(s) removed !
1500 atom(s) inserted !

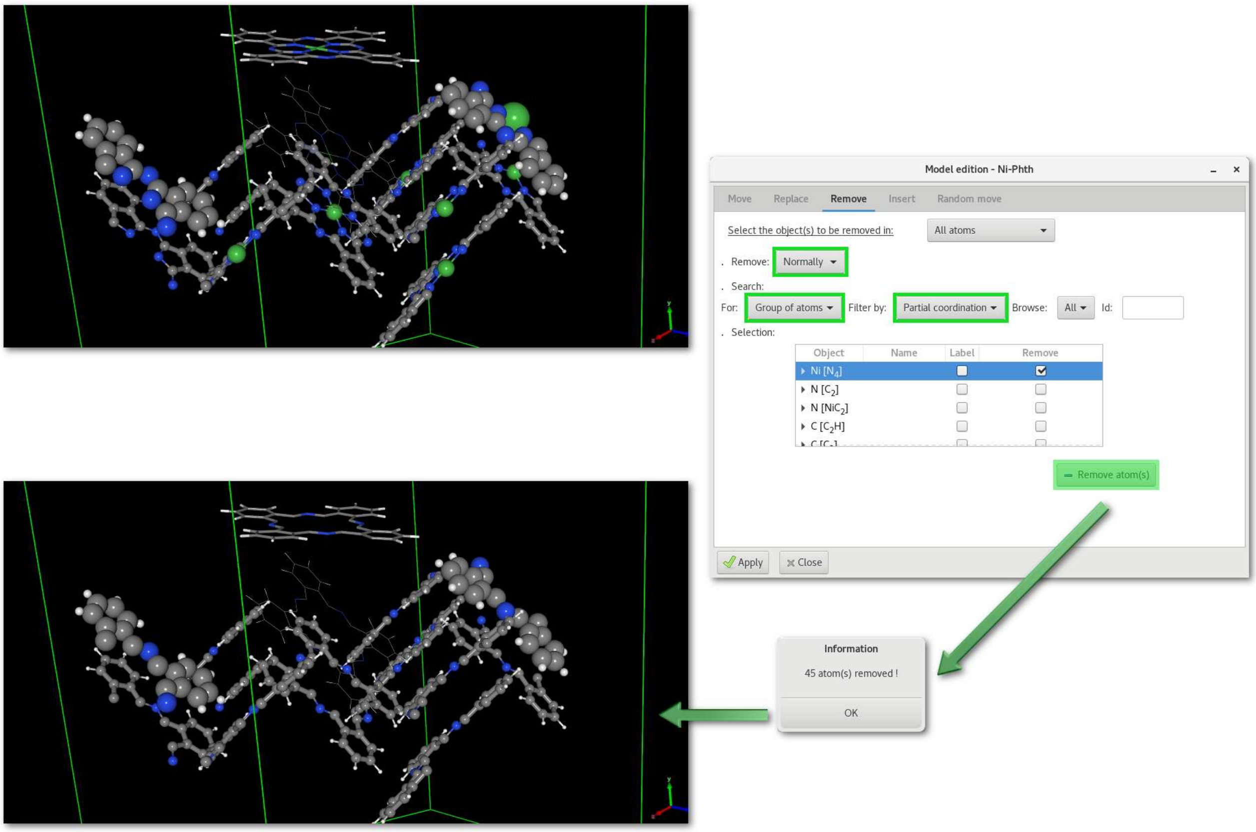
Figure 6.18 *Random substitution of 500 "`Si`" atoms by "`water`" molecules.*

Notes:

- Irreversible: the replacement is irreversible (at least not directly, but it is always possible to perform another backward substitution) therefore remember to save your work before replacing any object(s) in your model.
- Selection: At the end of the substitution process, and therefore after the insertion of the new objects, all these new objects will appear surrounded by light blue color in the OpenGL window (see figure 6.18), and will therefore be selected, making further work on these new objects easier.
- Barycenters: the new object is inserted and centered at the barycenter of the atomic positions of the old object to be removed.

The "`Remove`" tab

The "`Remove`" tab allows to remove object(s), atom(s) or group of atoms, like for the "`Replace`" tab the action can also be performed randomly. An example is provided in figure 6.19 with the normal (one by one) removal of all "`Ni-[N4]`" coordination spheres atoms from the "`Ni-Phth`" project: for a Nickel atom, this means that this "`Ni`" atom as well as it surrounding "`N`" neighbours are all removed.



Select the object(s) to be removed in: All atoms

. Remove: Normally

. Search:

For: Group of atoms Filter by: Partial coordination Browse: All Id:

. Selection:

Object	Name	Label	Remove
Ni $[N_4]$		☐	☑
N $[C_2]$		☐	☐
N $[NiC_2]$		☐	☐
C $[C_2H]$		☐	☐

45 atom(s) removed !

Figure 6.19 *Normal removal of all "`Ni-[N4]`" coordination spheres from the model.*

The "`Insert`" tab

The "`Insert`" tab allows to insert new object(s) in the model:

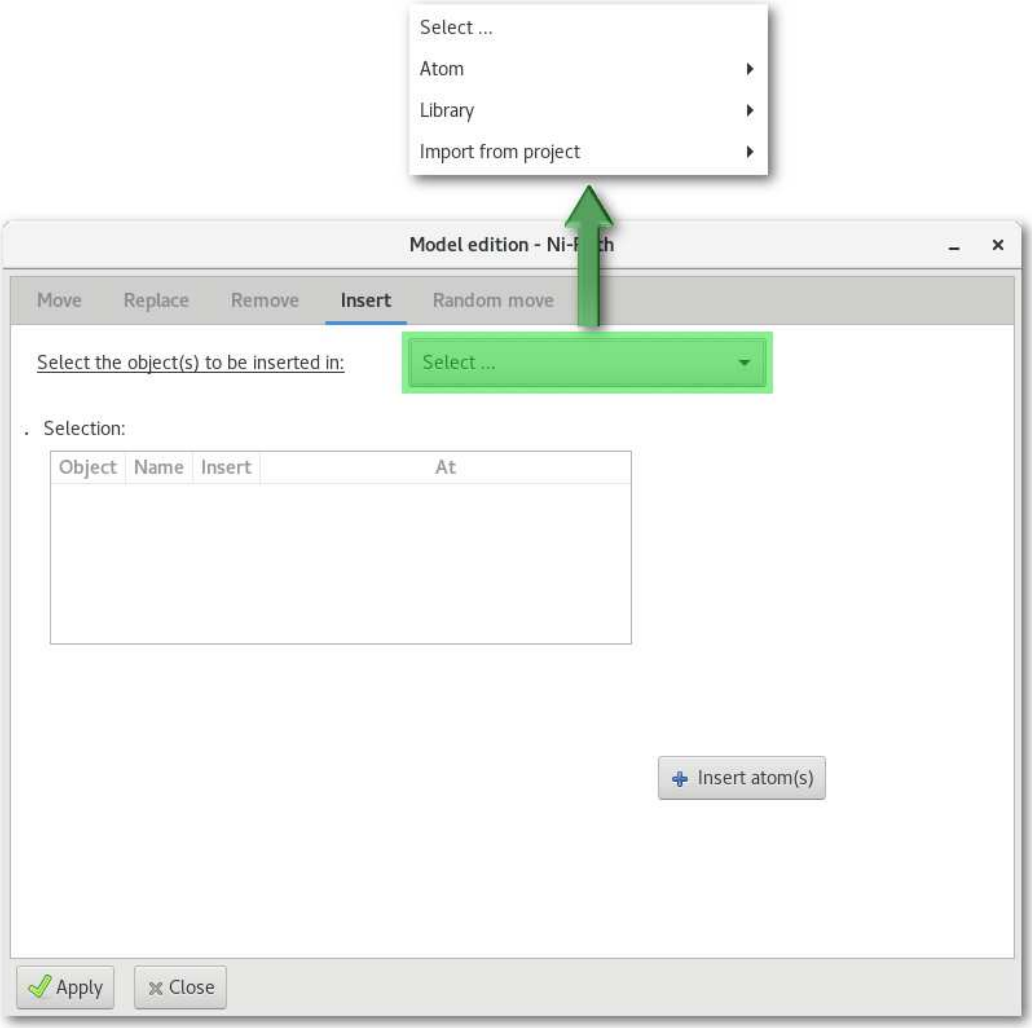


Figure 6.20 *The "`Insert`" tab, with the options to choose the object to be inserted and the position of insertion.*

The "`Select ...`" menu reproduces the one from the "`Replace`" tab, see the bottom part in figure 6.17, and allows to insert atom(s) [Fig. 6.17-c], molecular fragment(s) [Fig. 6.17-d] and atom(s) from any other project opened in the workspace [Fig. 6.17-e]. Selecting any object to insert will populate and update the tree bellow, with a new line. Each line describes the object to be inserted, and offers options to confirm the insertion and specify the position where to insert the object in the model.
An example is provided in figure 6.21 where a fullerene "C_{240}" is inserted in the "`Ni-Phth`" project modified after the removal example illustrated in figure 6.19.

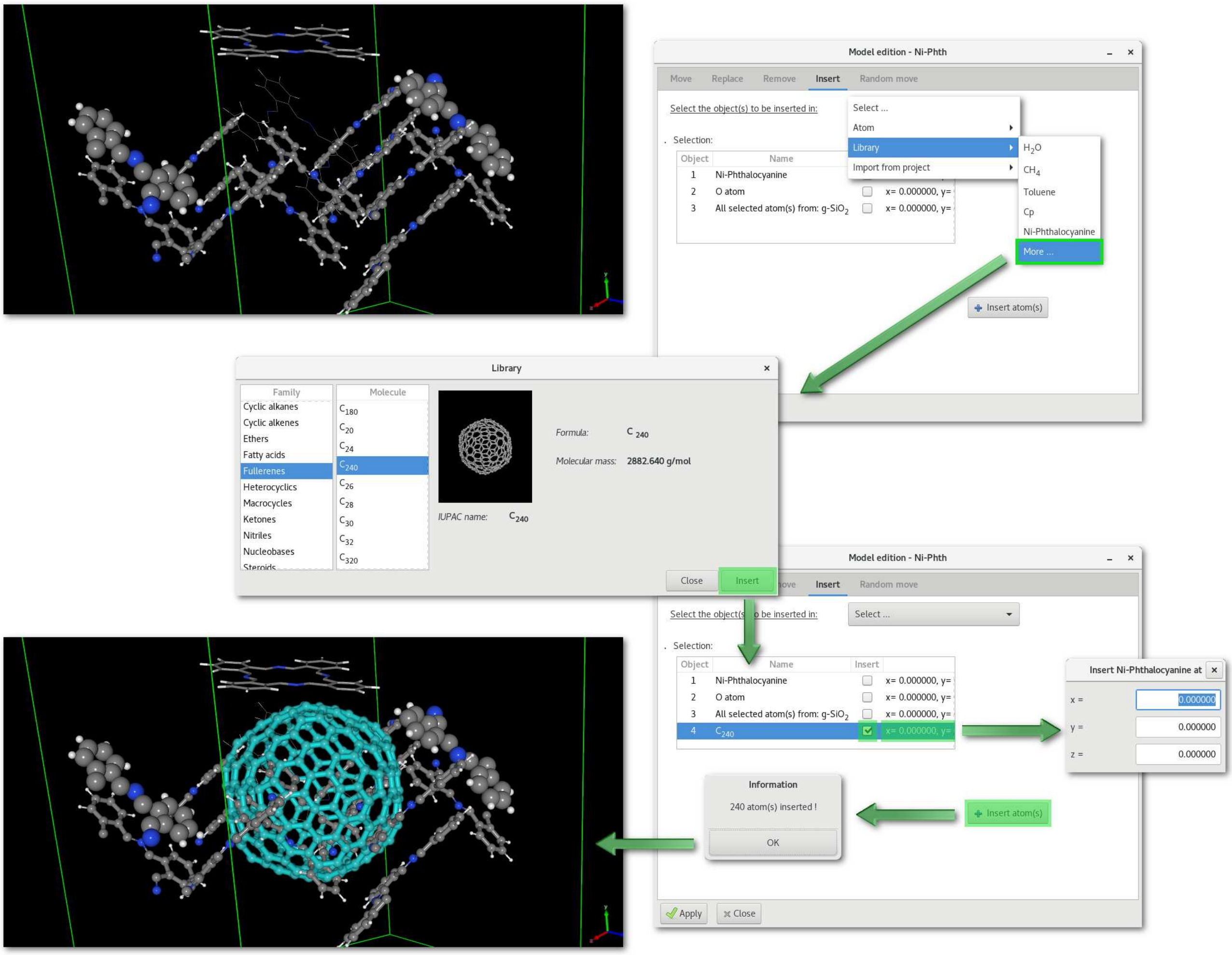


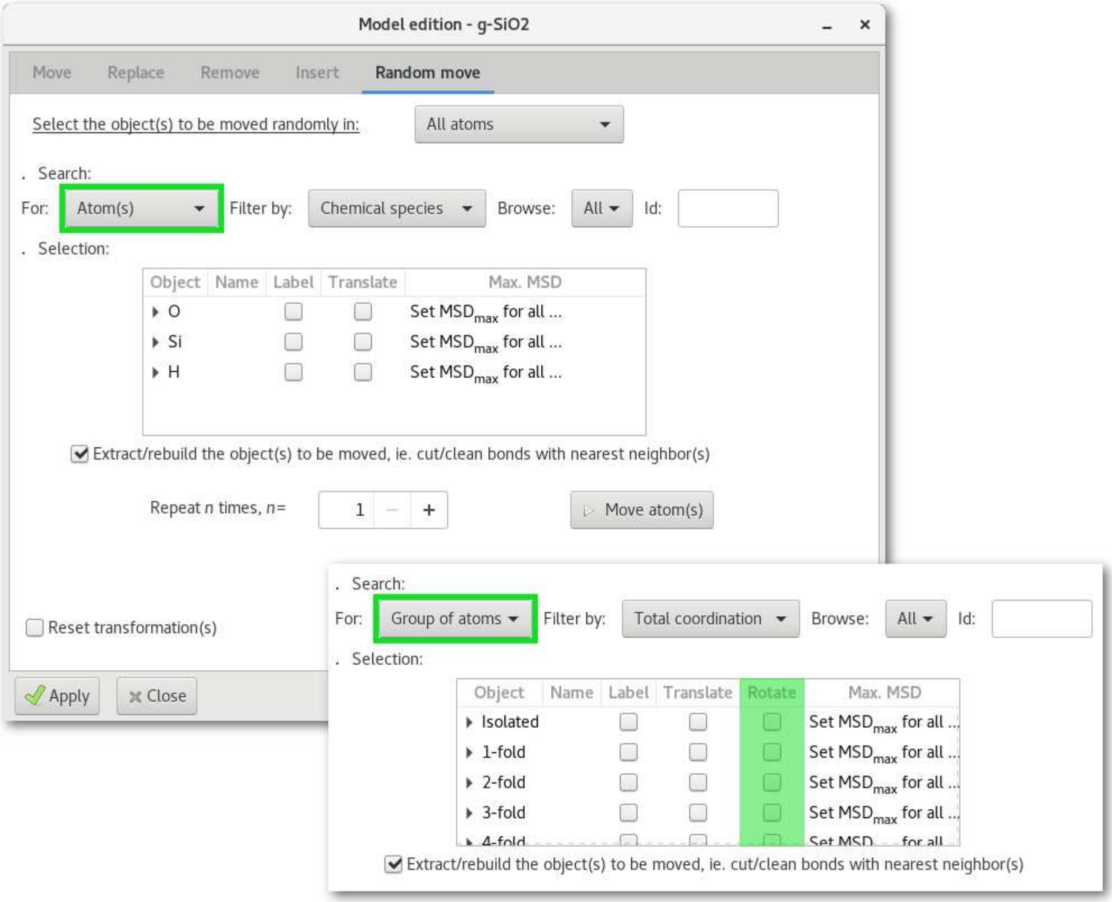
Figure 6.21 *Insertion of fullerene "C_{240}" in the "`Ni-Phth`" project modified after the removal example illustrated in figure 6.19.*

Notes:

- Irreversible: the insertion is irreversible (at least not directly, but it is always possible to remove all inserted atoms) therefore remember to save your work before inserting any object(s) in your model.
- Selection: After the insertion of the new objects, all these new objects will appear surrounded by light blue color (see figure 6.21)in the OpenGL window, and will therefore be selected, making further work on these new objects easier.
- Position: the coordinates (0.0, 0.0, 0.0) always refers to the center of the model, ie. the barycenter of all existing atomic coordinates.

The "`Random move`" tab

The "`Random move`" tab allows to disorder the model:



Select the object(s) to be moved randomly in: All atoms

Search:

For: Atom(s) Filter by: Chemical species Browse: All Id:

Selection:

Object	Name	Label	Translate	Max. MSD
O		☐	☐	Set MSD$_{max}$ for all ...
Si		☐	☐	Set MSD$_{max}$ for all ...
H		☐	☐	Set MSD$_{max}$ for all ...

☑ Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)

Repeat *n* times, *n*= 1

☐ Reset transformation(s)

Search:

For: Group of atoms Filter by: Total coordination Browse: All Id:

Selection:

Object	Name	Label	Translate	Rotate	Max. MSD
Isolated		☐	☐	☐	Set MSD$_{max}$ for all ...
1-fold		☐	☐	☐	Set MSD$_{max}$ for all ...
2-fold		☐	☐	☐	Set MSD$_{max}$ for all ...
3-fold		☐	☐	☐	Set MSD$_{max}$ for all ...
4-fold		☐	☐	☐	Set MSD$_{max}$ for all ...

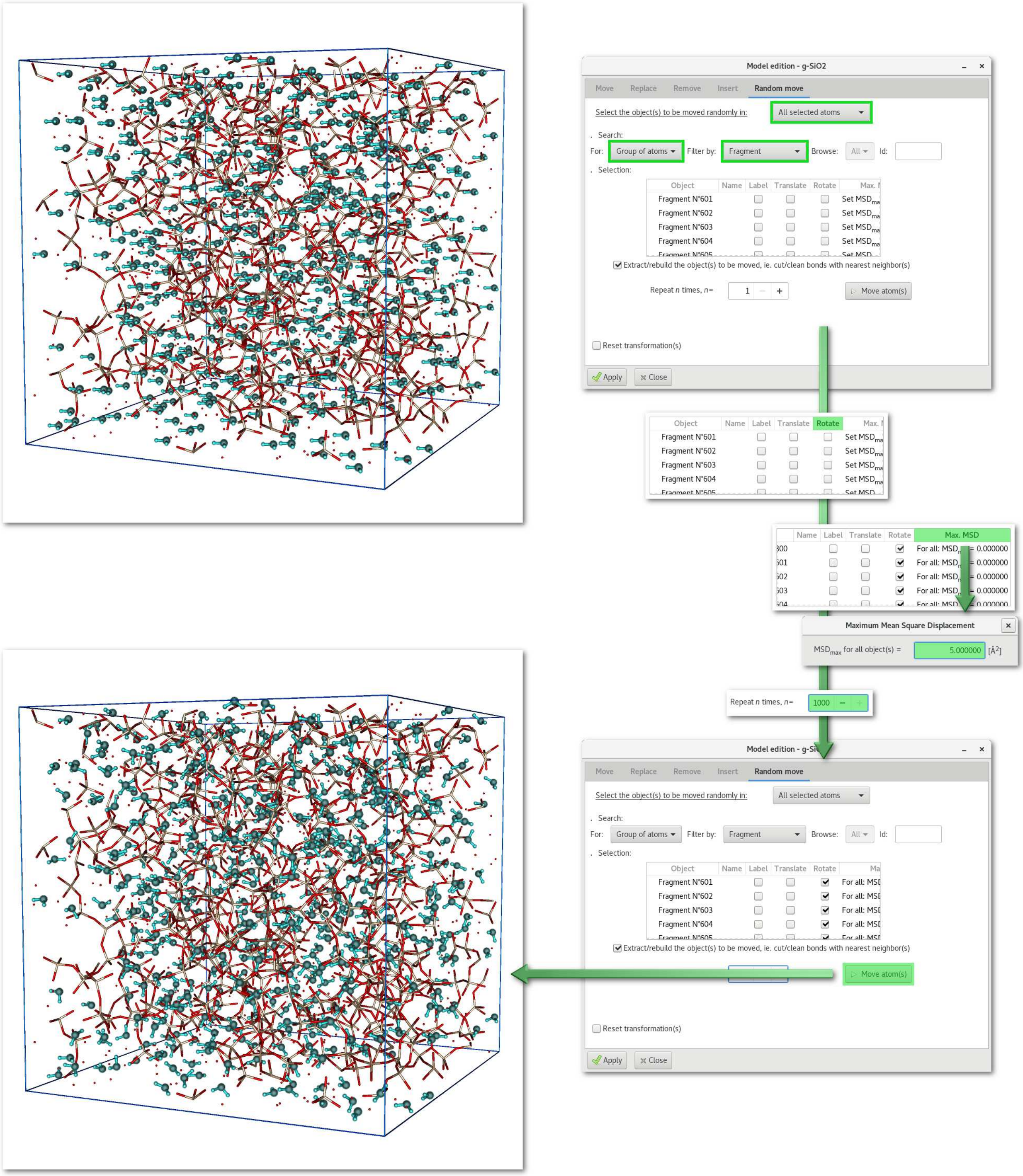
☑ Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)

Figure 6.22 *The "`Random move`" tab. With "`atom(s)`" selected as object(s) it is only possible to translate randomly, with "`Group of atoms`" it is also possible to rotate randomly and the corresponding column appears in the search tree.*

An example is provided in figure 6.23 with the random rotation of "`water`" molecules in the modified "`SiO`$_2$" project after the substitution example illustrated in figure 6.18. Indeed after the substitution "`water`" molecules were all perfectly aligned, to correct this unlikely organization **atomes** can rotate randomly and independently every water molecule in the model:

1. After the substitution all the "`H`" and "`O`" atoms of the newly inserted "`water`" molecules are selected, so search for selected atom(s) only [Fig. 6.13-1].
2. Then choose to apply the action to "`Group of atoms`" [Fig. 6.13-2].
3. Filter the selection using the "`Fragment`" option [Fig. 6.13-3].
4. After the steps 1, 2 and 3 the selection tree will correspond to the one in figure 6.23. To enable the random rotation simply click on the top header of the "`Rotate`"

column to select all object(s), actually all "`water`" molecules. It is required to enter a maximum MSD for each motion, click the top header of the "`MAX. MSD`" column to enter a suitable value. Optionally it is possible to iter the rotation process, at each step the rotation will be completely random.



Model edition - g-SiO2

Select the object(s) to be moved randomly in: All selected atoms

For: Group of atoms Filter by: Fragment Browse: All Id:

Object	Name	Label	Translate	Rotate	Max. MSD
Fragment N°601		☐	☐	☐	Set MSD_{max}
Fragment N°602		☐	☐	☐	Set MSD_{max}
Fragment N°603		☐	☐	☐	Set MSD_{max}
Fragment N°604		☐	☐	☐	Set MSD_{max}

☑ Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)

Repeat *n* times, *n*= 1

☐ Reset transformation(s)

Name	Label	Translate	Rotate	Max. MSD
	☐	☐	☑	For all: MSD_{max} = 0.000000
	☐	☐	☑	For all: MSD_{max} = 0.000000
	☐	☐	☑	For all: MSD_{max} = 0.000000
	☐	☐	☑	For all: MSD_{max} = 0.000000

Maximum Mean Square Displacement

MSD_{max} for all object(s) = 5.000000 [Å^2]

Repeat *n* times, *n*= 1000

Object	Name	Label	Translate	Rotate	Max. MSD
Fragment N°601		☐	☐	☑	For all: MSD
Fragment N°602		☐	☐	☑	For all: MSD
Fragment N°603		☐	☐	☑	For all: MSD
Fragment N°604		☐	☐	☑	For all: MSD

Figure 6.23 *Random rotation of "`water`" molecules in the "`SiO`$_2$" project modified after the substitution example illustrated in figure 6.18.*

Notes:

- Group of atoms: trying to move group of atoms that share atom(s) (ex: 2 coordination spheres with atom(s) in both coordination spheres) can lead to inaccurate results, the shared atom(s) being moved with each object they belong to.
- Rotation: the rotation is performed around the positional barycenter of the object's atomic coordinates. In the case of a repeated rotation the rotation center is preserved until the final step to avoid drifting. If both translation and rotation are repeated then the object is translated first, updating as well the position of the rotation center, and then rotated.
- Reconstruction: the check button labelled "`Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)`" offers the following option:
  - For "`Atom(s)`": if activated the object(s) to be moved will be extracted from the model and translated independently, otherwise chemical bond(s) will simply be stretched.
  - For "`Group of atom(s)`": if activated the atomic positions of the object(s) will be corrected to get only single piece object(s).

6.1.4 The "`Extract/rebuild`" buttons

As introduced in the previous pages these buttons allows to extract object(s) to be moved or copied/pasted from the model, into single piece object(s). The effect on motion is illustrated in sections 6.1.3 and 6.2.1, the effect on copy is the following:

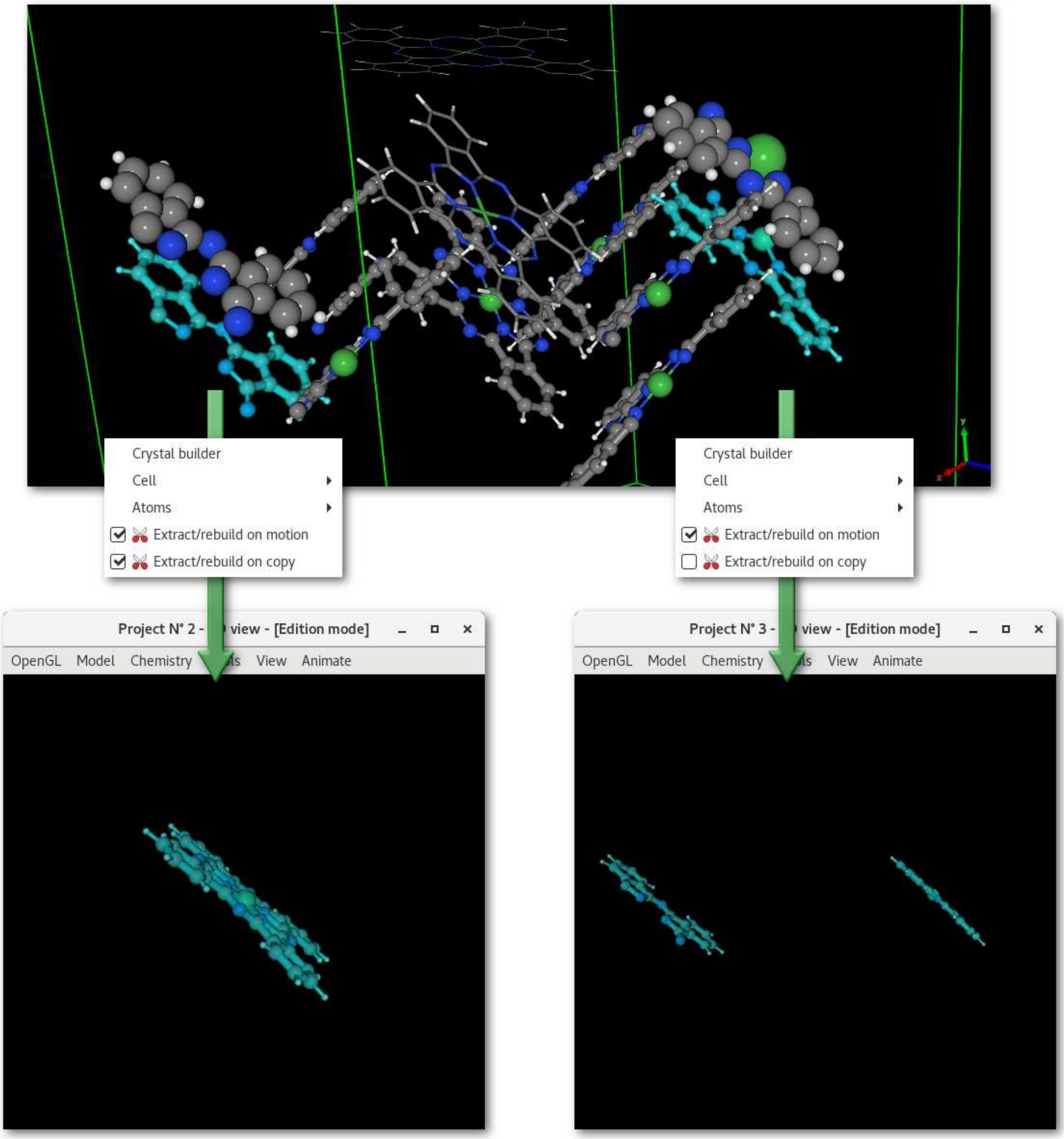


Figure 6.24 *Illustration of the rebuild process, a fragment is copied from the top figure and pasted back in new projects. That fragment appears split because of the PBC: on the left the fragment is rebuild as a singe object, on the right the 2 pieces remain separated.*

6.2 Mouse interaction with the OpenGL window: edition

It is possible to activate the mouse "`Edition`" using the "`Tools`" menu:

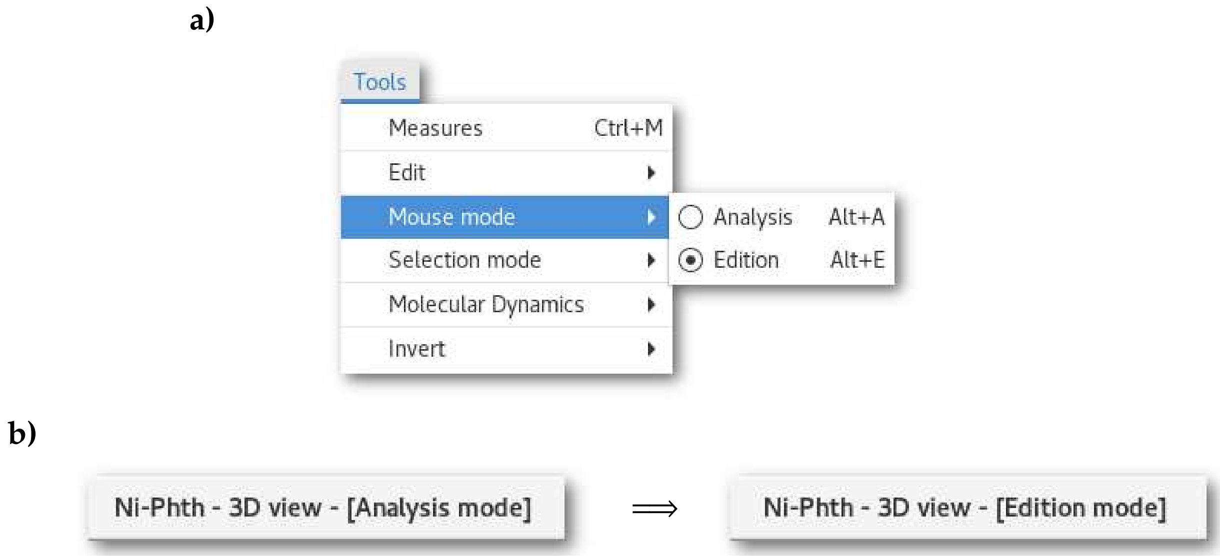


Figure 6.25 **a)** *Activating the mouse "*`Edition`*" mode using the "*`Tools`*" menu.* **b)** *when switching mode the title bar of the OpenGL window changes.*

It is also possible to use the Alt + e keyboard shortcut, and to switch back to "`Analysis`" mode using the Alt + a shortcut.
In "`Edition`" mode the mouse button functions are the following:

- **Left button**
    - *Single click on object*: object selection
    - *Pressed on background* + *motion*: **selected** (*only*) atomic coordinates rotation *
- **Scroll button**
    - *Scrolled*: zoom in/out
    - *Pressed* + *motion*: **selected** (*only*) atomic coordinates translation
- **Right button**
    - *Pressed on background*: edition contextual menu
    - *Pressed on object*: object edition contextual menu

* The rotation is performed around the coordinates barycenter of the selected atoms.

6.2.1 Atom selection

As for the "`Analysis`" mode object(s) can be selected using the mouse left click. In "`Edition`" mode selected atoms/objects are subjects to motion interactions using the mouse and it becomes complicated to check motion information with visual measurements. However using the "`Tools`" menu it is possible to activate the "`Measures`" selection mode (available when using the "`Model edition`" dialog (see section 6.1.3):

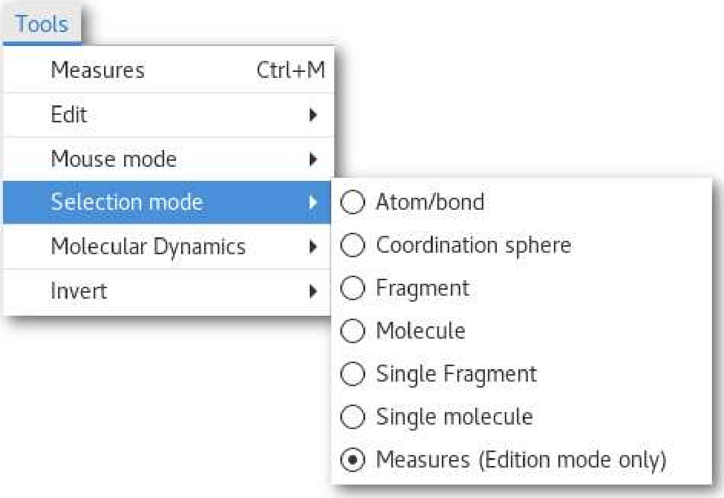
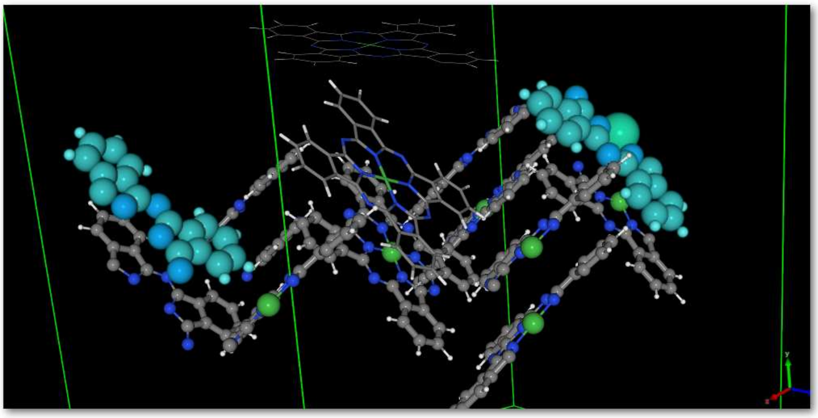


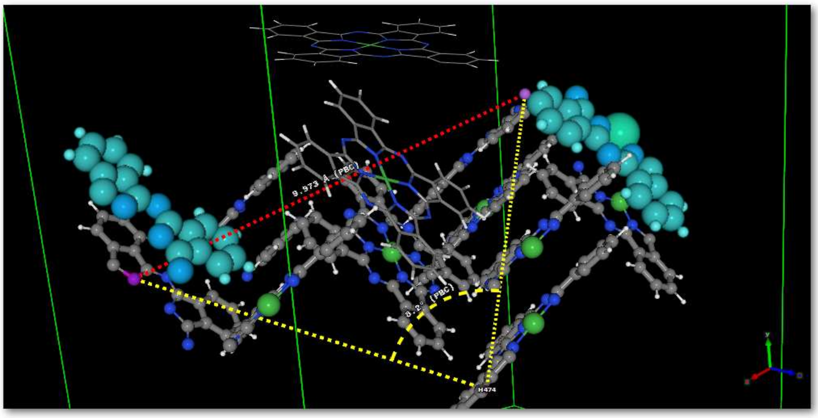
Figure 6.26 *Activating the "`Measures`" selection mode using the "`Tools`" menu.*

The following provides an example of utilization of the "`Measures`" selection mode:

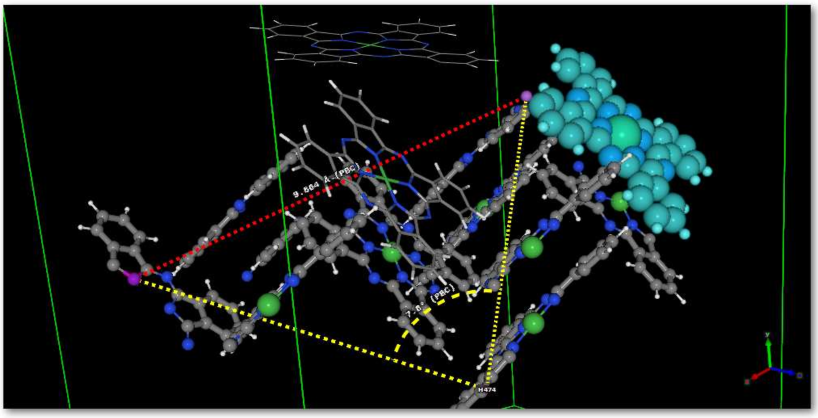
1. Select a fragment in the model:



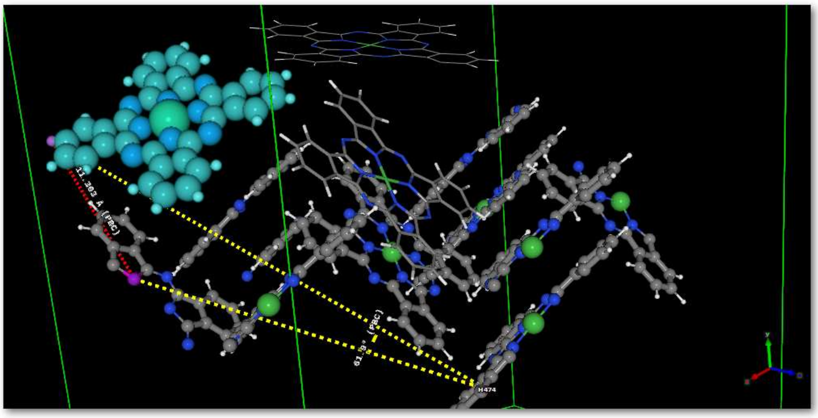
2. Switch to "`Edition`" mode (if not done already) and change the "`Mouse selection mode`" to "`Measures (Edition mode only)`". Then select some atoms in the model, and open the "`Measures`" dialog (see section 5.1.4) to display some measurements:



3. Start to move the selected fragment using the mouse left click+motion to rotate or mouse scroll click+motion to translate, by default, and if divided because of the PBC, **atomes** will reconstruct the fragment (see figure 6.27 to modify that behavior):



4. You will see that when moving the fragment with the mouse the information displayed (inter-atomic distances and angles) is instantaneously refreshed:



6.2.2 The edition contextual menu

The mouse right click button on the background of the OpenGL window opens the edition contextual menu:

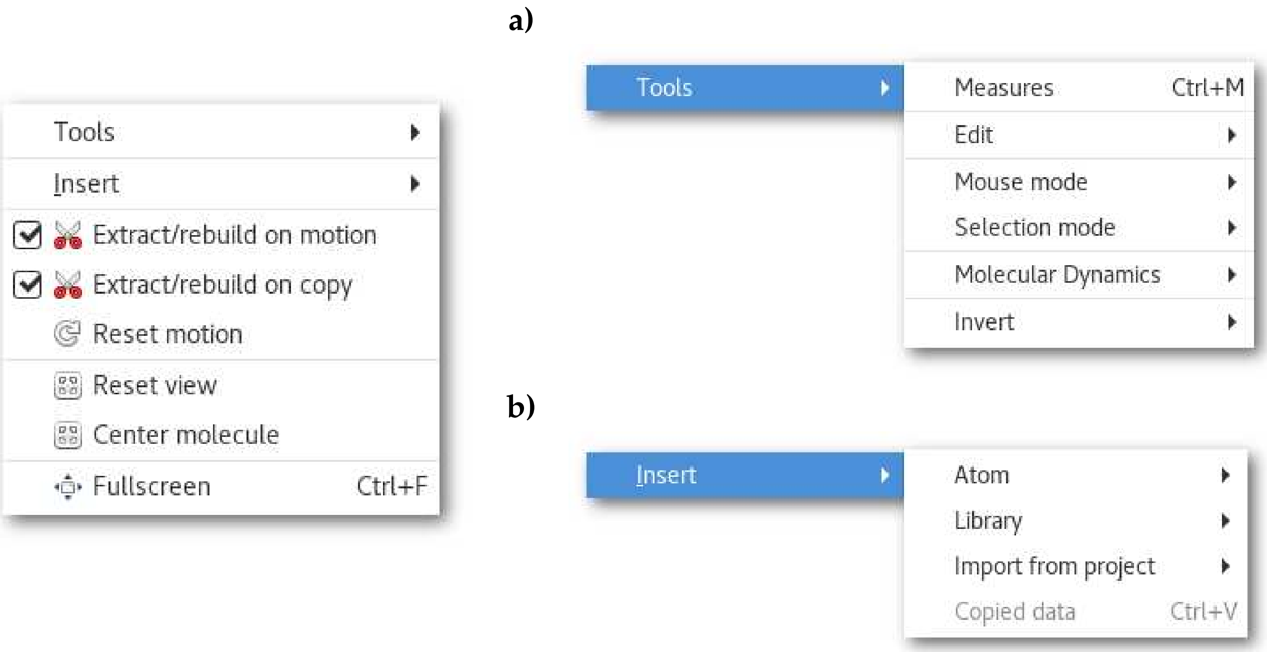
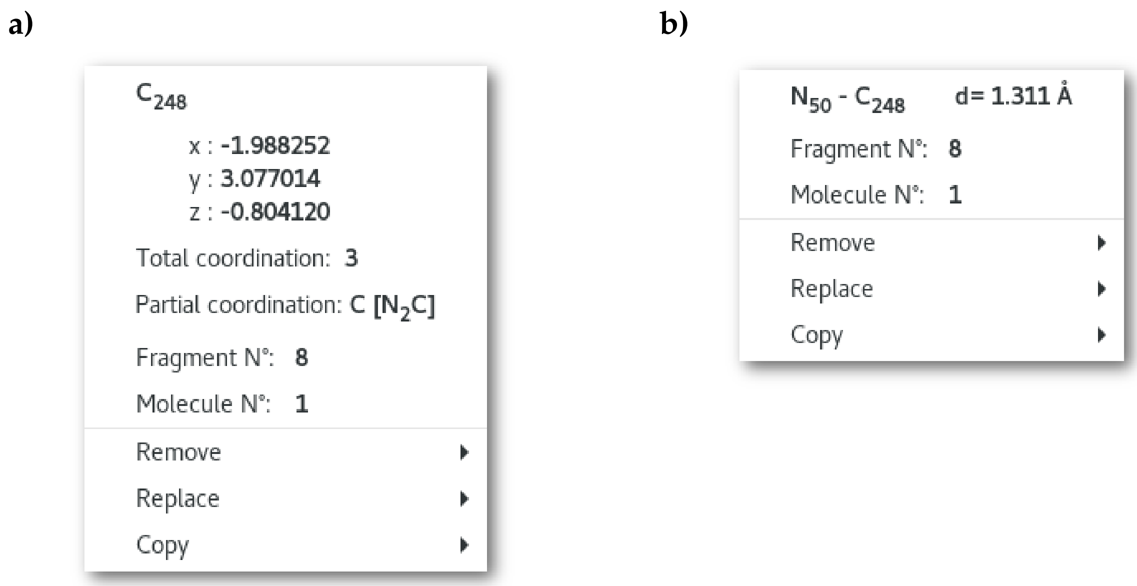


Figure 6.27 *The right button contextual menu on the background of the OpenGL window.*

- The "`Tools`" submenu [Fig. 6.27-a] reproduces the corresponding top bar menu.
- The "`Insert`" submenu [Fig. 6.27-b] offers shortcuts to insert objects in the model, and is similar to the "`Select ...`" menus described in section 6.1.3 for the "`Replace`" and "`Remove`" tabs of the "`Model edition`" dialog.
- The "`Extract/rebuild on motion`" button:
  - For "`Atom(s)`": if activated the object(s) to be moved will be extracted from the model and translated independently, otherwise chemical bond(s) will simply be stretched.
  - For "`Group of atom(s)`": if activated the atomic positions of the object(s) will be corrected to get only single piece object(s).
- The "`Reset motion`" button will reset all atomic coordinates to the value immediately saved when:
  - Entering the "`Edition`" mode: **if no atoms were inserted or removed in the model.**
  - Replacing/removing/inserting atom(s): **if any atom was inserted or removed in the model.**

6.2.3 The object edition contextual menu

Pressed over any atom/bond the right button opens the object edition contextual menu:



a)

C_{248}

x : -1.988252
y : 3.077014
z : -0.804120

Total coordination: 3

Partial coordination: C [N_2C]

Fragment N°: 8

Molecule N°: 1

b)

N_{50} - C_{248} d= 1.311 Å

Fragment N°: 8

Molecule N°: 1

Figure 6.28 *The object edition contextual menu:* **a)** *for an atom,* **b)** *for a chemical bond.*

The object edition contextual menu in figure 6.28 follows exactly the construction described in section 5.2.2 and 5.2.2 for the object contextual menu in "`Analysis`" mode. The object edition contextual menu offers shortcuts to "`Remove`", "`Replace`" and "`Copy`" object(s) in the model.

6.3 Keyboard shortcuts

- Single key shortcuts:
  - Colors:
    - a : change atom(s) colormap
    - p : change polyhedra(ons) colormap
  - Styles:
    - b : change default style to "`Ball and stick`"
    - c : change default style to "`Cylinders`"
    - d : change default style to "`Dots`"
    - s : change default style to "`Spheres`"
    - o : change default style to "`Covalent radius`"
    - i : change default style to "`Ionic radius`"
    - v : change default style to "`van Der Waals radius`"
    - r : change default style to "`In cristal radius`"
    - w : change default style to "`Wireframe`"
  - Measures:
    - m : show all measures for the selection, if pressed:
      - * once: display inter-atomic distance(s)
      - * twice: display inter-atomic angles
      - * a third time: hide measures
  - Atomic coordinates rotation:
    - → : rotate atomic coordinates right
    - ← : rotate atomic coordinates left
    - ↑ : rotate atomic coordinates up
    - ↓ : rotate atomic coordinates down
  - Misc:
    - Esc : exit fullscreen mode
    - Del : Delete all selected atom(s)

- Combined keys shortcuts:
  - Mouse mode:

    Alt + a : enter mouse "`Analysis`" mode
    Alt + e : enter mouse "`Edition`" mode

  - Selection:

    Ctrl + a : select / unselect all atoms
    Ctrl + c : copy all selected atom(s)
    Ctrl + v : paste copied selection (if the model is not a MD trajectory)
    Ctrl + x : copy, then delete selection
    Ctrl + n : create new (empty project)

  - Atomic coordinates translation:

    Ctrl + → : translate atomic coordinates right
    Ctrl + ← : translate atomic coordinates left
    Ctrl + ↑ : translate atomic coordinates up
    Ctrl + ↓ : translate atomic coordinates down
    Shift ⇑ + ↑ : zoom out
    Shift ⇑ + ↓ : zoom in

  - Misc:

    Ctrl + l : label / unlabel all atoms
    Ctrl + e : open the "`Environments configuration`" window [Sec. 5.1.3]
    Ctrl + m : open the "`Measures`" dialog [Sec. 5.1.4]
    Ctrl + r : open the "`Recorder`" dialog [Sec. 5.1.6]
    Ctrl + f : enter / exit fullscreen mode

Preparing molecular dynamics calculations in atomes

atomes proposes assistants dedicated to the creation/preparation/modification of input files for (massively parallel) molecular dynamics calculations:

- Classical MD:
  - DL-POLY [1]
  - LAMMPS [2]
- *ab-initio* MD:
  - CPMD [3]
  - CP2K [4]
- QM-MM (Mixed *ab-initio* - classical) MD:
  - CPMD [3]
  - CP2K [4]

7.1 Classical MD

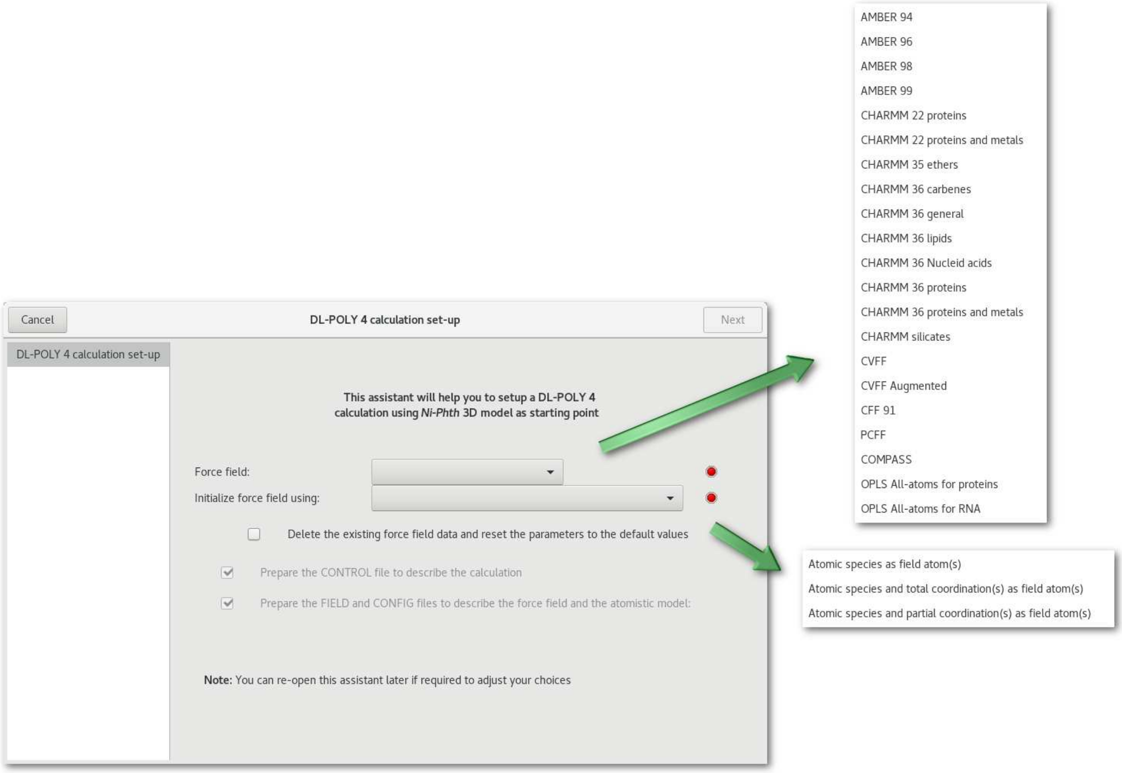
7.1.1 DL-POLY v4.09

The **atomes** helper for the DL-POLY calculation offers to prepare input files for **DL-POLY v4.09**. The **CONTROL**, **FIELD** and **CONFIG** files can be entirely designed. Before going further it is strongly advised to read the DL-POLY user manual:

ftp://ftp.dl.ac.uk/ccp5/DL_POLY/DL_POLY_4.0/DOCUMENTS/USRMAN4.pdf

7.1.1.1 Initializing the force field

The mandatory first step in the DL-POLY calculation assistant is to initialize the force field, as illustrated in figure 7.1 it required to select both:



This assistant will help you to setup a DL-POLY 4 calculation using *Ni-Phth* 3D model as starting point

Force field:

Initialize force field using:

☐ Delete the existing force field data and reset the parameters to the default values

☑ Prepare the CONTROL file to describe the calculation

☑ Prepare the FIELD and CONFIG files to describe the force field and the atomistic model:

Note: You can re-open this assistant later if required to adjust your choices

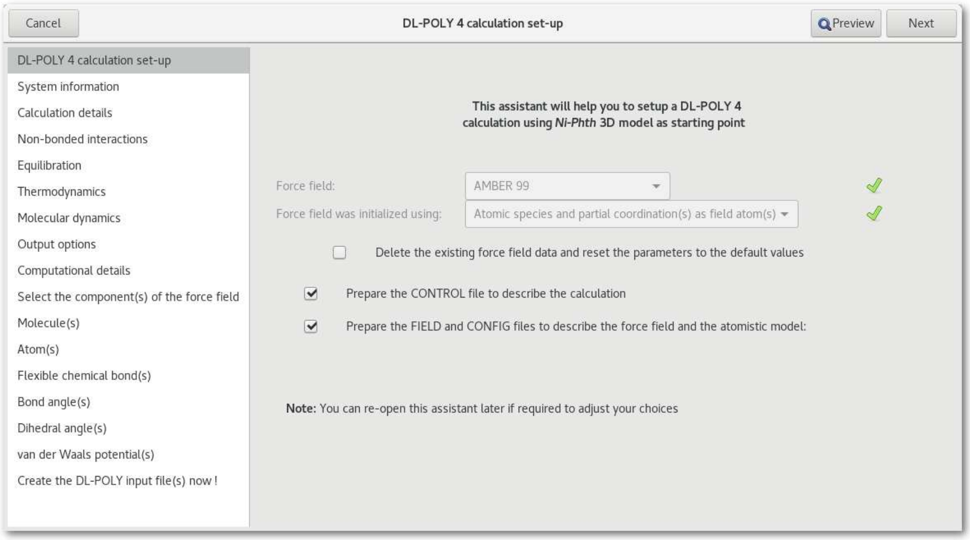
Figure 7.1 *Initializing the force field in the DL-POLY calculation assistant.*

- The force field to be used, ie. the data source for many of the "`FIELD`" file parameters including: bonds, angles, dihedrals and inversions.
  The **FIELD** file parameters can be imported from the following force fields:
  - **OPLS force fields**:
    - OPLS All-atoms for proteins
    - OPLS All-atoms for RNA
  - **CHARMM force fields**:
    - CHARMM 22 proteins
    - CHARMM 22 proteins and metals
    - CHARMM 35 ethers
    - CHARMM 36 carbenes
    - CHARMM 36 general
    - CHARMM 36 lipids
    - CHARMM 36 Nucleid acids
    - CHARMM 36 proteins
    - CHARMM 36 proteins and metals
    - CHARMM silicates
  - **AMBER force fields**:
    - AMBER 94
    - AMBER 96
    - AMBER 98
    - AMBER 99
  - **Consistent force fields**:
    - CVFF
    - CVFF Augmented
    - CFF 91
    - PCFF
    - COMPASS

Theses parameters are read by **atomes** on the fly / by request from the corresponding files located in the directory: "`bin/library/force_fields`".

- The atoms description to initiate the force field, ie. the first "rough" type of field atoms for the initial description of the force field:
  - The atomic species
  - The atomic species and the total coordination(s)
  - The atomic species and the partial coordination(s)

Once the force field has been initialized the default pages populates the assistant:



This assistant will help you to setup a DL-POLY 4 calculation using *Ni-Phth* 3D model as starting point

Force field: AMBER 99 ✓

Force field was initialized using: Atomic species and partial coordination(s) as field atom(s) ✓

☐ Delete the existing force field data and reset the parameters to the default values

☑ Prepare the CONTROL file to describe the calculation

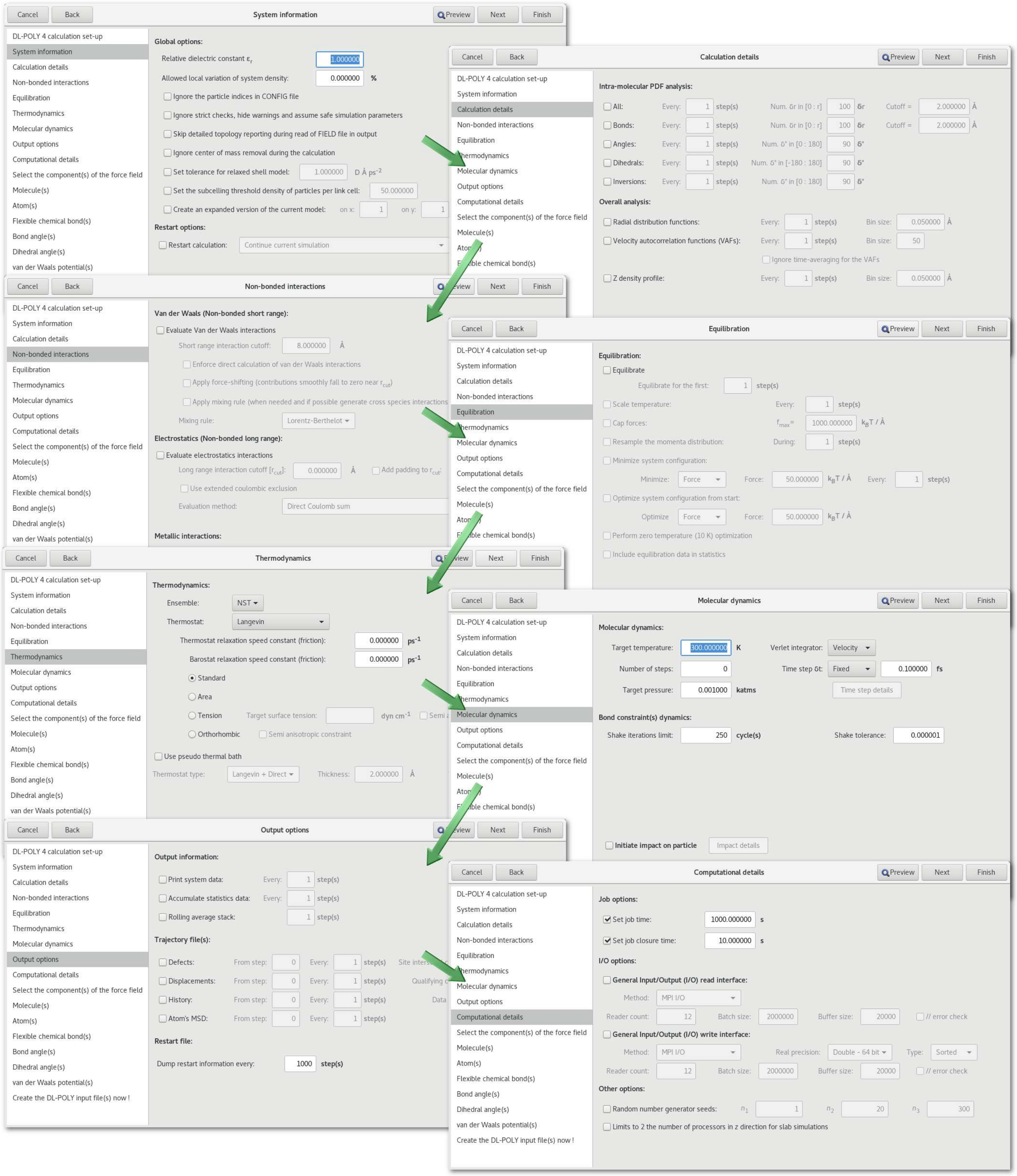
☑ Prepare the FIELD and CONFIG files to describe the force field and the atomistic model:

Note: You can re-open this assistant later if required to adjust your choices

Figure 7.2 *The initialized force field in the DL-POLY calculation assistant.*

7.1.1.2 The "`CONTROL`" file

When the force field has been initialized and providing the "`CONTROL`" file is to be prepared, it is possible to adjust the corresponding options.
These options are regrouped in 8 tabs illustrated in figure 7.3, and almost all options from the DL-POLY user guide are available, with the exception of the Plumed calculation options and some options for the two-temperature "`ttm`" model.



System information

Global options:
Relative dielectric constant ε_r: 1.000000
Allowed local variation of system density: 0.000000 %
☐ Ignore the particle indices in CONFIG file
☐ Ignore strict checks, hide warnings and assume safe simulation parameters
☐ Skip detailed topology reporting during read of FIELD file in output
☐ Ignore center of mass removal during the calculation
☐ Set tolerance for relaxed shell model: 1.000000 D Å ps^{-2}
☐ Set the subcelling threshold density of particles per link cell: 50.000000
☐ Create an expanded version of the current model: on x: 1 on y: 1
Restart options:
☐ Restart calculation: Continue current simulation

Calculation details

Intra-molecular PDF analysis:
☐ All: Every: 1 step(s) Num. δr in [0 : r] 100 δr Cutoff = 2.000000 Å
☐ Bonds: Every: 1 step(s) Num. δr in [0 : r] 100 δr Cutoff = 2.000000 Å
☐ Angles: Every: 1 step(s) Num. δ° in [0 : 180] 90 δ°
☐ Dihedrals: Every: 1 step(s) Num. δ° in [-180 : 180] 90 δ°
☐ Inversions: Every: 1 step(s) Num. δ° in [0 : 180] 90 δ°
Overall analysis:
☐ Radial distribution functions: Every: 1 step(s) Bin size: 0.050000 Å
☐ Velocity autocorrelation functions (VAFs): Every: 1 step(s) Bin size: 50
☐ Ignore time-averaging for the VAFs
☐ Z density profile: Every: 1 step(s) Bin size: 0.050000 Å

Non-bonded interactions

Van der Waals (Non-bonded short range):
☐ Evaluate Van der Waals interactions
Short range interaction cutoff: 8.000000 Å
☐ Enforce direct calculation of van der Waals interactions
☐ Apply force-shifting (contributions smoothly fall to zero near r_{cut})
☐ Apply mixing rule (when needed and if possible generate cross species interactions
Mixing rule: Lorentz-Berthelot
Electrostatics (Non-bonded long range):
☐ Evaluate electrostatics interactions
Long range interaction cutoff [r_{cut}]: 0.000000 Å ☐ Add padding to r_{cut}
☐ Use extended coulombic exclusion
Evaluation method: Direct Coulomb sum
Metallic interactions:

Equilibration

Equilibration:
☐ Equilibrate
Equilibrate for the first: 1 step(s)
☐ Scale temperature: Every: 1 step(s)
☐ Cap forces: f_{max} = 1000.000000 k_BT / Å
☐ Resample the momenta distribution: During: 1 step(s)
☐ Minimize system configuration:
Minimize: Force Force: 50.000000 k_BT / Å Every: 1 step(s)
☐ Optimize system configuration from start:
Optimize Force Force: 50.000000 k_BT / Å
☐ Perform zero temperature (10 K) optimization
☐ Include equilibration data in statistics

Thermodynamics

Thermodynamics:
Ensemble: NST
Thermostat: Langevin
Thermostat relaxation speed constant (friction): 0.000000 ps^{-1}
Barostat relaxation speed constant (friction): 0.000000 ps^{-1}
● Standard
○ Area
○ Tension Target surface tension: dyn cm^{-1} ☐ Semi
○ Orthorhombic ☐ Semi anisotropic constraint
☐ Use pseudo thermal bath
Thermostat type: Langevin + Direct Thickness: 2.000000 Å

Molecular dynamics

Molecular dynamics:
Target temperature: 300.000000 K Verlet integrator: Velocity
Number of steps: 0 Time step δt: Fixed 0.100000 fs
Target pressure: 0.001000 katms Time step details
Bond constraint(s) dynamics:
Shake iterations limit: 250 cycle(s) Shake tolerance: 0.000001
☐ Initiate impact on particle Impact details

Output options

Output information:
☐ Print system data: Every: 1 step(s)
☐ Accumulate statistics data: Every: 1 step(s)
☐ Rolling average stack: 1 step(s)
Trajectory file(s):
☐ Defects: From step: 0 Every: 1 step(s) Site inters
☐ Displacements: From step: 0 Every: 1 step(s) Qualifying
☐ History: From step: 0 Every: 1 step(s) Data
☐ Atom's MSD: From step: 0 Every: 1 step(s)
Restart file:
Dump restart information every: 1000 step(s)

Computational details

Job options:
☑ Set job time: 1000.000000 s
☑ Set job closure time: 10.000000 s
I/O options:
☐ General Input/Output (I/O) read interface:
Method: MPI I/O
Reader count: 12 Batch size: 2000000 Buffer size: 20000 ☐ // error check
☐ General Input/Output (I/O) write interface:
Method: MPI I/O Real precision: Double - 64 bit Type: Sorted
Reader count: 12 Batch size: 2000000 Buffer size: 20000 ☐ // error check
Other options:
☐ Random number generator seeds: n_1 1 n_2 20 n_3 300
☐ Limits to 2 the number of processors in z direction for slab simulations

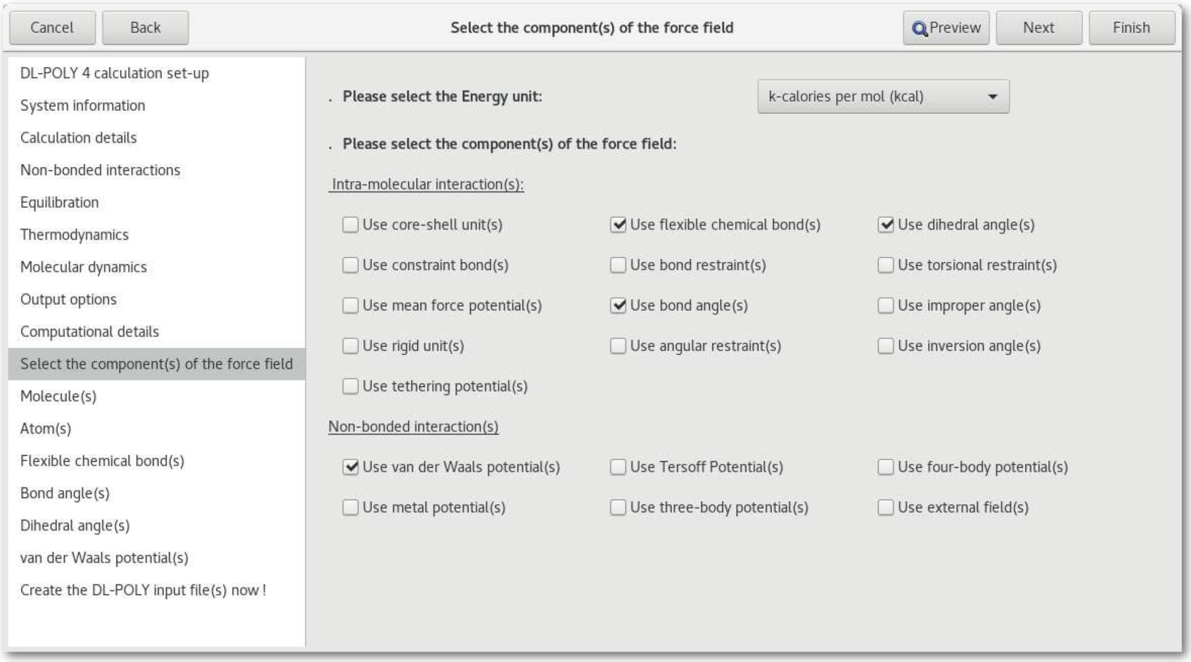
Figure 7.3 *The "`CONTROL`" file options in the DL-POLY calculation assistant.*

7.1.1.3 The "`FIELD`" file

If the "`FIELD`" file is to be prepared then the corresponding tabs are also made available in the assistant.

Force field elements

The first tab related to the "`FIELD`" file allows to enable or disable all kind of component(s) for the force field to be created:



. Please select the Energy unit: k-calories per mol (kcal)

. Please select the component(s) of the force field:

Intra-molecular interaction(s):

☐ Use core-shell unit(s)	☑ Use flexible chemical bond(s)	☑ Use dihedral angle(s)
☐ Use constraint bond(s)	☐ Use bond restraint(s)	☐ Use torsional restraint(s)
☐ Use mean force potential(s)	☑ Use bond angle(s)	☐ Use improper angle(s)
☐ Use rigid unit(s)	☐ Use angular restraint(s)	☐ Use inversion angle(s)
☐ Use tethering potential(s)		

Non-bonded interaction(s)

☑ Use van der Waals potential(s)	☐ Use Tersoff Potential(s)	☐ Use four-body potential(s)
☐ Use metal potential(s)	☐ Use three-body potential(s)	☐ Use external field(s)

Figure 7.4 *"`Select the component(s) of the force field`" tab in the DL-POLY calculation assistant.*

The "`Energy unit`" combo box, allows to change the energy units for the field parameters, please note that changing the energy unit will convert all parameters in the "`FIELD`" file to the new unit.

The other options are divided in 2 categories, the "`Intra-molecular interaction(s)`" options and the "`Non-bonded interaction(s)`" options. To enable / disable any feature simply check / uncheck the corresponding button in this tab, then the associated page will be inserted / removed from the list of pages available in the assistant.

General behavior of the "`FIELD`" file part of the assistant

Each page of the assistant is dedicated to a particular property, the first pages (up to 13 pages) being dedicated to intra-molecular interactions and the latest pages (up to 6 pages) being dedicated to non-bonded interactions.

Each page contains a table presenting the list of the associated properties, double clicking on a line with the mouse left button will allow to edit the corresponding line/property, while the mouse right button will open a contextual menu with different set of actions including the edition available otherwise.

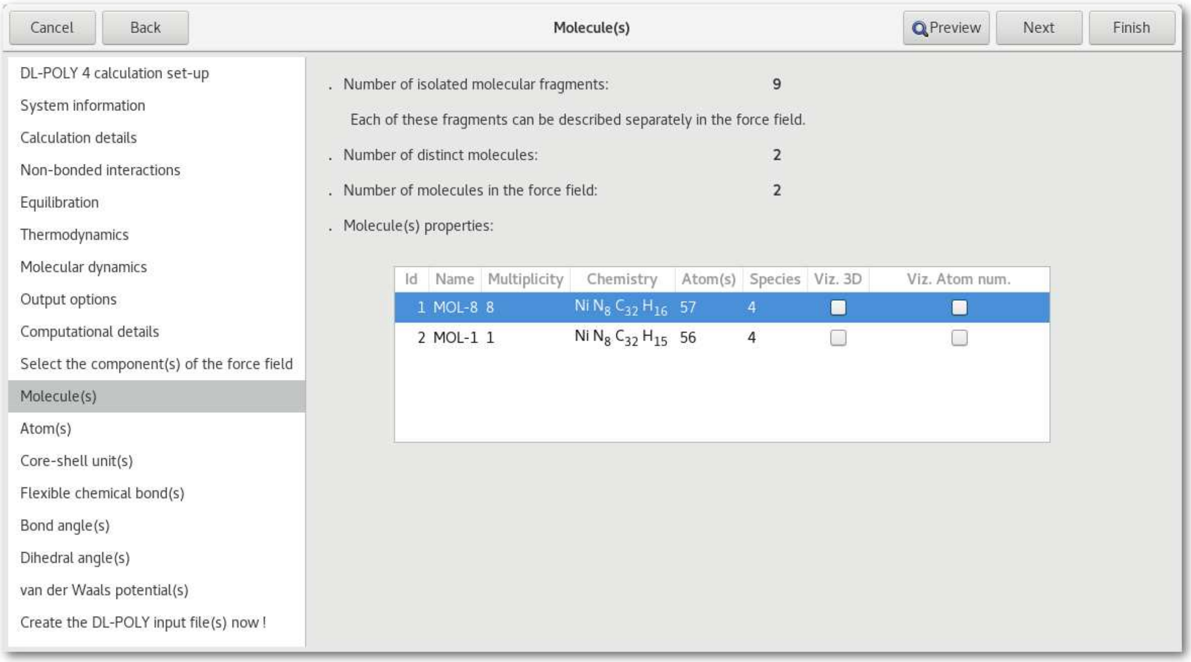
For almost each and every intra or inter-molecular property listed in the corresponding tab, corresponds a "`Use`" check button. It is mandatory to check-in the "`Use`" button for the property to be used when building the "`FIELD`" (remember that few are mutually exclusive), if not then the information is simply stored for further usage.

Any objects selection is associated with a visualization in the model, ie. if an atom/a bond/an angle ... is selected then this object will be highlighted with a particular color in the 3D window, also the associated line in the selection dialog will be colored as well and using the same color.

Each page will be briefly introduced thereafter.

The "`Molecule(s)`" tab

The "`Molecule(s)`" tab, see figure 7.5, lists all the different molecules in the model:



. Number of isolated molecular fragments: 9

Each of these fragments can be described separately in the force field.

. Number of distinct molecules: 2

. Number of molecules in the force field: 2

. Molecule(s) properties:

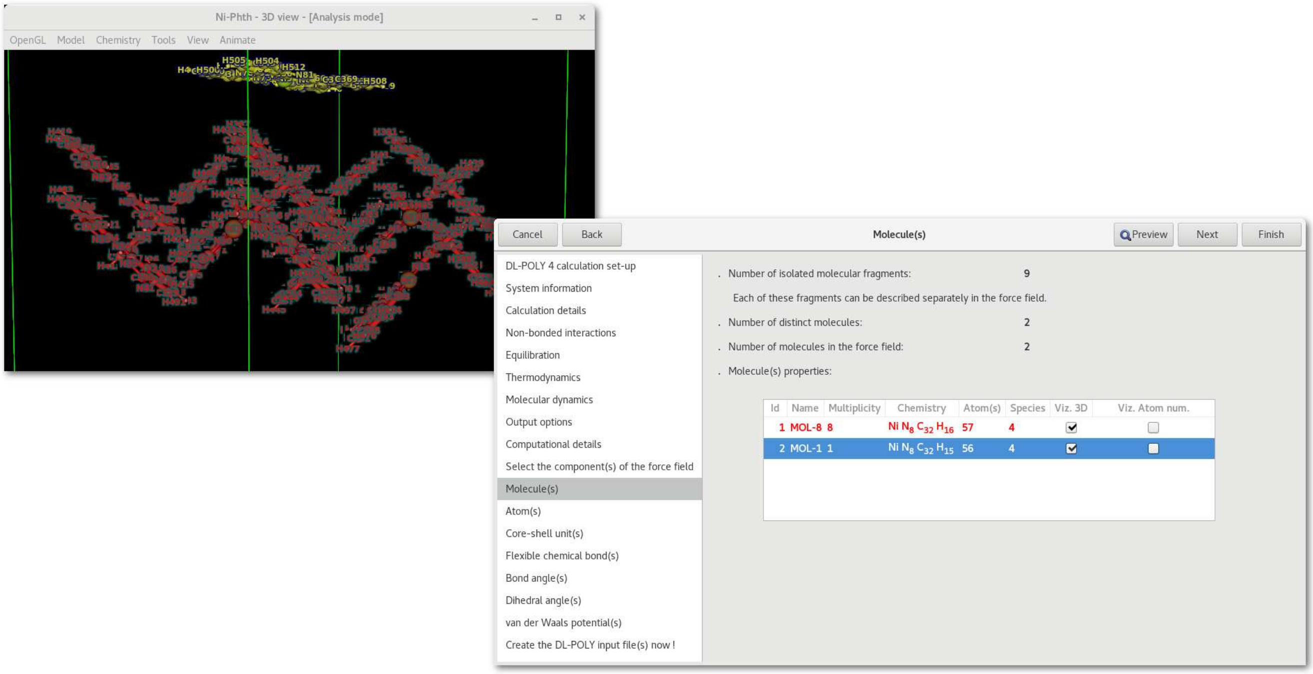
Id	Name	Multiplicity	Chemistry	Atom(s)	Species	Viz. 3D	Viz. Atom num.
1	MOL-8	8	$NiN_8C_{32}H_{16}$	57	4	☐	☐
2	MOL-1	1	$NiN_8C_{32}H_{15}$	56	4	☐	☐

Figure 7.5 *"`Molecule(s)`" tab in the DL-POLY calculation assistant.*

Each line corresponds to a molecule, and for each molecule the information is as follow:

1. ID in the force field
2. Name in the force field (can be changed by double clicking on the line)
3. Multiplicity (number of times the same molecule appears in the model)
4. Chemistry
5. Total number of atoms
6. Number of chemical species
7. Check button to visualize the molecule in the model
8. Check button to visualize the atom number within the molecule

In the "`Ni-Phth`" example used here, two distinct molecules are found, 8 identical and standard Ni-phthalocyanine molecules that constitute the bottom surface and 1 modified Ni-phthalocyanine molecule, with a H atom missing on top of it.
As illustrated in figure 7.6 the effect of the first check button 7 is to help visualizing the different molecule(s) in the model. For each molecule a color is defined and applied to both the atom(s) in the model and the corresponding line in the "`Molecule(s)`" tab.



. Number of isolated molecular fragments: 9

Each of these fragments can be described separately in the force field.

. Number of distinct molecules: 2

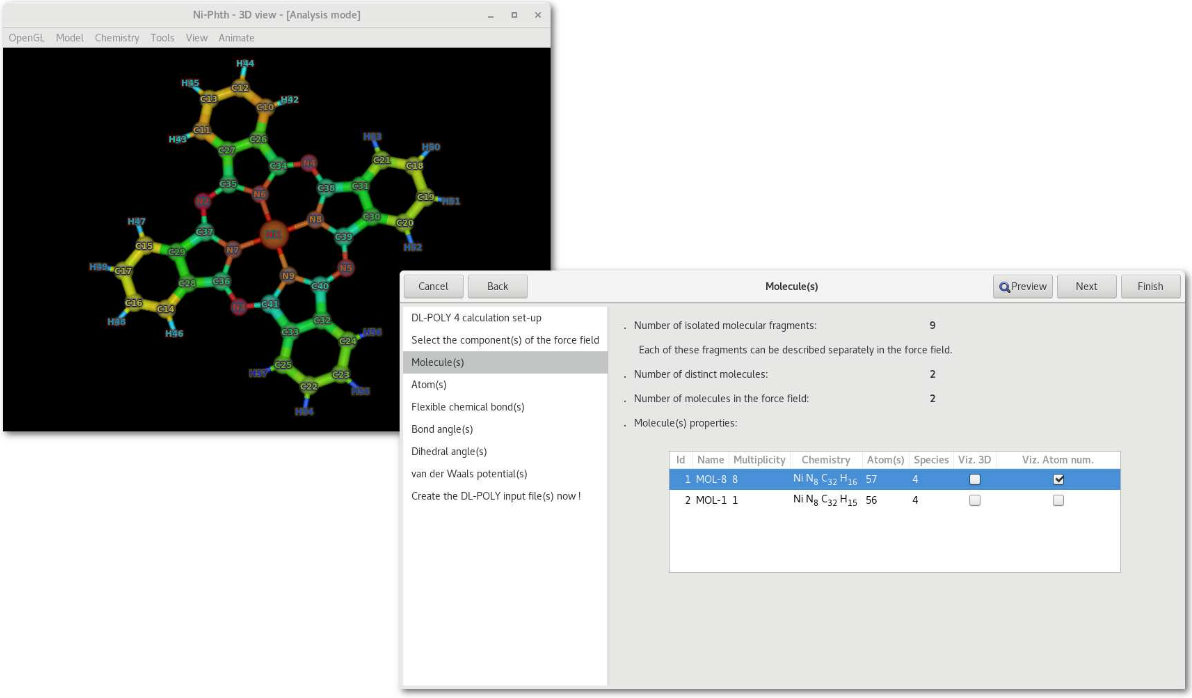
. Number of molecules in the force field: 2

. Molecule(s) properties:

Id	Name	Multiplicity	Chemistry	Atom(s)	Species	Viz. 3D	Viz. Atom num.
1	MOL-8	8	Ni N_8 C_{32} H_{16}	57	4	☑	☐
2	MOL-1	1	Ni N_8 C_{32} H_{15}	56	4	☑	☐

Figure 7.6 *Visualizing the "`Molecule(s)`" using the DL_POLY calculation assistant.*

Whereas as illustrated in figure 7.7 the effect of the second check button 8 is to help visualizing the atom numbers as assigned in the "`FIELD`" file, numbers range from 1 to the total number of atom(s) in the molecule.



. Number of isolated molecular fragments: 9

Each of these fragments can be described separately in the force field.

. Number of distinct molecules: 2

. Number of molecules in the force field: 2

. Molecule(s) properties:

Id	Name	Multiplicity	Chemistry	Atom(s)	Species	Viz. 3D	Viz. Atom num.
1	MOL-8	8	Ni N_8 C_{32} H_{16}	57	4	☐	☑
2	MOL-1	1	Ni N_8 C_{32} H_{15}	56	4	☐	☐

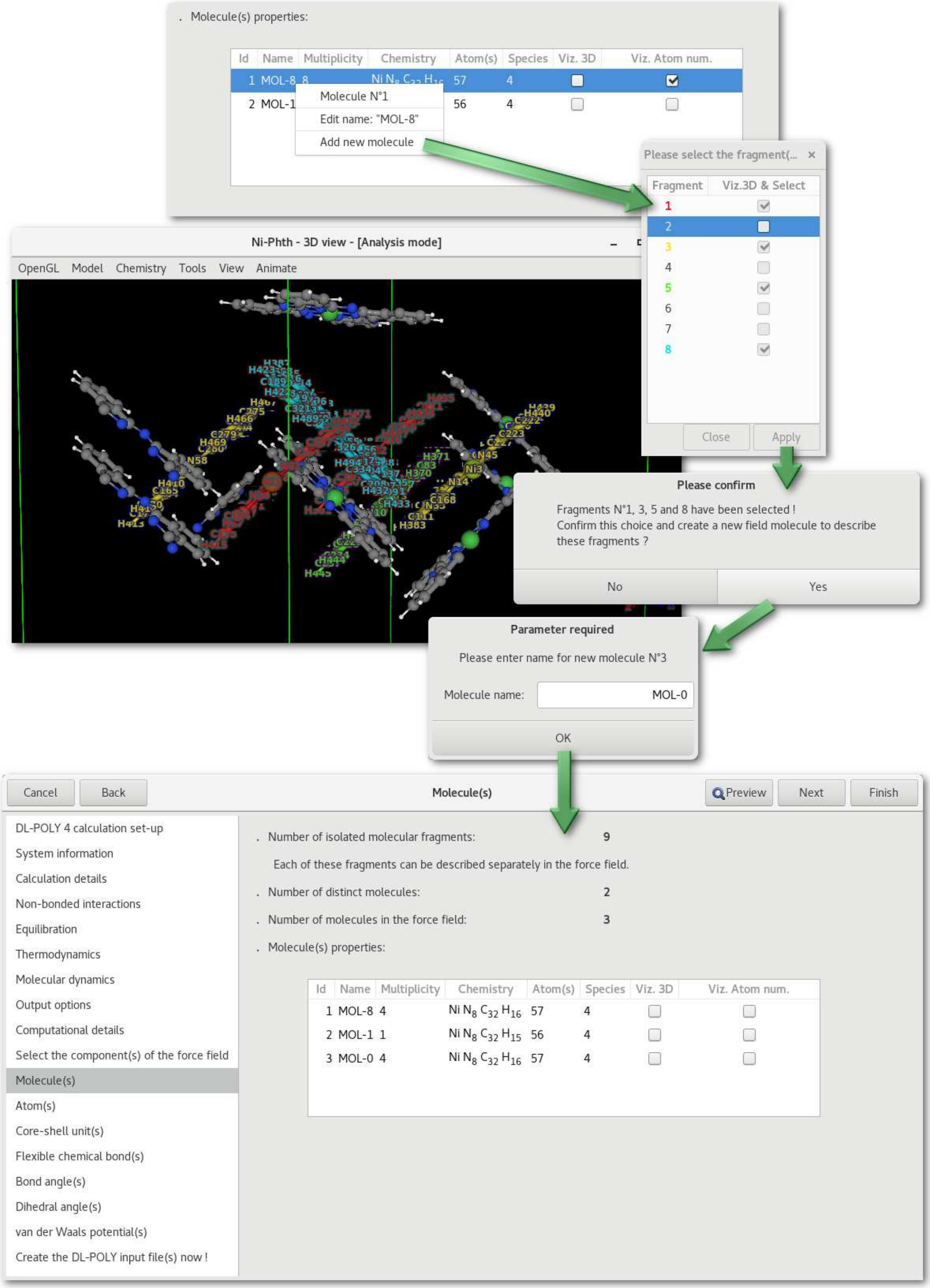
Figure 7.7 *Visualizing the atom(s) number(s) within the "`Molecule(s)`", to clarify the representation a single fragment from the "`NiPhth`" example is displayed.*

Some mouse options are available in the "`Molecule(s)`" tab:

- Double click anywhere on the line to edit the name of the molecule.
- Use the right click to open the contextual menu to edit the name/add/remove molecule(s).

As illustrated in figures 7.8 and 7.9 it is possible to add molecule(s) to the force field, or to merge existing molecules from the force field into a single description:

- Providing that the multiplicity of a molecule is higher than 1, and therefore than several identical molecular fragment exist, it is possible to split the existing molecule, preserving the old description for the non-selected fragment(s) and creating a copy for the selected fragment(s). This process is illustrated in figure 7.8.
- Providing that some molecules in the force field have the same chemistry and connectivity it is possible to merge the description this two separates molecules as one. This process is illustrated in figure 7.9.



. Molecule(s) properties:

Id	Name	Multiplicity	Chemistry	Atom(s)	Species	Viz. 3D	Viz. Atom num.
1	MOL-8	8	Ni N_8 C_{32} H_{16}	57	4	☐	☑
2	MOL-1			56	4	☐	☐

Please select the fragment(...

Fragment	Viz.3D & Select
1	☑
2	☐
3	☑
4	☐
5	☑
6	☐
7	☐
8	☑

Please confirm

Fragments N°1, 3, 5 and 8 have been selected !
Confirm this choice and create a new field molecule to describe these fragments ?

Parameter required

Please enter name for new molecule N°3

Molecule name: MOL-0

. Number of isolated molecular fragments: 9

Each of these fragments can be described separately in the force field.

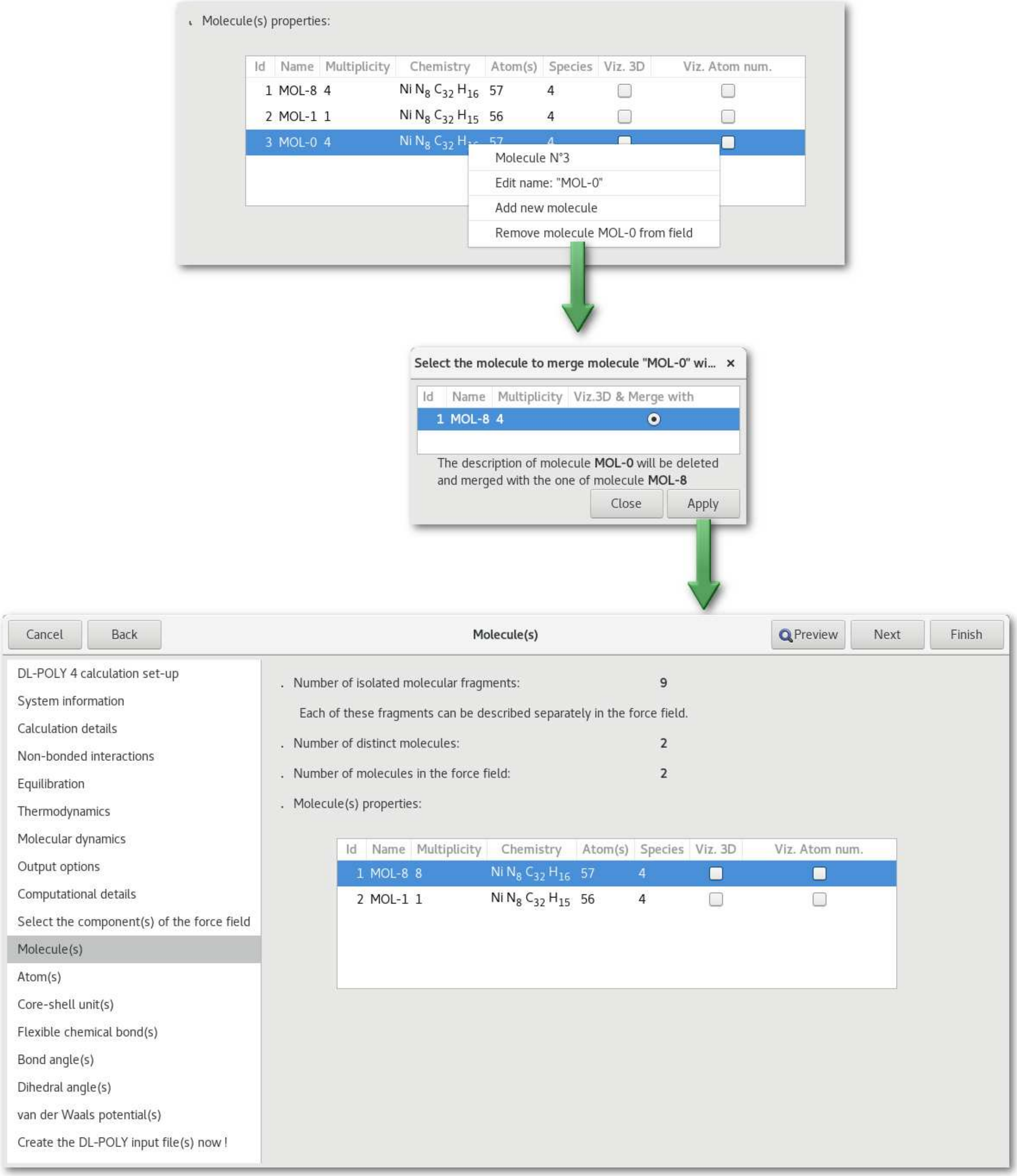
. Number of distinct molecules: 2

. Number of molecules in the force field: 3

. Molecule(s) properties:

Id	Name	Multiplicity	Chemistry	Atom(s)	Species	Viz. 3D	Viz. Atom num.
1	MOL-8	4	Ni N_8 C_{32} H_{16}	57	4	☐	☐
2	MOL-1	1	Ni N_8 C_{32} H_{15}	56	4	☐	☐
3	MOL-0	4	Ni N_8 C_{32} H_{16}	57	4	☐	☐

Figure 7.8 *Adding molecules to the force field using the DL_POLY calculation assistant.*



. Molecule(s) properties:

Id	Name	Multiplicity	Chemistry	Atom(s)	Species	Viz. 3D	Viz. Atom num.
1	MOL-8	4	Ni N_8 C_{32} H_{16}	57	4	☐	☐
2	MOL-1	1	Ni N_8 C_{32} H_{15}	56	4	☐	☐
3	MOL-0	4	Ni N_8 C_{32} H	57	4	☐	☐

Select the molecule to merge molecule "MOL-0" wi...

Id	Name	Multiplicity	Viz.3D & Merge with
1	MOL-8	4	●

The description of molecule **MOL-0** will be deleted and merged with the one of molecule **MOL-8**

. Number of isolated molecular fragments: 9

Each of these fragments can be described separately in the force field.

. Number of distinct molecules: 2

. Number of molecules in the force field: 2

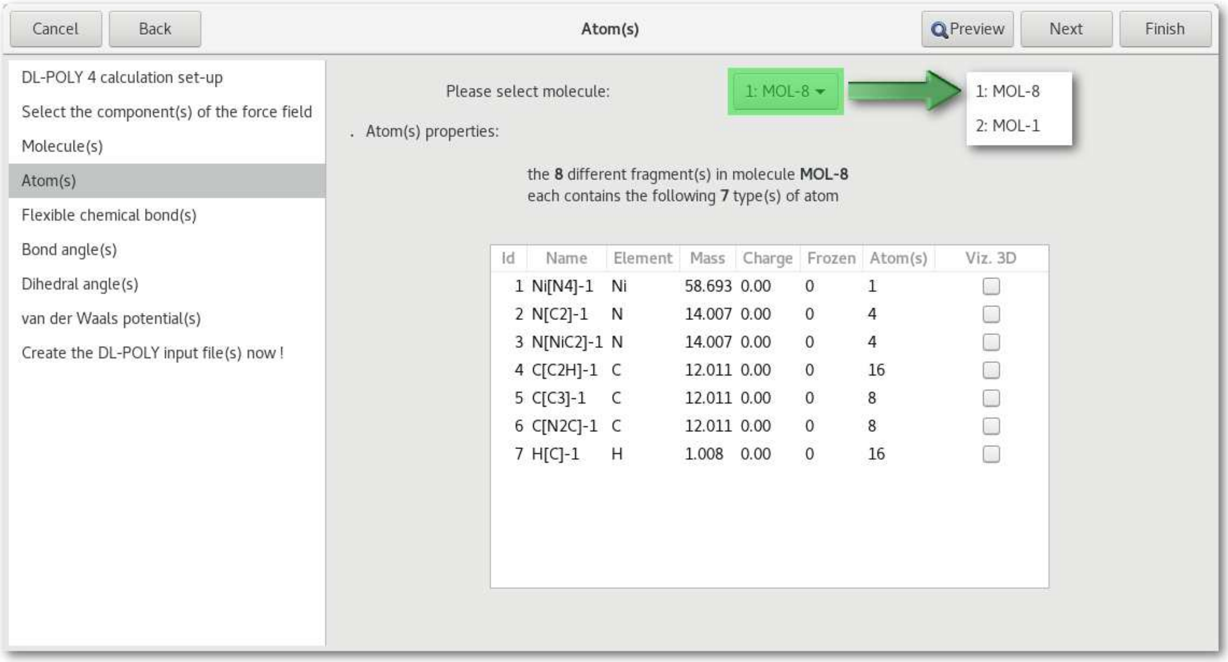
. Molecule(s) properties:

Id	Name	Multiplicity	Chemistry	Atom(s)	Species	Viz. 3D	Viz. Atom num.
1	MOL-8	8	Ni N_8 C_{32} H_{16}	57	4	☐	☐
2	MOL-1	1	Ni N_8 C_{32} H_{15}	56	4	☐	☐

Figure 7.9 *Merging molecules from the force field using the DL_POLY calculation assistant.*

The "`Atom(s)`" tab

When molecules have been properly defined, the next tab allows to configure the atom(s) description, this has to be done for each molecule:



Please select molecule: 1: MOL-8

Atom(s) properties:

the **8** different fragment(s) in molecule **MOL-8**
each contains the following **7** type(s) of atom

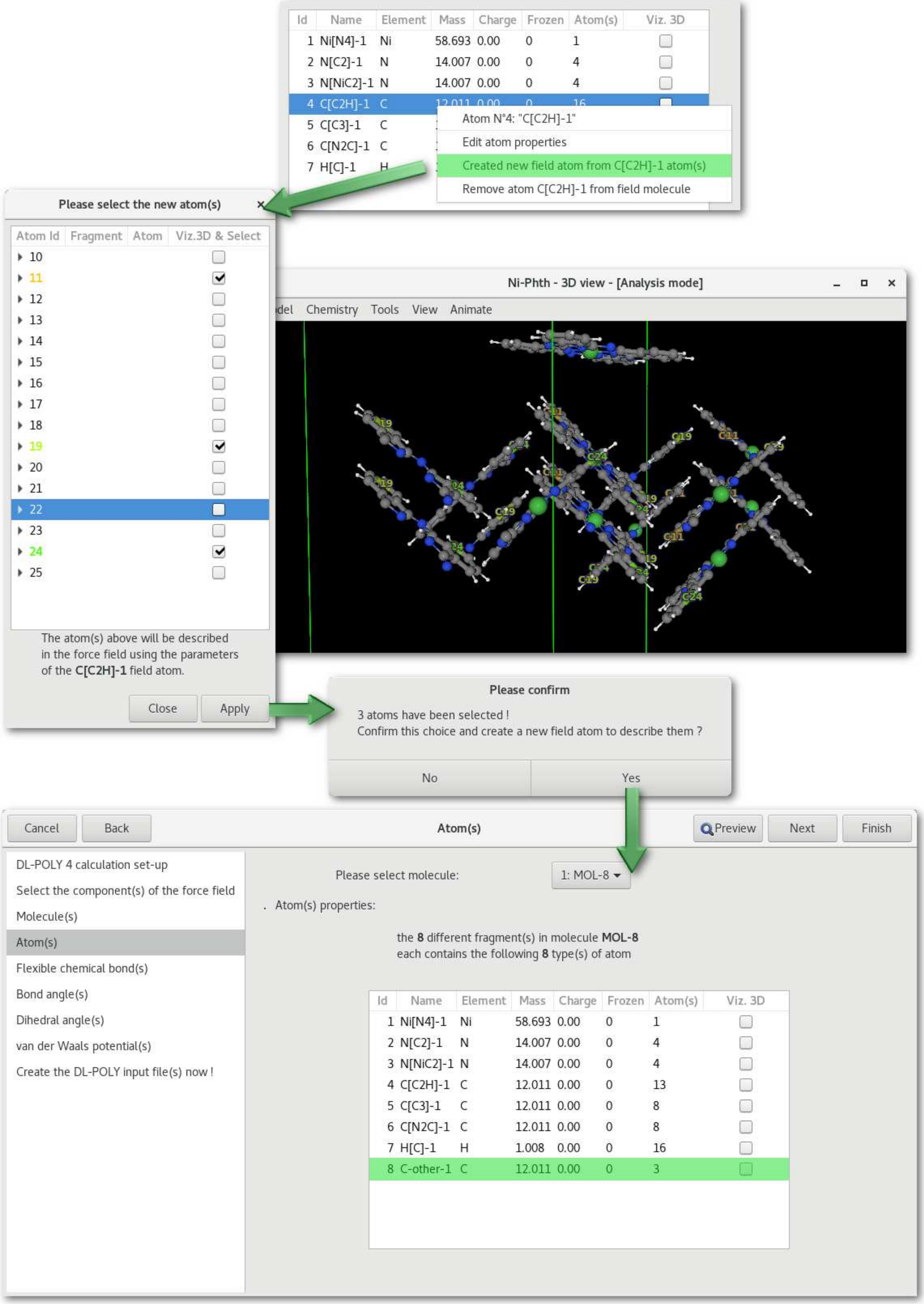
Id	Name	Element	Mass	Charge	Frozen	Atom(s)	Viz. 3D
1	Ni[N4]-1	Ni	58.693	0.00	0	1	☐
2	N[C2]-1	N	14.007	0.00	0	4	☐
3	N[NiC2]-1	N	14.007	0.00	0	4	☐
4	C[C2H]-1	C	12.011	0.00	0	16	☐
5	C[C3]-1	C	12.011	0.00	0	8	☐
6	C[N2C]-1	C	12.011	0.00	0	8	☐
7	H[C]-1	H	1.008	0.00	0	16	☐

Figure 7.10 *The "`Atom(s)`" tab in the DL-POLY assistant.*

As illustrated in figure 7.10 the first element to notice in the "`Atom(s)`" tab is the combo box for the choice of the molecule to work on, that same combo box will be inserted in any tab dedicated to intra-molecular interactions.

Each line corresponds to a particular atom for the molecule specified above, and for each atom the information is as follow:

1. ID in the molecule
2. Name in the molecule
3. Element
4. Mass
5. Charge
6. Number of frozen atoms for this type
7. Total number of atoms for this type
8. Check button to visualize the atom in the model



Id	Name	Element	Mass	Charge	Frozen	Atom(s)	Viz. 3D
1	Ni[N4]-1	Ni	58.693	0.00	0	1	☐
2	N[C2]-1	N	14.007	0.00	0	4	☐
3	N[NiC2]-1	N	14.007	0.00	0	4	☐
4	C[C2H]-1	C	12.011	0.00	0	16	☐
5	C[C3]-1	C					
6	C[N2C]-1	C					
7	H[C]-1	H					

Please select the new atom(s)

Atom Id	Fragment	Atom	Viz.3D & Select
10			☐
11			☑
12			☐
13			☐
14			☐
15			☐
16			☐
17			☐
18			☐
19			☑
20			☐
21			☐
22			☐
23			☐
24			☑
25			☐

The atom(s) above will be described in the force field using the parameters of the **C[C2H]-1** field atom.

Please confirm

3 atoms have been selected !
Confirm this choice and create a new field atom to describe them ?

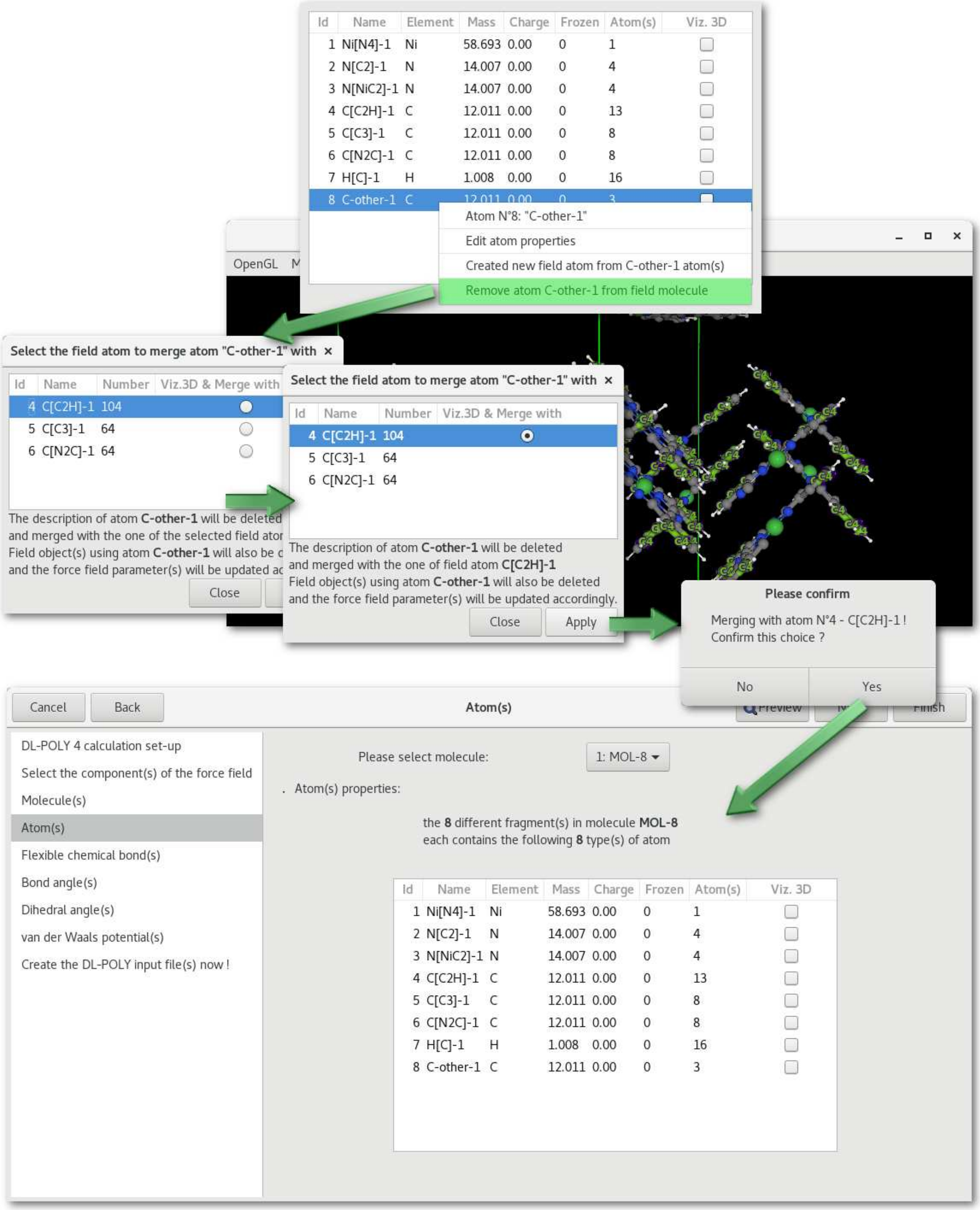
Please select molecule: 1: MOL-8

Atom(s) properties:

the **8** different fragment(s) in molecule **MOL-8**
each contains the following **8** type(s) of atom

Id	Name	Element	Mass	Charge	Frozen	Atom(s)	Viz. 3D
1	Ni[N4]-1	Ni	58.693	0.00	0	1	☐
2	N[C2]-1	N	14.007	0.00	0	4	☐
3	N[NiC2]-1	N	14.007	0.00	0	4	☐
4	C[C2H]-1	C	12.011	0.00	0	13	☐
5	C[C3]-1	C	12.011	0.00	0	8	☐
6	C[N2C]-1	C	12.011	0.00	0	8	☐
7	H[C]-1	H	1.008	0.00	0	16	☐
8	C-other-1	C	12.011	0.00	0	3	☐

Figure 7.11 *Inserting a new atom description in the "`Atom(s)`" tab.*



Id	Name	Element	Mass	Charge	Frozen	Atom(s)	Viz. 3D
1	Ni[N4]-1	Ni	58.693	0.00	0	1	☐
2	N[C2]-1	N	14.007	0.00	0	4	☐
3	N[NiC2]-1	N	14.007	0.00	0	4	☐
4	C[C2H]-1	C	12.011	0.00	0	13	☐
5	C[C3]-1	C	12.011	0.00	0	8	☐
6	C[N2C]-1	C	12.011	0.00	0	8	☐
7	H[C]-1	H	1.008	0.00	0	16	☐
8	C-other-1	C	12.011	0.00	0	3	☐

Select the field atom to merge atom "C-other-1" with

Id	Name	Number	Viz.3D & Merge with
4	C[C2H]-1	104	○
5	C[C3]-1	64	○
6	C[N2C]-1	64	○

The description of atom **C-other-1** will be deleted
and merged with the one of the selected field ator
Field object(s) using atom **C-other-1** will also be c
and the force field parameter(s) will be updated ac

Select the field atom to merge atom "C-other-1" with

Id	Name	Number	Viz.3D & Merge with
4	C[C2H]-1	104	●
5	C[C3]-1	64	
6	C[N2C]-1	64	

The description of atom **C-other-1** will be deleted
and merged with the one of field atom **C[C2H]-1**
Field object(s) using atom **C-other-1** will also be deleted
and the force field parameter(s) will be updated accordingly.

Please confirm

Merging with atom N°4 - C[C2H]-1 !
Confirm this choice ?

Please select molecule: 1: MOL-8

Atom(s) properties:

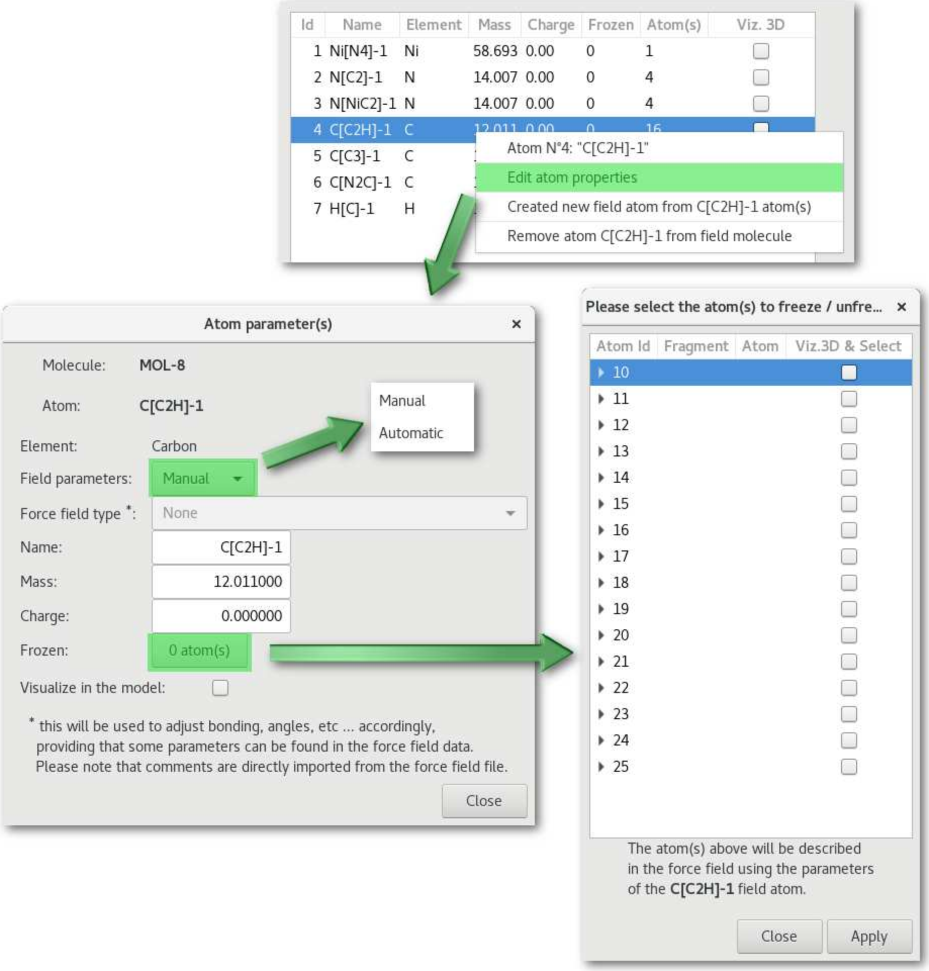
the **8** different fragment(s) in molecule **MOL-8**
each contains the following **8** type(s) of atom

Id	Name	Element	Mass	Charge	Frozen	Atom(s)	Viz. 3D
1	Ni[N4]-1	Ni	58.693	0.00	0	1	☐
2	N[C2]-1	N	14.007	0.00	0	4	☐
3	N[NiC2]-1	N	14.007	0.00	0	4	☐
4	C[C2H]-1	C	12.011	0.00	0	13	☐
5	C[C3]-1	C	12.011	0.00	0	8	☐
6	C[N2C]-1	C	12.011	0.00	0	8	☐
7	H[C]-1	H	1.008	0.00	0	16	☐
8	C-other-1	C	12.011	0.00	0	3	☐

Figure 7.12 *Merging two existing atom descriptions in the "`Atom(s)`" tab.*

Before editing an atom property it might be necessary to add or remove some atom types from the existing description, these actions are available using the mouse right button contextual menu. As illustrated in figure 7.11 it is possible to create a new type of atom from an existing atom type that contains more that 1 atom. And as illustrated in figure 7.12 it is possible to merge an existing atom description with any other atom type of the same chemical species. Whether it is for inserting or merging an atom it is important to specify that all existing atomic descriptions, a part for the new one or the one to be removed, will be preserved and thus that no information will be lost in this process.

Editing an atom properties, by double clicking on the atom line or using the contextual menu, will open the "`Atom parameter(s)`" dialog:



Id	Name	Element	Mass	Charge	Frozen	Atom(s)	Viz. 3D
1	Ni[N4]-1	Ni	58.693	0.00	0	1	☐
2	N[C2]-1	N	14.007	0.00	0	4	☐
3	N[NiC2]-1	N	14.007	0.00	0	4	☐
4	C[C2H]-1	C	12.011	0.00	0	16	☐
5	C[C3]-1	C					
6	C[N2C]-1	C					
7	H[C]-1	H					

Atom parameter(s)

Molecule: MOL-8

Atom: C[C2H]-1

Element: Carbon

Field parameters: Manual

Force field type *: None

Name: C[C2H]-1

Mass: 12.011000

Charge: 0.000000

Frozen: 0 atom(s)

Visualize in the model: ☐

* this will be used to adjust bonding, angles, etc ... accordingly, providing that some parameters can be found in the force field data. Please note that comments are directly imported from the force field file.

Please select the atom(s) to freeze / unfre...

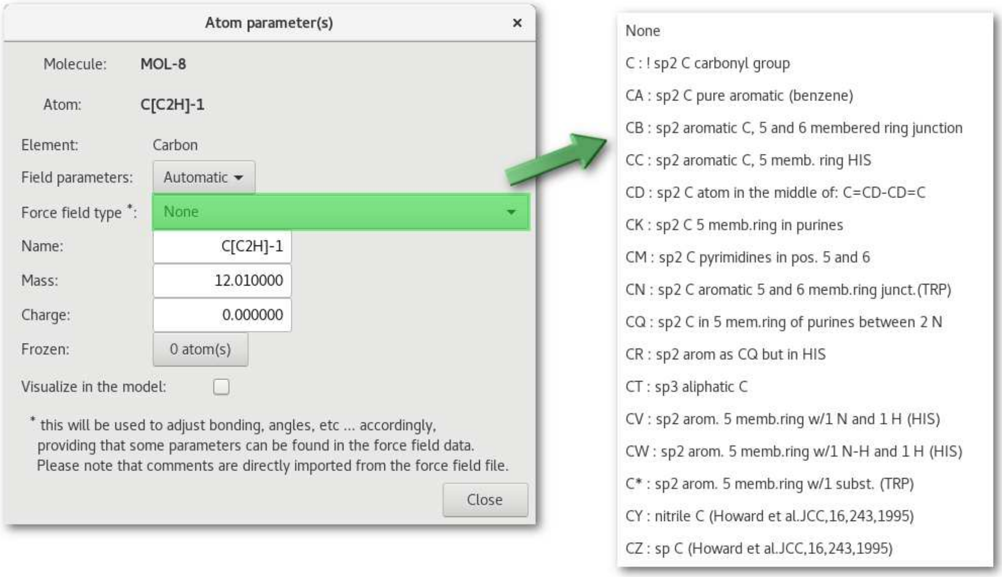
Atom Id	Fragment	Atom	Viz.3D & Select
10			☐
11			☐
12			☐
13			☐
14			☐
15			☐
16			☐
17			☐
18			☐
19			☐
20			☐
21			☐
22			☐
23			☐
24			☐
25			☐

The atom(s) above will be described in the force field using the parameters of the **C[C2H]-1** field atom.

Figure 7.13 *Editing an atom description in the "`Atom(s)`" tab.*

The "`Field parameters`" combo allows to switch between "`Manual`" (user defined only) and "`Automatic`" force field parameters (if any available). By default the choice is set on "`Manual`" and the "`Force field type`" combo is inactive. The "`Frozen`" button allows to pick atom(s) to be frozen among the edited atom type (see figure 7.13).

When selecting "`Automatic`" for the "`Field parameters`" combo, providing that some force field parameters are found "`Force field type`" combo becomes active and offers to choose between available description(s):



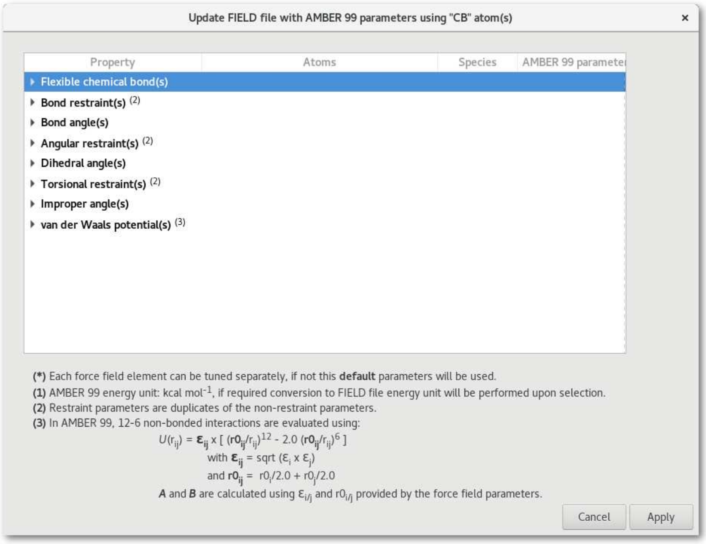
Molecule: MOL-8
Atom: C[C2H]-1
Element: Carbon
Field parameters: Automatic
Force field type *: None
Name: C[C2H]-1
Mass: 12.010000
Charge: 0.000000
Frozen: 0 atom(s)
Visualize in the model: ☐

* this will be used to adjust bonding, angles, etc ... accordingly, providing that some parameters can be found in the force field data. Please note that comments are directly imported from the force field file.

None
C : ! sp2 C carbonyl group
CA : sp2 C pure aromatic (benzene)
CB : sp2 aromatic C, 5 and 6 membered ring junction
CC : sp2 aromatic C, 5 memb. ring HIS
CD : sp2 C atom in the middle of: C=CD-CD=C
CK : sp2 C 5 memb.ring in purines
CM : sp2 C pyrimidines in pos. 5 and 6
CN : sp2 C aromatic 5 and 6 memb.ring junct.(TRP)
CQ : sp2 C in 5 mem.ring of purines between 2 N
CR : sp2 arom as CQ but in HIS
CT : sp3 aliphatic C
CV : sp2 arom. 5 memb.ring w/1 N and 1 H (HIS)
CW : sp2 arom. 5 memb.ring w/1 N-H and 1 H (HIS)
C* : sp2 arom. 5 memb.ring w/1 subst. (TRP)
CY : nitrile C (Howard et al.JCC,16,243,1995)
CZ : sp C (Howard et al.JCC,16,243,1995)

Figure 7.14 *Choosing a force field description for the atom type in the "`Atom(s)`" tab. In this example available parameters are from the Amber 99 force field.*

As soon as a selection has been made a dialog (see fig. 7.15) pops up to update the "`FIELD`" file with the available parameters in the force field selected at the initializing stage of the assistant (Amber 99 in this example).



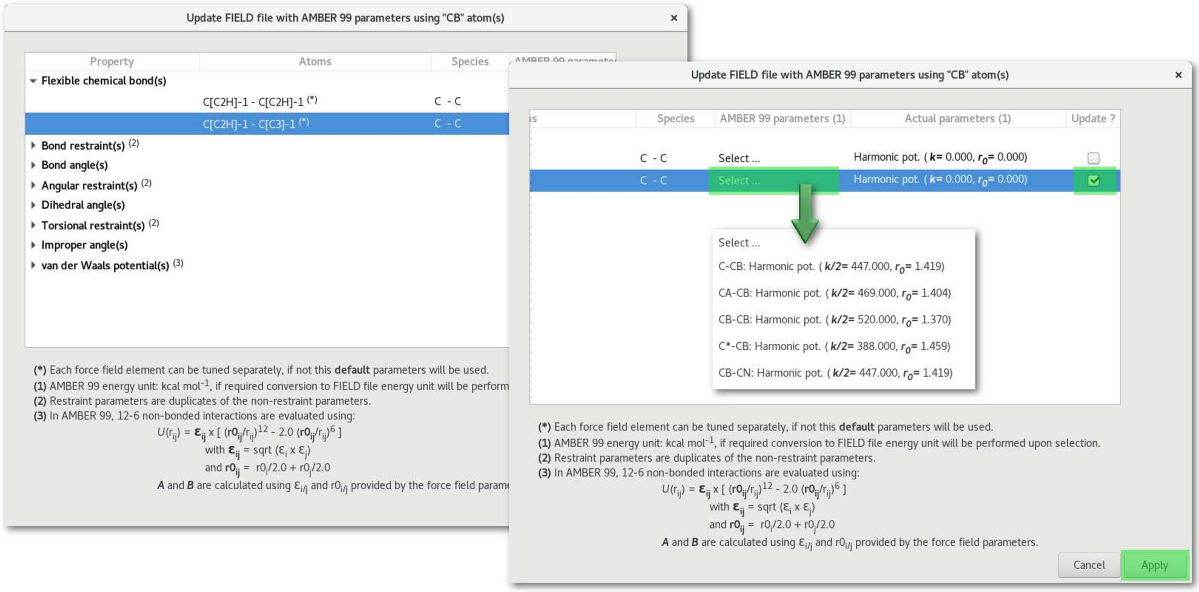
(*) Each force field element can be tuned separately, if not this **default** parameters will be used.
(1) AMBER 99 energy unit: kcal mol^{-1}, if required conversion to FIELD file energy unit will be performed upon selection.
(2) Restraint parameters are duplicates of the non-restraint parameters.
(3) In AMBER 99, 12-6 non-bonded interactions are evaluated using:

$$U(r_{ij}) = \boldsymbol{\varepsilon}_{ij} \times [(\mathbf{r0}_{ij}/r_{ij})^{12} - 2.0\ (\mathbf{r0}_{ij}/r_{ij})^{6}]$$
$$\text{with } \boldsymbol{\varepsilon}_{ij} = \text{sqrt}\ (\varepsilon_i \times \varepsilon_j)$$
$$\text{and } \mathbf{r0}_{ij} = r0_i/2.0 + r0_j/2.0$$

A and **B** are calculated using $\varepsilon_{i/j}$ and $r0_{i/j}$ provided by the force field parameters.

Figure 7.15 *The "`Update FIELD file with the force field parameters`" dialog.*

The number of lines in the table in figure 7.15 depends on both the option(s) ("`Flexible chemical bond(s), Bond angle(s) ...`") selected to create the "`FIELD`" file, the line will appears only if the option was selected, and the availability of the data for that particular type of atom in the selected force field. In this example all the properties presented were selected to create the "`FIELD`" file and some data exist in the force field for the "`CB`" atom type with each particular property. This dialog helps to update quickly any parameters to be used to create the "`FIELD`" file:



Update FIELD file with AMBER 99 parameters using "CB" atom(s)

Property	Atoms	Species
Flexible chemical bond(s)		
	C[C2H]-1 - C[C2H]-1 (*)	C - C
	C[C2H]-1 - C[C3]-1 (*)	C - C
Bond restraint(s) (2)		
Bond angle(s)		
Angular restraint(s) (2)		
Dihedral angle(s)		
Torsional restraint(s) (2)		
Improper angle(s)		
van der Waals potential(s) (3)		

Update FIELD file with AMBER 99 parameters using "CB" atom(s)

Species	AMBER 99 parameters (1)	Actual parameters (1)	Update ?
C - C	Select ...	Harmonic pot. (**k**= 0.000, r_0= 0.000)	☐
C - C	Select ...	Harmonic pot. (**k**= 0.000, r_0= 0.000)	☑

Select ...
C-CB: Harmonic pot. (**k/2**= 447.000, r_0= 1.419)
CA-CB: Harmonic pot. (**k/2**= 469.000, r_0= 1.404)
CB-CB: Harmonic pot. (**k/2**= 520.000, r_0= 1.370)
C*-CB: Harmonic pot. (**k/2**= 388.000, r_0= 1.459)
CB-CN: Harmonic pot. (**k/2**= 447.000, r_0= 1.419)

(*) Each force field element can be tuned separately, if not this **default** parameters will be used.
(1) AMBER 99 energy unit: kcal mol^{-1}, if required conversion to FIELD file energy unit will be performed upon selection.
(2) Restraint parameters are duplicates of the non-restraint parameters.
(3) In AMBER 99, 12-6 non-bonded interactions are evaluated using:

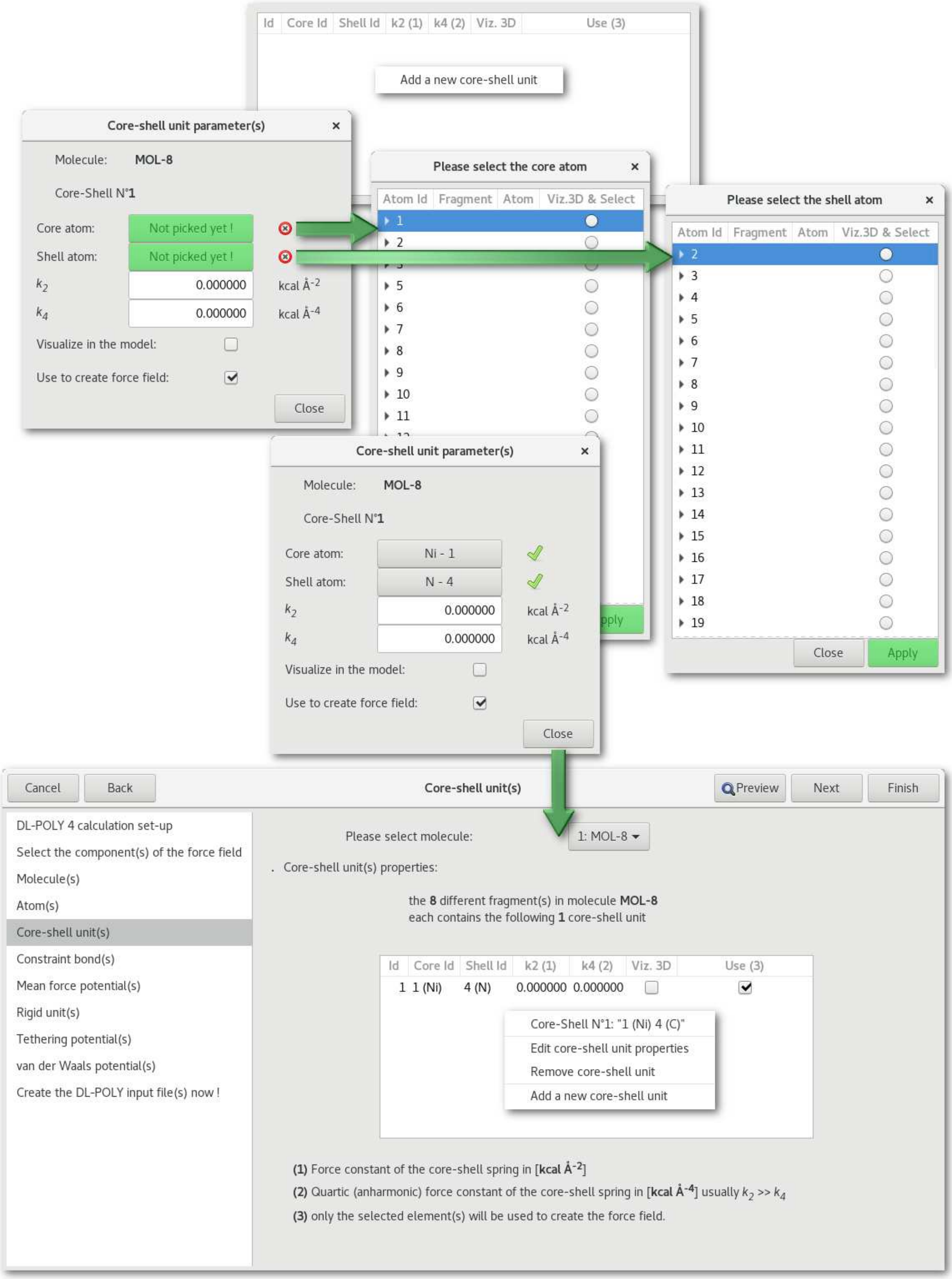
$$U(r_{ij}) = \boldsymbol{\varepsilon}_{ij} \times [\ (\mathbf{r0}_{ij}/r_{ij})^{12} - 2.0\ (\mathbf{r0}_{ij}/r_{ij})^{6}\ ]$$
$$\text{with } \boldsymbol{\varepsilon}_{ij} = \text{sqrt}\ (\varepsilon_i \times \varepsilon_j)$$
$$\text{and } \mathbf{r0}_{ij} = r0_i/2.0 + r0_j/2.0$$

A and ***B*** are calculated using $\varepsilon_{i/j}$ and $r0_{i/j}$ provided by the force field parameters.

Figure 7.16 *Updating parameters for the "`FIELD`" file, using field parameters for the "`CB`" atom(s) in the "`Amber 99`" force field.*

As illustrated in figure 7.16 to update any "`FIELD`" file value simply browse the property tree, select the desired force field parameters among available data, remember to check the "`update`" button at the end of the line, and finally pressed the "`Apply`" button.

"Core-shell unit(s)"



Core-shell unit parameter(s)

Molecule: **MOL-8**

Core-Shell N°**1**

Core atom: Not picked yet !

Shell atom: Not picked yet !

k_2 0.000000 kcal Å^{-2}

k_4 0.000000 kcal Å^{-4}

Visualize in the model: ☐

Use to create force field: ☑

Atom Id	Fragment	Atom	Viz.3D & Select
1			●
2			○
3			○
5			○
6			○
7			○
8			○
9			○
10			○
11			○

Atom Id	Fragment	Atom	Viz.3D & Select
2			●
3			○
4			○
5			○
6			○
7			○
8			○
9			○
10			○
11			○
12			○
13			○
14			○
15			○
16			○
17			○
18			○
19			○

Core-shell unit parameter(s)

Molecule: **MOL-8**

Core-Shell N°**1**

Core atom: Ni - 1 ✓

Shell atom: N - 4 ✓

k_2 0.000000 kcal Å^{-2}

k_4 0.000000 kcal Å^{-4}

Visualize in the model: ☐

Use to create force field: ☑

Please select molecule: 1: MOL-8

. Core-shell unit(s) properties:

the **8** different fragment(s) in molecule **MOL-8**
each contains the following **1** core-shell unit

Id	Core Id	Shell Id	k2 (1)	k4 (2)	Viz. 3D	Use (3)
1	1 (Ni)	4 (N)	0.000000	0.000000	☐	☑

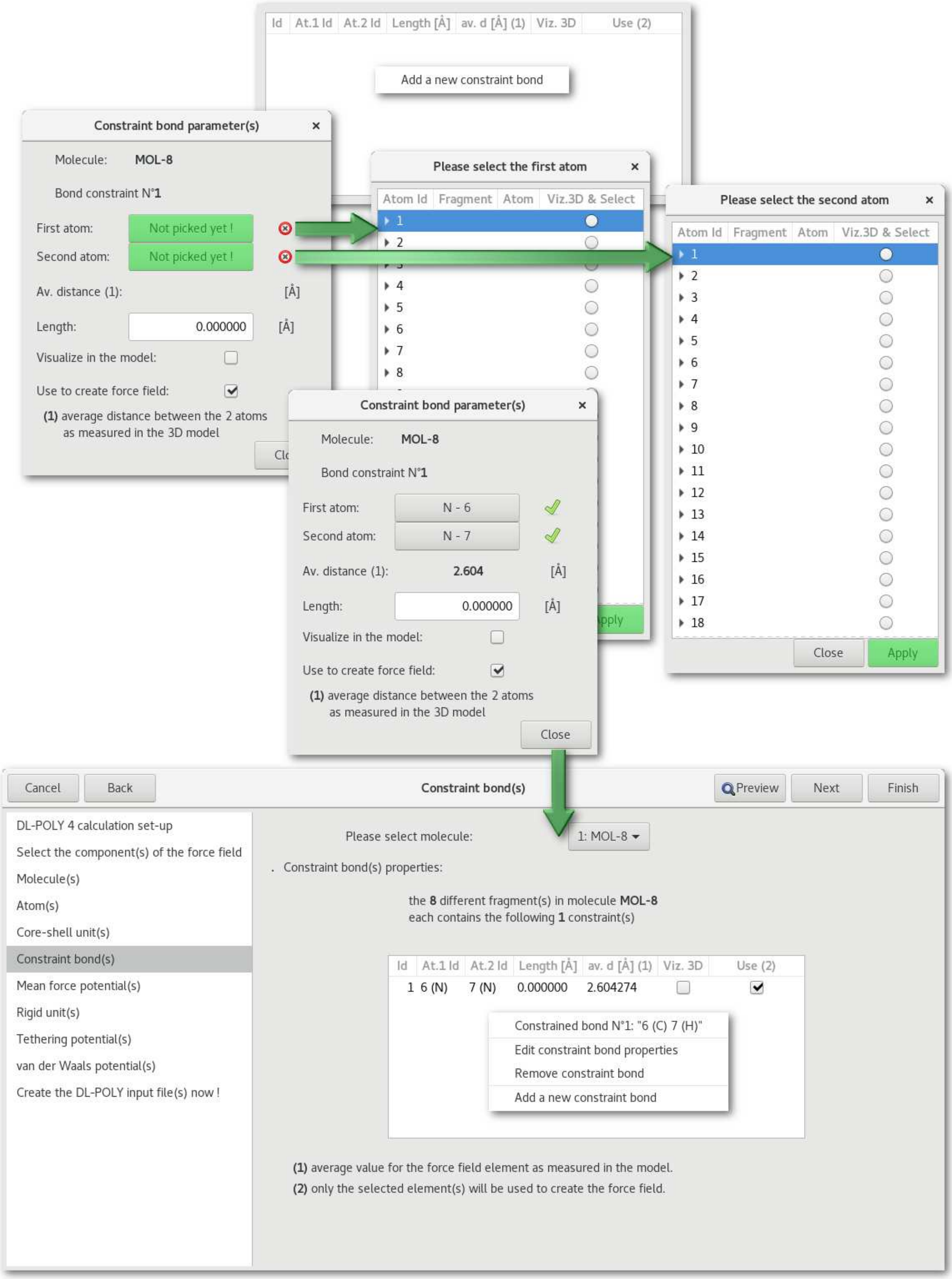
(1) Force constant of the core-shell spring in [**kcal Å^{-2}**]

(2) Quartic (anharmonic) force constant of the core-shell spring in [**kcal Å^{-4}**] usually $k_2 >> k_4$

(3) only the selected element(s) will be used to create the force field.

Figure 7.17 *"`Core-shell unit(s)`" tab in the "`DL-POLY`" assistant.*

`"Constraint bond(s)"`



Constraint bond parameter(s)

Molecule: **MOL-8**

Bond constraint N°**1**

First atom: Not picked yet !

Second atom: Not picked yet !

Av. distance (1): [Å]

Length: 0.000000 [Å]

Visualize in the model: ☐

Use to create force field: ☑

(1) average distance between the 2 atoms as measured in the 3D model

Constraint bond parameter(s)

Molecule: **MOL-8**

Bond constraint N°**1**

First atom: N - 6 ✓

Second atom: N - 7 ✓

Av. distance (1): **2.604** [Å]

Length: 0.000000 [Å]

Visualize in the model: ☐

Use to create force field: ☑

(1) average distance between the 2 atoms as measured in the 3D model

Please select molecule: 1: MOL-8

. Constraint bond(s) properties:

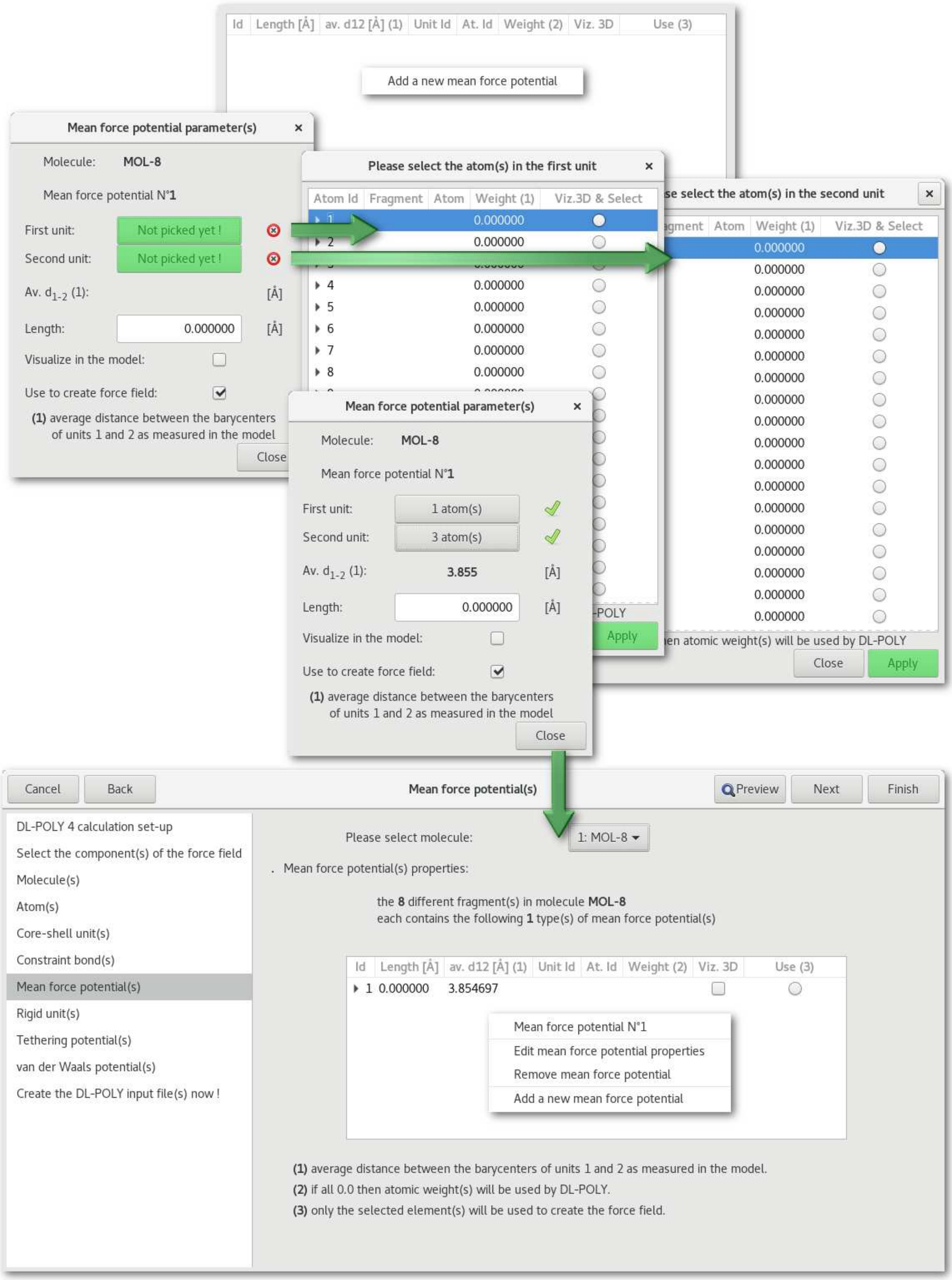
the **8** different fragment(s) in molecule **MOL-8**
each contains the following **1** constraint(s)

Id	At.1 Id	At.2 Id	Length [Å]	av. d [Å] (1)	Viz. 3D	Use (2)
1	6 (N)	7 (N)	0.000000	2.604274	☐	☑

(1) average value for the force field element as measured in the model.
(2) only the selected element(s) will be used to create the force field.

Figure 7.18 *"`Constrains bond(s)`" tab in the "`DL-POLY`" assistant.*

"`Mean force potential(s)`"



Id	Length [Å]	av. d12 [Å] (1)	Unit Id	At. Id	Weight (2)	Viz. 3D	Use (3)

Molecule: **MOL-8**

Mean force potential N°**1**

First unit: Not picked yet !

Second unit: Not picked yet !

Av. d_{1-2} (1): [Å]

Length: 0.000000 [Å]

Visualize in the model: ☐

Use to create force field: ☑

(1) average distance between the barycenters of units 1 and 2 as measured in the model

Atom Id	Fragment	Atom	Weight (1)	Viz.3D & Select
1			0.000000	○
2			0.000000	○
4			0.000000	○
5			0.000000	○
6			0.000000	○
7			0.000000	○
8			0.000000	○

gment	Atom	Weight (1)	Viz.3D & Select
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○
		0.000000	○

en atomic weight(s) will be used by DL-POLY

Molecule: **MOL-8**

Mean force potential N°**1**

First unit: 1 atom(s) ✓

Second unit: 3 atom(s) ✓

Av. d_{1-2} (1): **3.855** [Å]

Length: 0.000000 [Å]

Visualize in the model: ☐

Use to create force field: ☑

(1) average distance between the barycenters of units 1 and 2 as measured in the model

Please select molecule: 1: MOL-8

. Mean force potential(s) properties:

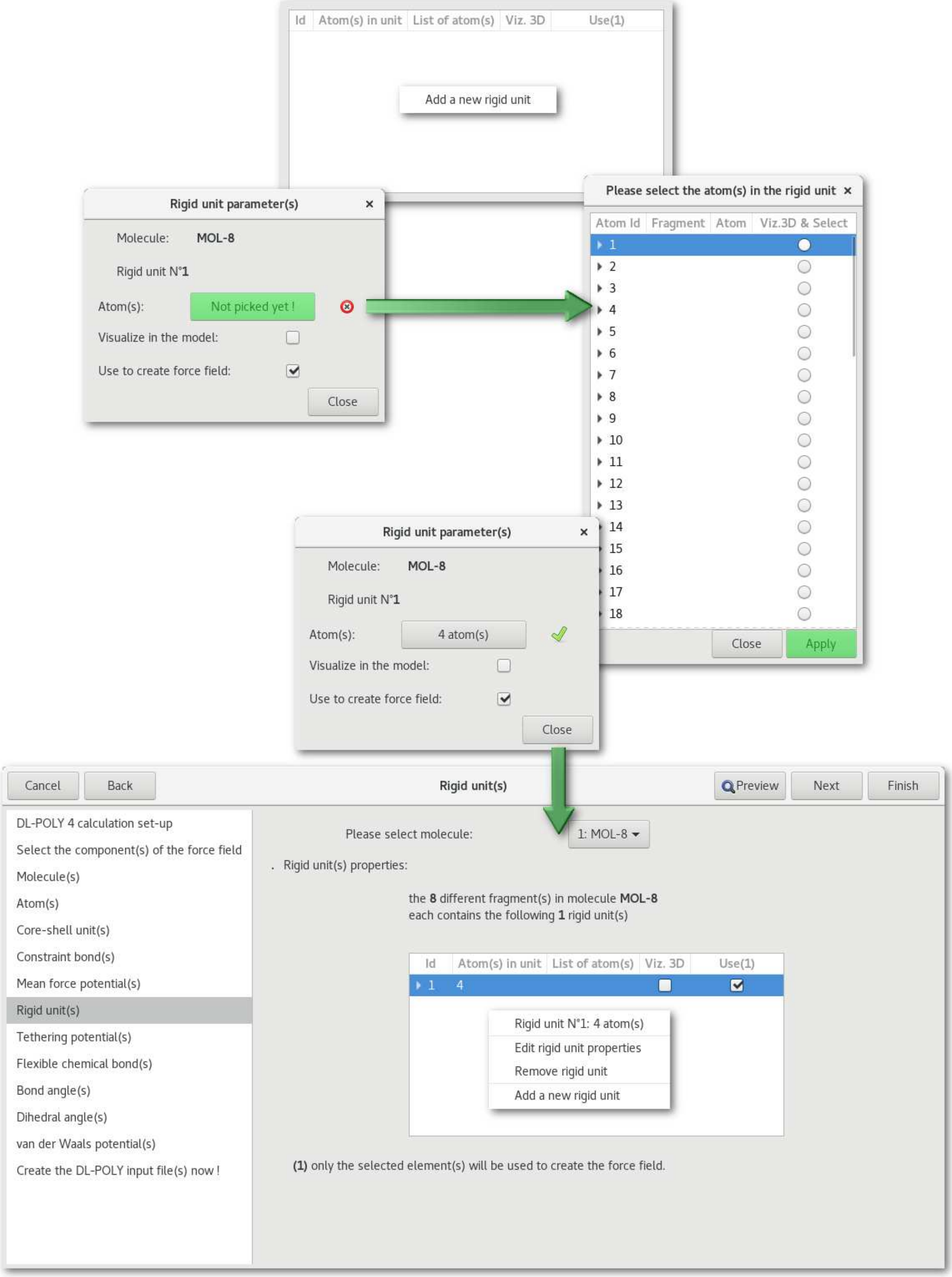
the **8** different fragment(s) in molecule **MOL-8**
each contains the following **1** type(s) of mean force potential(s)

Id	Length [Å]	av. d12 [Å] (1)	Unit Id	At. Id	Weight (2)	Viz. 3D	Use (3)
1	0.000000	3.854697				☐	○

(1) average distance between the barycenters of units 1 and 2 as measured in the model.
(2) if all 0.0 then atomic weight(s) will be used by DL-POLY.
(3) only the selected element(s) will be used to create the force field.

Figure 7.19 *"`Mean force potential(s)`" tab in the "`DL-POLY`" assistant.*

"Rigid unit(s)"



Molecule: **MOL-8**

Rigid unit N°**1**

Atom(s): Not picked yet !

Visualize in the model: ☐

Use to create force field: ☑

Molecule: **MOL-8**

Rigid unit N°**1**

Atom(s): 4 atom(s) ✓

Visualize in the model: ☐

Use to create force field: ☑

Please select molecule: 1: MOL-8

. Rigid unit(s) properties:

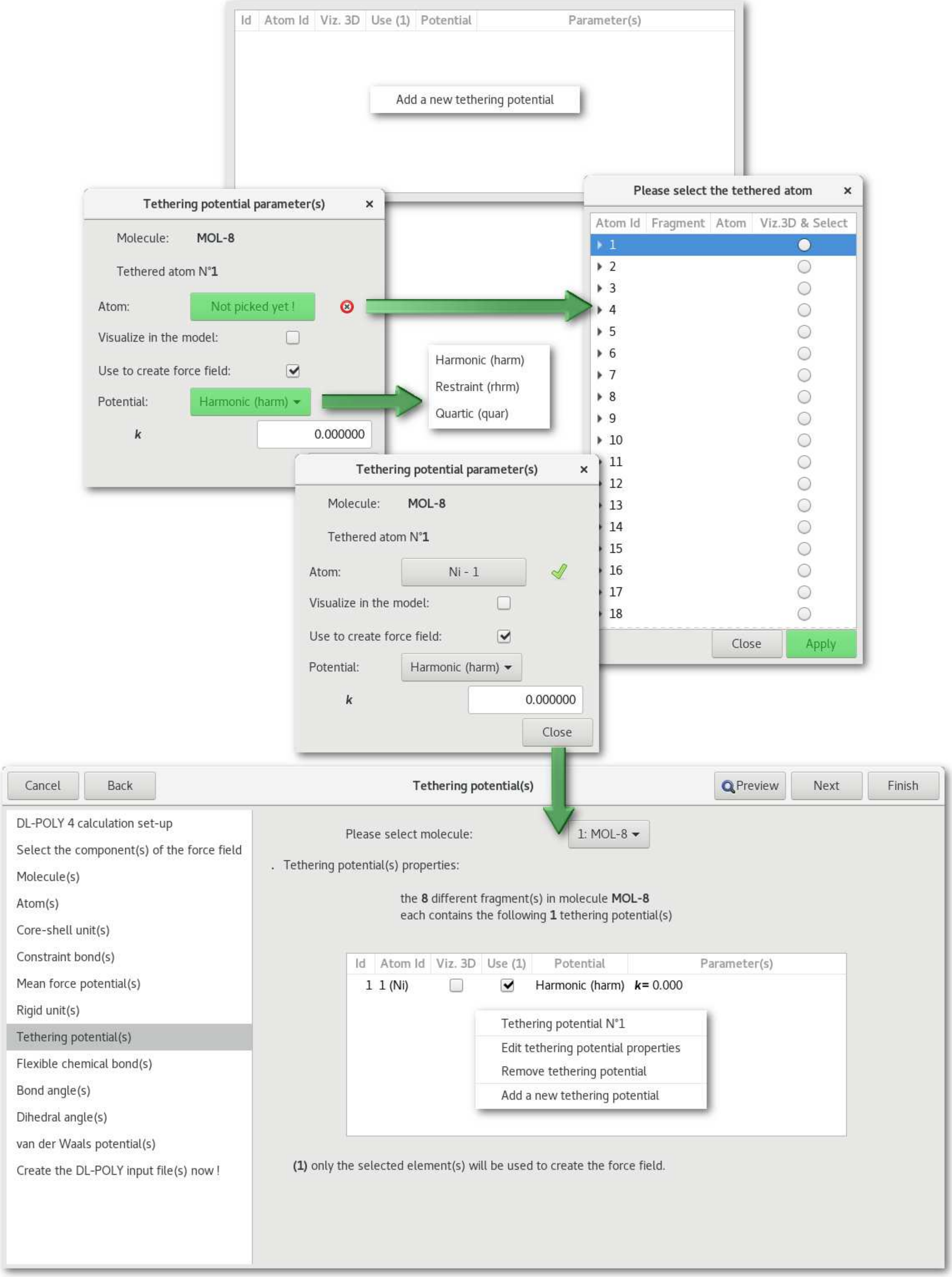
the **8** different fragment(s) in molecule **MOL-8**
each contains the following **1** rigid unit(s)

Id	Atom(s) in unit	List of atom(s)	Viz. 3D	Use(1)
1	4		☐	☑

(1) only the selected element(s) will be used to create the force field.

Figure 7.20 *"`Rigid unit(s)`" tab in the "`DL-POLY`" assistant.*

"`Tethering potential(s)`"



Molecule: **MOL-8**

Tethered atom N°**1**

Atom: Not picked yet !

Visualize in the model: ☐

Use to create force field: ☑

Potential: Harmonic (harm)

k 0.000000

Molecule: **MOL-8**

Tethered atom N°**1**

Atom: Ni - 1 ✓

Visualize in the model: ☐

Use to create force field: ☑

Potential: Harmonic (harm)

k 0.000000

Please select molecule: 1: MOL-8

. Tethering potential(s) properties:

the **8** different fragment(s) in molecule **MOL-8**
each contains the following **1** tethering potential(s)

Id	Atom Id	Viz. 3D	Use (1)	Potential	Parameter(s)
1	1 (Ni)	☐	☑	Harmonic (harm)	***k***= 0.000

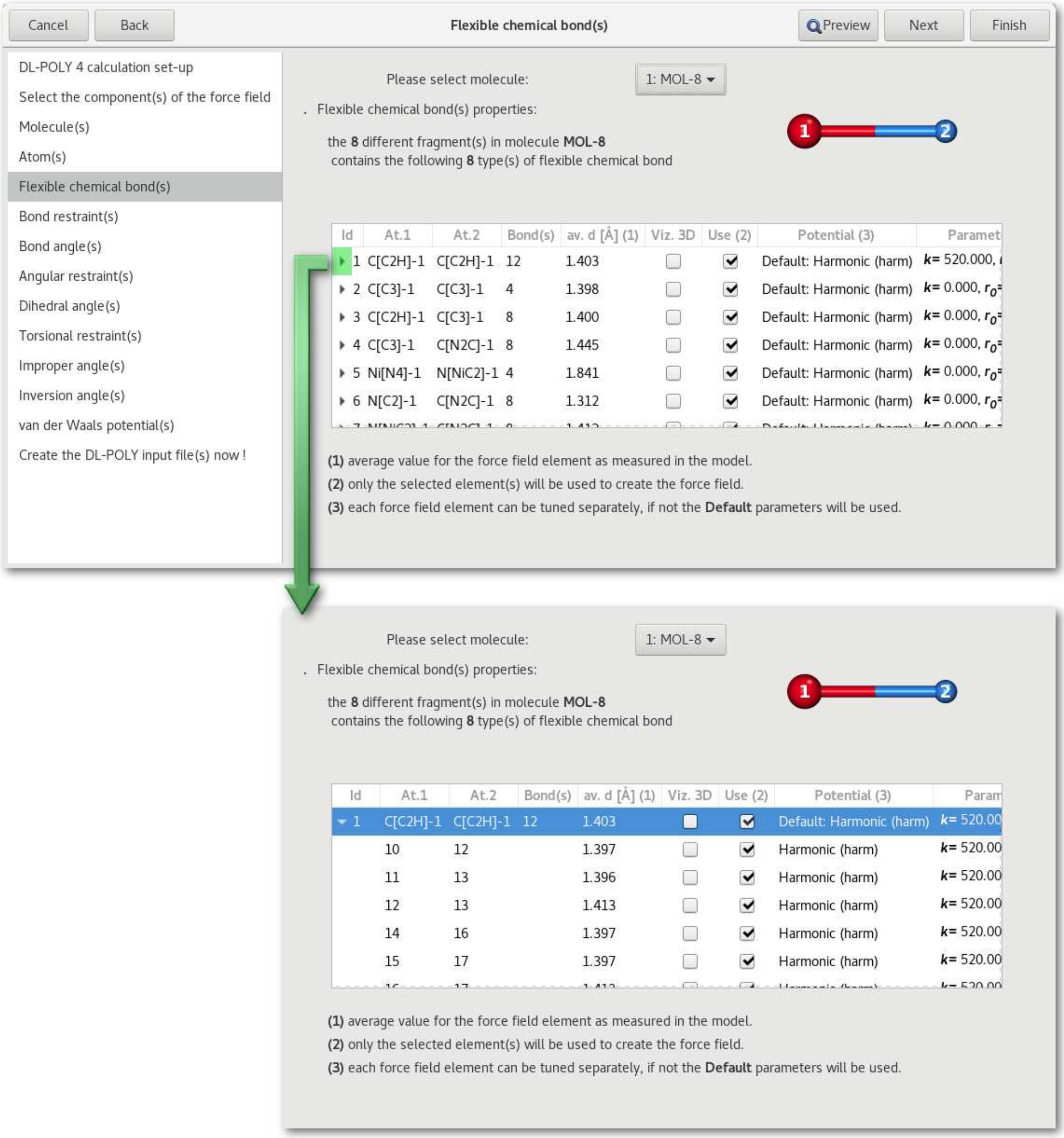
(1) only the selected element(s) will be used to create the force field.

Figure 7.21 *"`Tethering potential(s)`" tab in the "`DL-POLY`" assistant.*

"`Flexible chemical bond(s)`" and "`Bond restraint(s)`"

The tabs for the "`Flexible chemical bond(s)`" and the "`Bond restraint(s)`" being extremely similar, this manual presents only the part related to "`Flexible chemical bond(s)`".

As illustrated in figure 7.22 the bonds, for the selected molecule, are listed by type depending on the nature of the field atoms involved, also for each type of bond it is possible to display every single bond in the molecule.



Please select molecule: 1: MOL-8

. Flexible chemical bond(s) properties:

the **8** different fragment(s) in molecule **MOL-8**
contains the following **8** type(s) of flexible chemical bond

Id	At.1	At.2	Bond(s)	av. d [Å] (1)	Viz. 3D	Use (2)	Potential (3)	Paramet
▸ 1	C[C2H]-1	C[C2H]-1	12	1.403	☐	☑	Default: Harmonic (harm)	**k**= 520.000,
▸ 2	C[C3]-1	C[C3]-1	4	1.398	☐	☑	Default: Harmonic (harm)	**k**= 0.000, r_0=
▸ 3	C[C2H]-1	C[C3]-1	8	1.400	☐	☑	Default: Harmonic (harm)	**k**= 0.000, r_0=
▸ 4	C[C3]-1	C[N2C]-1	8	1.445	☐	☑	Default: Harmonic (harm)	**k**= 0.000, r_0=
▸ 5	Ni[N4]-1	N[NiC2]-1	4	1.841	☐	☑	Default: Harmonic (harm)	**k**= 0.000, r_0=
▸ 6	N[C2]-1	C[N2C]-1	8	1.312	☐	☑	Default: Harmonic (harm)	**k**= 0.000, r_0=

(1) average value for the force field element as measured in the model.
(2) only the selected element(s) will be used to create the force field.
(3) each force field element can be tuned separately, if not the **Default** parameters will be used.

Please select molecule: 1: MOL-8

. Flexible chemical bond(s) properties:

the **8** different fragment(s) in molecule **MOL-8**
contains the following **8** type(s) of flexible chemical bond

Id	At.1	At.2	Bond(s)	av. d [Å] (1)	Viz. 3D	Use (2)	Potential (3)	Param
▾ 1	C[C2H]-1	C[C2H]-1	12	1.403	☐	☑	Default: Harmonic (harm)	**k**= 520.00
	10	12		1.397	☐	☑	Harmonic (harm)	**k**= 520.00
	11	13		1.396	☐	☑	Harmonic (harm)	**k**= 520.00
	12	13		1.413	☐	☑	Harmonic (harm)	**k**= 520.00
	14	16		1.397	☐	☑	Harmonic (harm)	**k**= 520.00
	15	17		1.397	☐	☑	Harmonic (harm)	**k**= 520.00

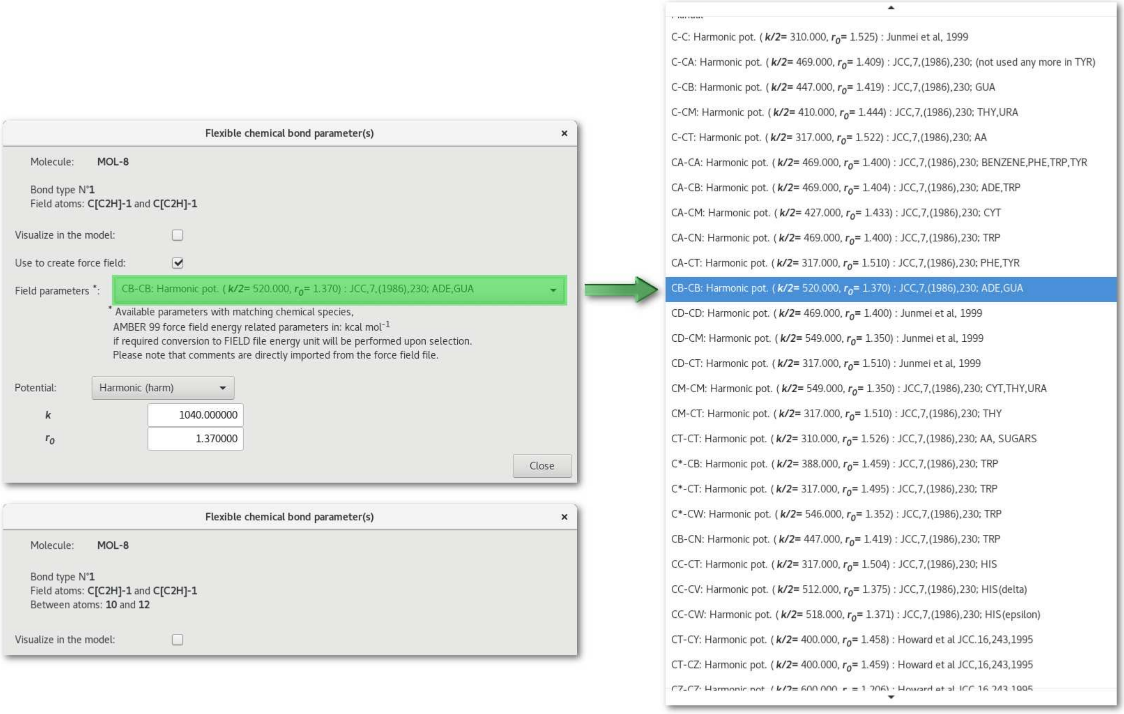
(1) average value for the force field element as measured in the model.
(2) only the selected element(s) will be used to create the force field.
(3) each force field element can be tuned separately, if not the **Default** parameters will be used.

Figure 7.22 *"`Flexible chemical bond(s)`" tab in the "`DL-POLY`" assistant.*

Each line corresponds to a either to a bond type, or a particular bond, for the molecule specified above, and for each bond the information is as follow:

1. ID in the molecule (if the line refers to a bond type).
2. Name for atom type 1 (bond type), or field number for atom 1 (bond).
3. Name for atom type 2 (bond type), or field number for atom 2 (bond).
4. Value measured in the model: average for all bonds for that type, or, value (or average if the multiplicity for the molecule is > 1) for that particular bond.
5. Visualize all bonds of that type or that particular bond in the model.
6. Use to create the "`FIELD`" file, if not checked the bond / type will not be used.
7. Potential to use to describe all bonds of that type ("`Default:`" value) or that particular bond in the model.
8. Numerical value(s) for the parameters of the selected potential.

The description of the bond(s) can be modified simultaneously for all bond(s) of the same type using the root line that type, or one by one by browsing the list and picking any line. It is therefore possible to choose a different parametrization for every single bond in the molecule. Some parameters can be modified directly in the table, otherwise a simple double click using the mouse left button will open the bond edition dialog illustrated in figure 7.23.



Molecule: **MOL-8**

Bond type N°**1**
Field atoms: **C[C2H]-1** and **C[C2H]-1**

Visualize in the model: ☐

Use to create force field: ☑

Field parameters *: CB-CB: Harmonic pot. (**k/2=** 520.000, r_0= 1.370) : JCC,7,(1986),230; ADE,GUA

* Available parameters with matching chemical species,
AMBER 99 force field energy related parameters in: kcal mol^{-1}
if required conversion to FIELD file energy unit will be performed upon selection.
Please note that comments are directly imported from the force field file.

Potential: Harmonic (harm)

k: 1040.000000

r_0: 1.370000

Molecule: **MOL-8**

Bond type N°**1**
Field atoms: **C[C2H]-1** and **C[C2H]-1**
Between atoms: **10** and **12**

Visualize in the model: ☐

C-C: Harmonic pot. (**k/2=** 310.000, r_0= 1.525) : Junmei et al, 1999
C-CA: Harmonic pot. (**k/2=** 469.000, r_0= 1.409) : JCC,7,(1986),230; (not used any more in TYR)
C-CB: Harmonic pot. (**k/2=** 447.000, r_0= 1.419) : JCC,7,(1986),230; GUA
C-CM: Harmonic pot. (**k/2=** 410.000, r_0= 1.444) : JCC,7,(1986),230; THY,URA
C-CT: Harmonic pot. (**k/2=** 317.000, r_0= 1.522) : JCC,7,(1986),230; AA
CA-CA: Harmonic pot. (**k/2=** 469.000, r_0= 1.400) : JCC,7,(1986),230; BENZENE,PHE,TRP,TYR
CA-CB: Harmonic pot. (**k/2=** 469.000, r_0= 1.404) : JCC,7,(1986),230; ADE,TRP
CA-CM: Harmonic pot. (**k/2=** 427.000, r_0= 1.433) : JCC,7,(1986),230; CYT
CA-CN: Harmonic pot. (**k/2=** 469.000, r_0= 1.400) : JCC,7,(1986),230; TRP
CA-CT: Harmonic pot. (**k/2=** 317.000, r_0= 1.510) : JCC,7,(1986),230; PHE,TYR
CB-CB: Harmonic pot. (**k/2=** 520.000, r_0= 1.370) : JCC,7,(1986),230; ADE,GUA
CD-CD: Harmonic pot. (**k/2=** 469.000, r_0= 1.400) : Junmei et al, 1999
CD-CM: Harmonic pot. (**k/2=** 549.000, r_0= 1.350) : Junmei et al, 1999
CD-CT: Harmonic pot. (**k/2=** 317.000, r_0= 1.510) : Junmei et al, 1999
CM-CM: Harmonic pot. (**k/2=** 549.000, r_0= 1.350) : JCC,7,(1986),230; CYT,THY,URA
CM-CT: Harmonic pot. (**k/2=** 317.000, r_0= 1.510) : JCC,7,(1986),230; THY
CT-CT: Harmonic pot. (**k/2=** 310.000, r_0= 1.526) : JCC,7,(1986),230; AA, SUGARS
C*-CB: Harmonic pot. (**k/2=** 388.000, r_0= 1.459) : JCC,7,(1986),230; TRP
C*-CT: Harmonic pot. (**k/2=** 317.000, r_0= 1.495) : JCC,7,(1986),230; TRP
C*-CW: Harmonic pot. (**k/2=** 546.000, r_0= 1.352) : JCC,7,(1986),230; TRP
CB-CN: Harmonic pot. (**k/2=** 447.000, r_0= 1.419) : JCC,7,(1986),230; TRP
CC-CT: Harmonic pot. (**k/2=** 317.000, r_0= 1.504) : JCC,7,(1986),230; HIS
CC-CV: Harmonic pot. (**k/2=** 512.000, r_0= 1.375) : JCC,7,(1986),230; HIS(delta)
CC-CW: Harmonic pot. (**k/2=** 518.000, r_0= 1.371) : JCC,7,(1986),230; HIS(epsilon)
CT-CY: Harmonic pot. (**k/2=** 400.000, r_0= 1.458) : Howard et al JCC.16,243,1995
CT-CZ: Harmonic pot. (**k/2=** 400.000, r_0= 1.459) : Howard et al JCC,16,243,1995
CZ-CZ: Harmonic pot. (**k/2=** 600.000, r_0= 1.206) : Howard et al JCC,16,243,1995

Figure 7.23 *"`Flexible chemical bond(s)`" edition dialog in the "`DL-POLY`" assistant.*

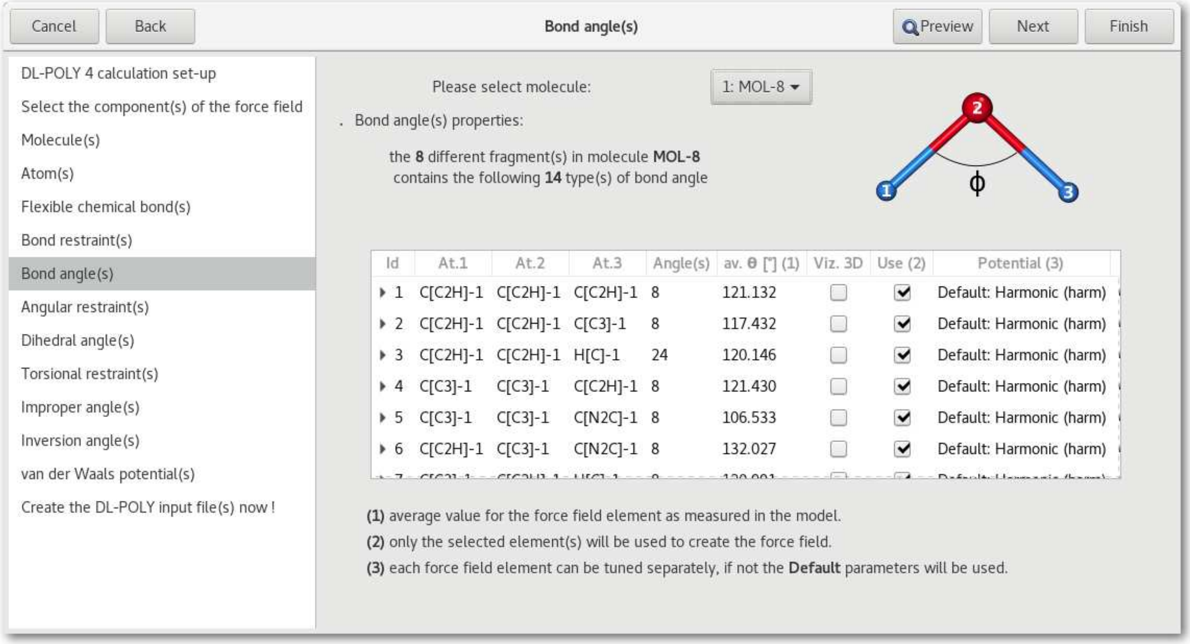
In figure 7.23 the "`Field parameters`" combo box presents the list of matching parameters, chemical species wise, found in the force field selected at the initialization stage.

The next tabs of the assistant dedicated to intra-molecular properties are as follow:

- "`Bond angle(s)`"
- "`Angular restraint(s)`"
- "`Dihedral angle(s)`"
- "`Torsional restraint(s)`"
- "`Improper angle(s)`"
- "`Inversion angle(s)`"

For all these properties the philosophy is similar to the one presented above for the "`Flexible chemical bond(s)`". Hence will only briefly illustrate the different tabs without more details.

"`Bond angle(s)`" and "`Angular restraint(s)`"



Please select molecule: 1: MOL-8

. Bond angle(s) properties:

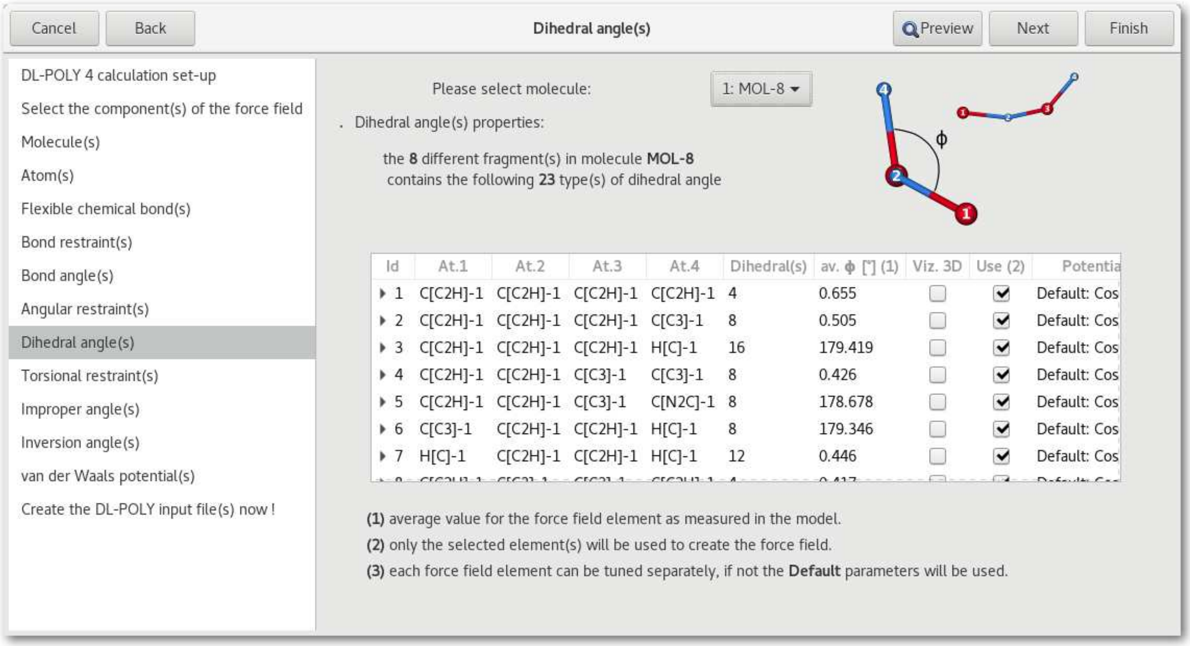
the **8** different fragment(s) in molecule **MOL-8**
contains the following **14** type(s) of bond angle

Id	At.1	At.2	At.3	Angle(s)	av. θ [°] (1)	Viz. 3D	Use (2)	Potential (3)
▸ 1	C[C2H]-1	C[C2H]-1	C[C2H]-1	8	121.132	☐	☑	Default: Harmonic (harm)
▸ 2	C[C2H]-1	C[C2H]-1	C[C3]-1	8	117.432	☐	☑	Default: Harmonic (harm)
▸ 3	C[C2H]-1	C[C2H]-1	H[C]-1	24	120.146	☐	☑	Default: Harmonic (harm)
▸ 4	C[C3]-1	C[C3]-1	C[C2H]-1	8	121.430	☐	☑	Default: Harmonic (harm)
▸ 5	C[C3]-1	C[C3]-1	C[N2C]-1	8	106.533	☐	☑	Default: Harmonic (harm)
▸ 6	C[C2H]-1	C[C3]-1	C[N2C]-1	8	132.027	☐	☑	Default: Harmonic (harm)

(1) average value for the force field element as measured in the model.
(2) only the selected element(s) will be used to create the force field.
(3) each force field element can be tuned separately, if not the **Default** parameters will be used.

Figure 7.24 *"`Bond angle(s)`" tab in the "`DL-POLY`" assistant.*

"`Dihedral angle(s)`" and "`Torsional restraint(s)`"



Please select molecule: 1: MOL-8

Dihedral angle(s) properties:

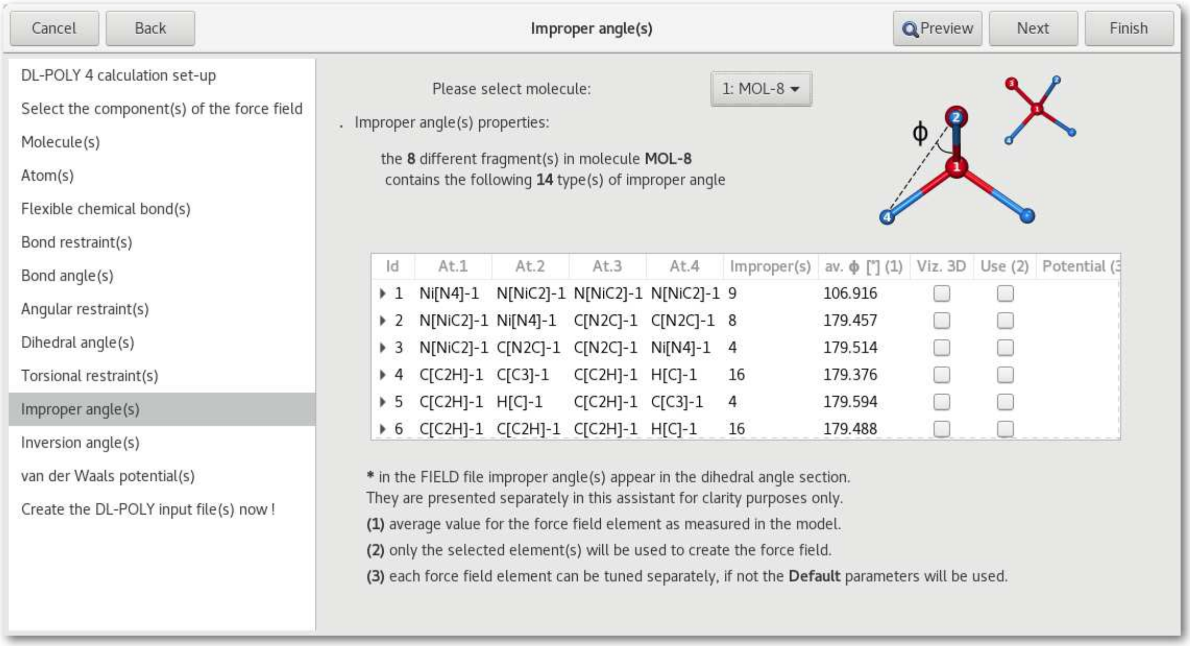
the **8** different fragment(s) in molecule **MOL-8**
contains the following **23** type(s) of dihedral angle

Id	At.1	At.2	At.3	At.4	Dihedral(s)	av. ϕ [°] (1)	Viz. 3D	Use (2)	Potentia
1	C[C2H]-1	C[C2H]-1	C[C2H]-1	C[C2H]-1	4	0.655	☐	☑	Default: Cos
2	C[C2H]-1	C[C2H]-1	C[C2H]-1	C[C3]-1	8	0.505	☐	☑	Default: Cos
3	C[C2H]-1	C[C2H]-1	C[C2H]-1	H[C]-1	16	179.419	☐	☑	Default: Cos
4	C[C2H]-1	C[C2H]-1	C[C3]-1	C[C3]-1	8	0.426	☐	☑	Default: Cos
5	C[C2H]-1	C[C2H]-1	C[C3]-1	C[N2C]-1	8	178.678	☐	☑	Default: Cos
6	C[C3]-1	C[C2H]-1	C[C2H]-1	H[C]-1	8	179.346	☐	☑	Default: Cos
7	H[C]-1	C[C2H]-1	C[C2H]-1	H[C]-1	12	0.446	☐	☑	Default: Cos

(1) average value for the force field element as measured in the model.
(2) only the selected element(s) will be used to create the force field.
(3) each force field element can be tuned separately, if not the **Default** parameters will be used.

Figure 7.25 *"`Dihedral angle(s)`" tab in the "`DL-POLY`" assistant.*

"`Improper angle(s)`"



Please select molecule: 1: MOL-8

Improper angle(s) properties:

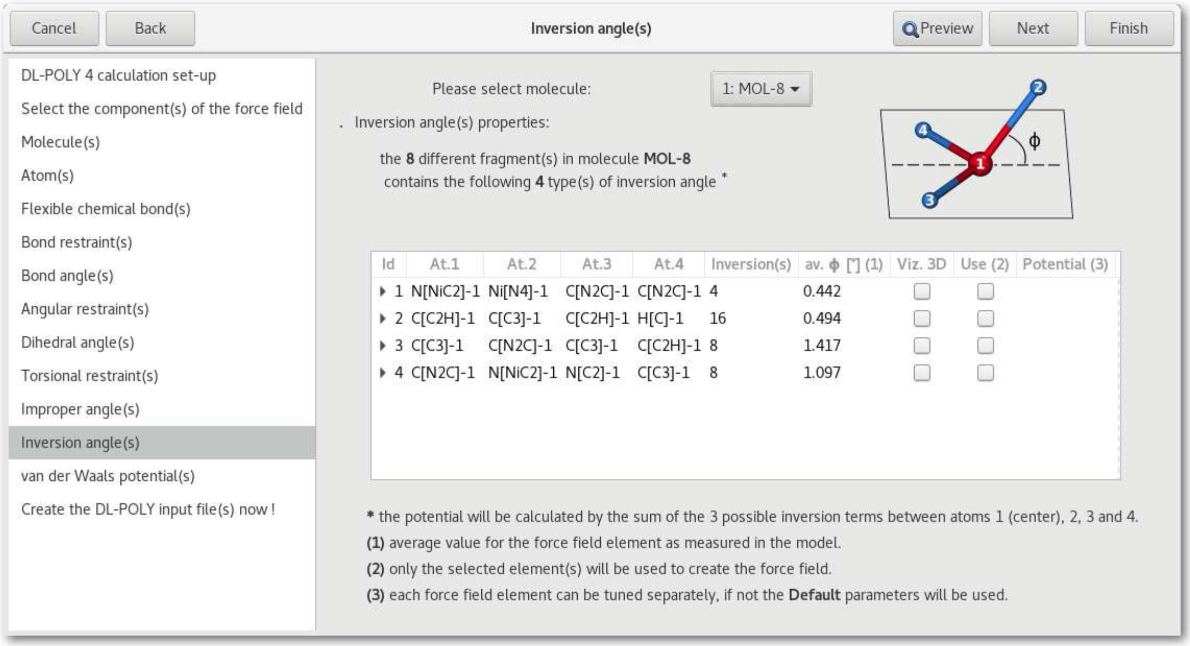
the **8** different fragment(s) in molecule **MOL-8**
contains the following **14** type(s) of improper angle

Id	At.1	At.2	At.3	At.4	Improper(s)	av. ϕ [°] (1)	Viz. 3D	Use (2)	Potential (3
1	Ni[N4]-1	N[NiC2]-1	N[NiC2]-1	N[NiC2]-1	9	106.916	☐	☐	
2	N[NiC2]-1	Ni[N4]-1	C[N2C]-1	C[N2C]-1	8	179.457	☐	☐	
3	N[NiC2]-1	C[N2C]-1	C[N2C]-1	Ni[N4]-1	4	179.514	☐	☐	
4	C[C2H]-1	C[C3]-1	C[C2H]-1	H[C]-1	16	179.376	☐	☐	
5	C[C2H]-1	H[C]-1	C[C2H]-1	C[C3]-1	4	179.594	☐	☐	
6	C[C2H]-1	C[C2H]-1	C[C2H]-1	H[C]-1	16	179.488	☐	☐	

***** in the FIELD file improper angle(s) appear in the dihedral angle section.
They are presented separately in this assistant for clarity purposes only.
(1) average value for the force field element as measured in the model.
(2) only the selected element(s) will be used to create the force field.
(3) each force field element can be tuned separately, if not the **Default** parameters will be used.

Figure 7.26 *"`Improper angle(s)`" tab in the "`DL-POLY`" assistant.*

`"Inversion angle(s)"`



Please select molecule: 1: MOL-8

Inversion angle(s) properties:

the **8** different fragment(s) in molecule **MOL-8**
contains the following **4** type(s) of inversion angle *

Id	At.1	At.2	At.3	At.4	Inversion(s)	av. ϕ [°] (1)	Viz. 3D	Use (2)	Potential (3)
1	N[NiC2]-1	Ni[N4]-1	C[N2C]-1	C[N2C]-1	4	0.442	☐	☐	
2	C[C2H]-1	C[C3]-1	C[C2H]-1	H[C]-1	16	0.494	☐	☐	
3	C[C3]-1	C[N2C]-1	C[C3]-1	C[C2H]-1	8	1.417	☐	☐	
4	C[N2C]-1	N[NiC2]-1	N[C2]-1	C[C3]-1	8	1.097	☐	☐	

***** the potential will be calculated by the sum of the 3 possible inversion terms between atoms 1 (center), 2, 3 and 4.

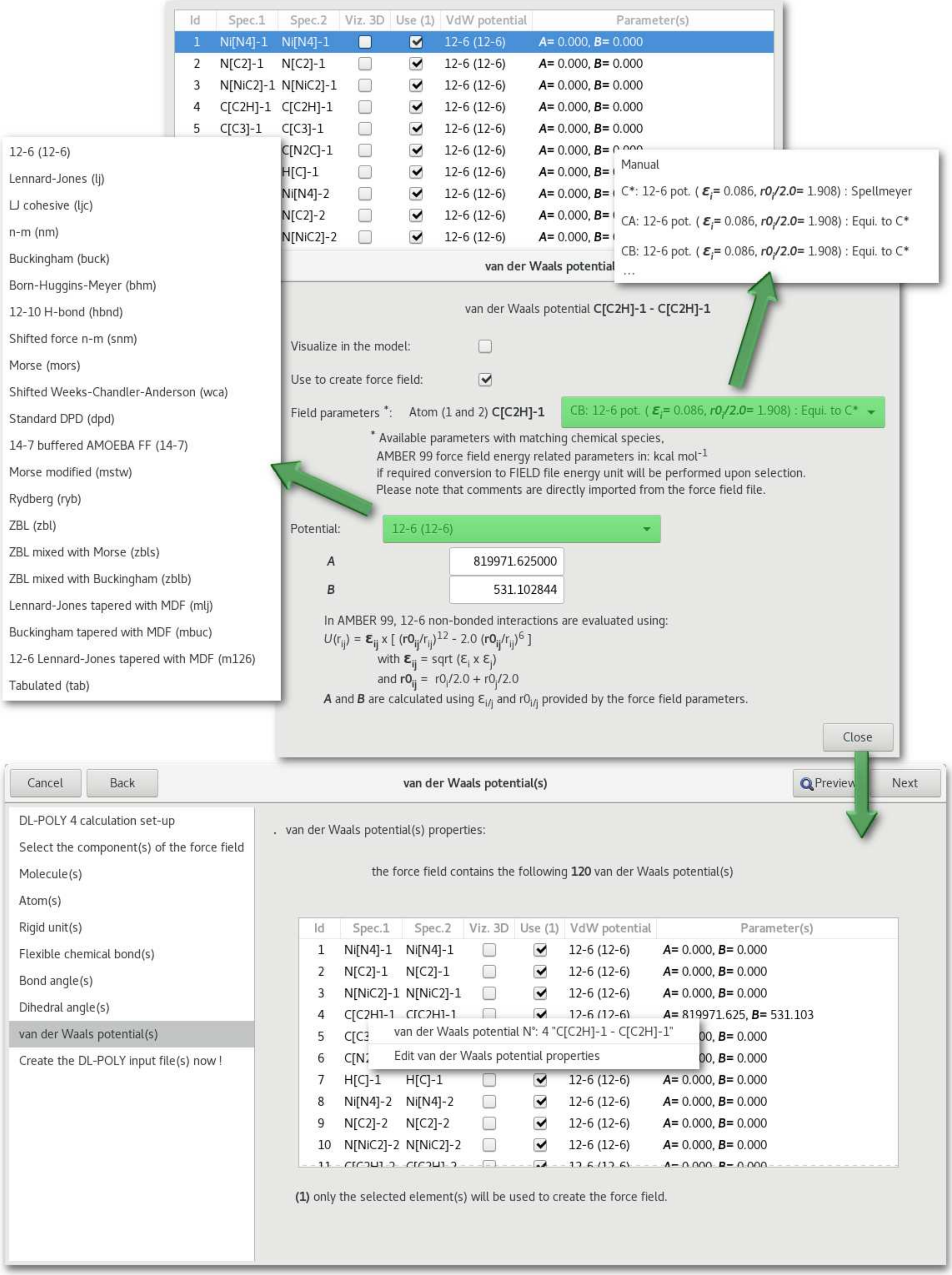
(1) average value for the force field element as measured in the model.

(2) only the selected element(s) will be used to create the force field.

(3) each force field element can be tuned separately, if not the **Default** parameters will be used.

Figure 7.27 *"`Inversion angle(s)`" tab in the "`DL-POLY`" assistant.*

`"van der Waals potential(s)"`



Id	Spec.1	Spec.2	Viz. 3D	Use (1)	VdW potential	Parameter(s)
1	Ni[N4]-1	Ni[N4]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
2	N[C2]-1	N[C2]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
3	N[NiC2]-1	N[NiC2]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
4	C[C2H]-1	C[C2H]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
5	C[C3]-1	C[C3]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
		C[N2C]-1	☐	☑	12-6 (12-6)	A= 0.000, B=
		H[C]-1	☐	☑	12-6 (12-6)	A= 0.000, B=
		Ni[N4]-2	☐	☑	12-6 (12-6)	A= 0.000, B=
		N[C2]-2	☐	☑	12-6 (12-6)	A= 0.000, B=
		N[NiC2]-2	☐	☑	12-6 (12-6)	A= 0.000, B=

van der Waals potential

van der Waals potential **C[C2H]-1 - C[C2H]-1**

Visualize in the model: ☐

Use to create force field: ☑

Field parameters *: Atom (1 and 2) **C[C2H]-1** CB: 12-6 pot. (ε_i= 0.086, $r0_i/2.0$= 1.908) : Equi. to C*

* Available parameters with matching chemical species,
AMBER 99 force field energy related parameters in: kcal mol^{-1}
if required conversion to FIELD file energy unit will be performed upon selection.
Please note that comments are directly imported from the force field file.

Potential: 12-6 (12-6)

A 819971.625000

B 531.102844

In AMBER 99, 12-6 non-bonded interactions are evaluated using:

$U(r_{ij}) = \varepsilon_{ij} \times [(r0_{ij}/r_{ij})^{12} - 2.0 (r0_{ij}/r_{ij})^6]$

with ε_{ij} = sqrt ($\varepsilon_i \times \varepsilon_j$)

and $r0_{ij}$ = $r0_i/2.0 + r0_j/2.0$

A and *B* are calculated using $\varepsilon_{i/j}$ and $r0_{i/j}$ provided by the force field parameters.

van der Waals potential(s)

. van der Waals potential(s) properties:

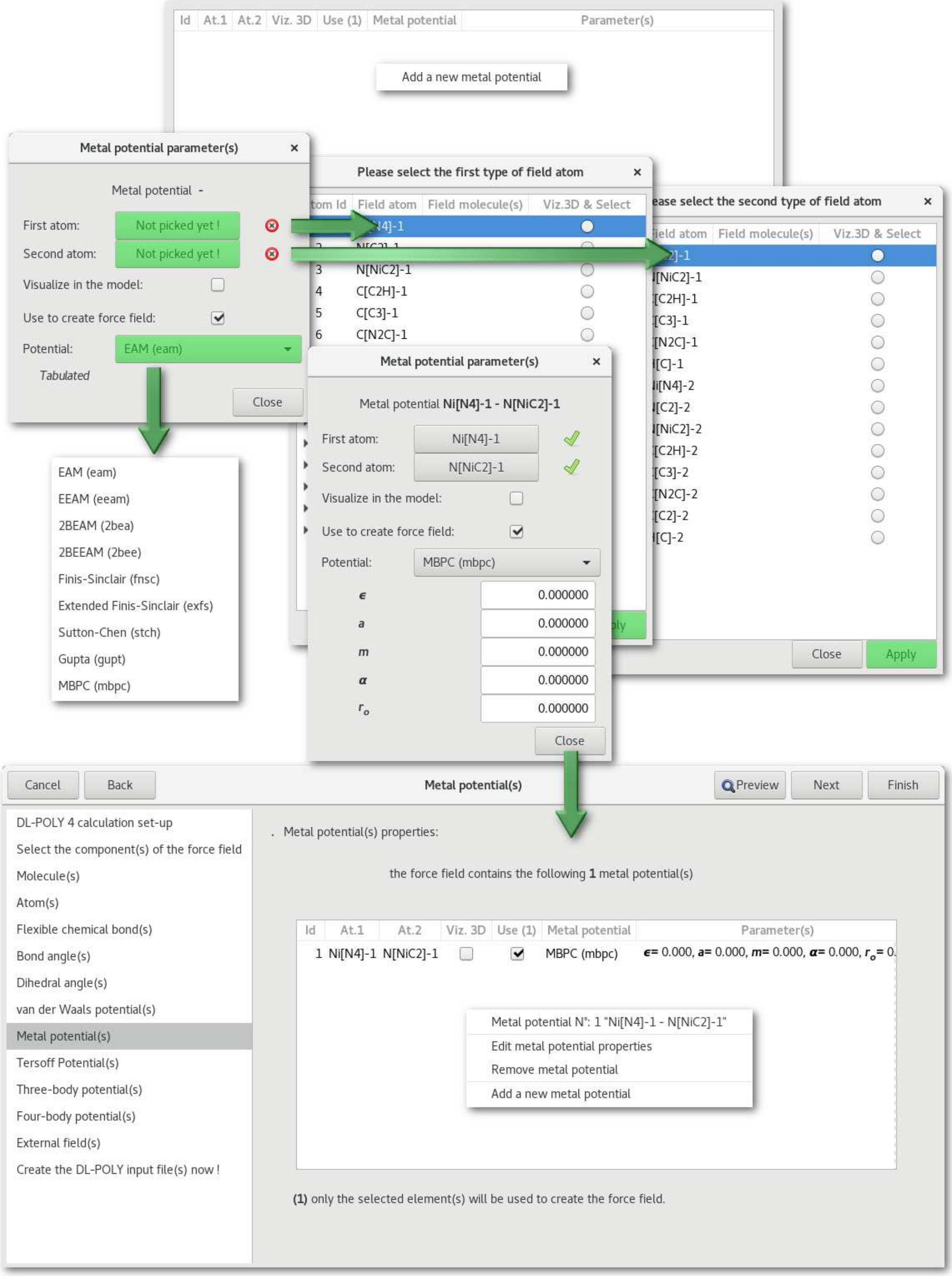
the force field contains the following **120** van der Waals potential(s)

Id	Spec.1	Spec.2	Viz. 3D	Use (1)	VdW potential	Parameter(s)
1	Ni[N4]-1	Ni[N4]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
2	N[C2]-1	N[C2]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
3	N[NiC2]-1	N[NiC2]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
4	C[C2H]-1	C[C2H]-1	☐	☑	12-6 (12-6)	A= 819971.625, B= 531.103
5	C[C3					00, B= 0.000
6	C[N2					00, B= 0.000
7	H[C]-1	H[C]-1	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
8	Ni[N4]-2	Ni[N4]-2	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
9	N[C2]-2	N[C2]-2	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000
10	N[NiC2]-2	N[NiC2]-2	☐	☑	12-6 (12-6)	A= 0.000, B= 0.000

(1) only the selected element(s) will be used to create the force field.

Figure 7.28 *"`van der Waals potential(s)`" tab in the "`DL-POLY`" assistant.*

"Metal potential(s)"



Metal potential -

First atom: Not picked yet !

Second atom: Not picked yet !

Potential: EAM (eam)

Atom Id	Field atom
1	…4]-1
2	N[C2]-1
3	N[NiC2]-1
4	C[C2H]-1
5	C[C3]-1
6	C[N2C]-1

Field atom
…2]-1
…[NiC2]-1
…[C2H]-1
…[C3]-1
…[N2C]-1
…[C]-1
…i[N4]-2
…[C2]-2
…[NiC2]-2
…[C2H]-2
…[C3]-2
…[N2C]-2
…[C2]-2
…[C]-2

Metal potential **Ni[N4]-1 - N[NiC2]-1**

First atom: Ni[N4]-1 ✓

Second atom: N[NiC2]-1 ✓

Visualize in the model: ☐

Use to create force field: ☑

Potential: MBPC (mbpc)

ϵ 0.000000

a 0.000000

m 0.000000

α 0.000000

r_o 0.000000

. Metal potential(s) properties:

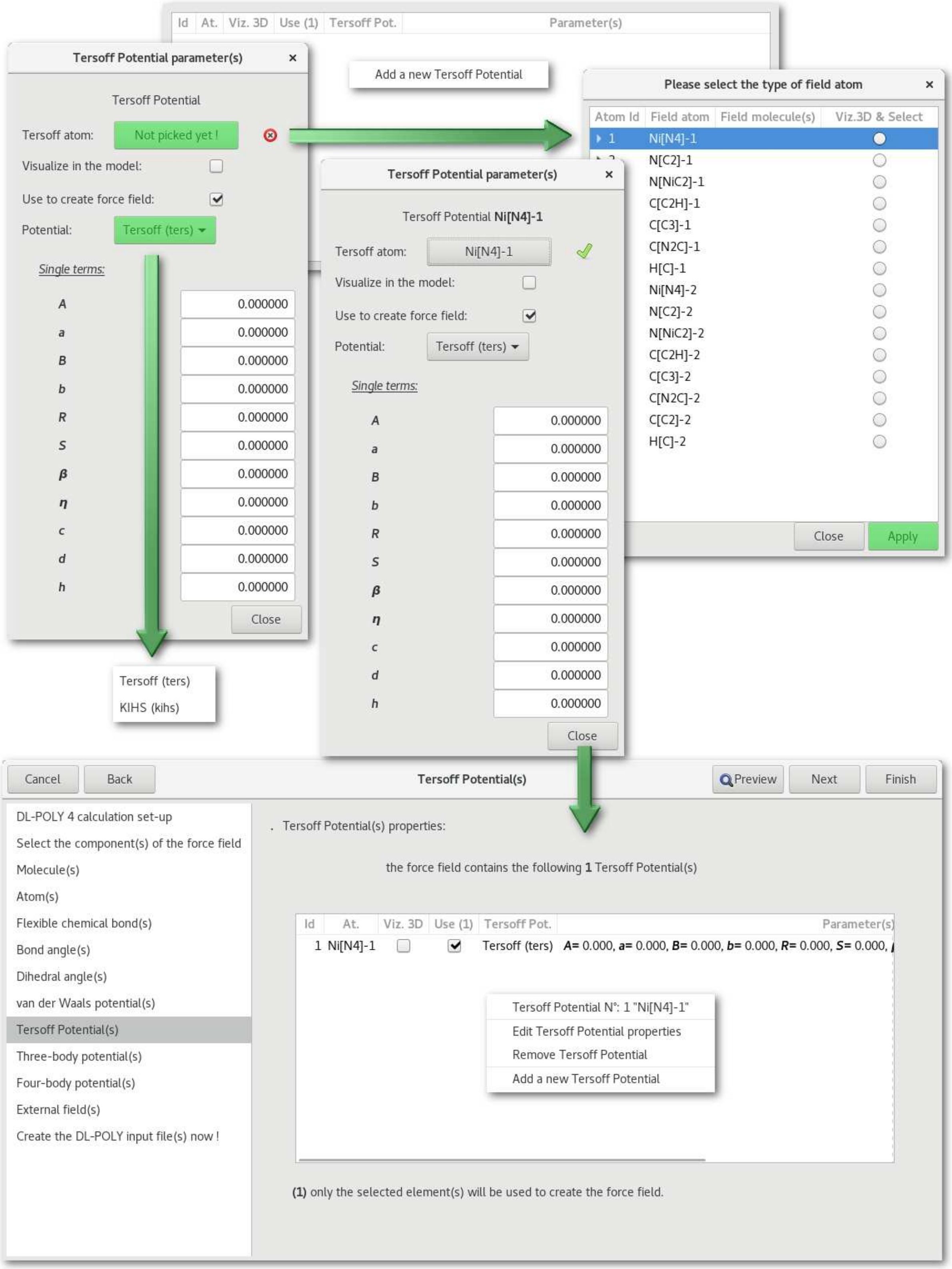
the force field contains the following **1** metal potential(s)

Id	At.1	At.2	Viz. 3D	Use (1)	Metal potential	Parameter(s)
1	Ni[N4]-1	N[NiC2]-1	☐	☑	MBPC (mbpc)	ϵ= 0.000, a= 0.000, m= 0.000, α= 0.000, r_o= 0.

(1) only the selected element(s) will be used to create the force field.

Figure 7.29 *"`Metal potential(s)`" tab in the "`DL-POLY`" assistant.*

"Tersoff potential(s)"



Tersoff Potential parameter(s)

Tersoff Potential

Tersoff atom: Not picked yet !

Visualize in the model: ☐

Use to create force field: ☑

Potential: Tersoff (ters)

Single terms:

A	0.000000
a	0.000000
B	0.000000
b	0.000000
R	0.000000
S	0.000000
β	0.000000
η	0.000000
c	0.000000
d	0.000000
h	0.000000

Please select the type of field atom

Atom Id	Field atom	Field molecule(s)	Viz.3D & Select
1	Ni[N4]-1		●
2	N[C2]-1		○
	N[NiC2]-1		○
	C[C2H]-1		○
	C[C3]-1		○
	C[N2C]-1		○
	H[C]-1		○
	Ni[N4]-2		○
	N[C2]-2		○
	N[NiC2]-2		○
	C[C2H]-2		○
	C[C3]-2		○
	C[N2C]-2		○
	C[C2]-2		○
	H[C]-2		○

Tersoff Potential parameter(s)

Tersoff Potential **Ni[N4]-1**

Tersoff atom: Ni[N4]-1 ✓

Visualize in the model: ☐

Use to create force field: ☑

Potential: Tersoff (ters)

Single terms:

A	0.000000
a	0.000000
B	0.000000
b	0.000000
R	0.000000
S	0.000000
β	0.000000
η	0.000000
c	0.000000
d	0.000000
h	0.000000

Tersoff Potential(s)

. Tersoff Potential(s) properties:

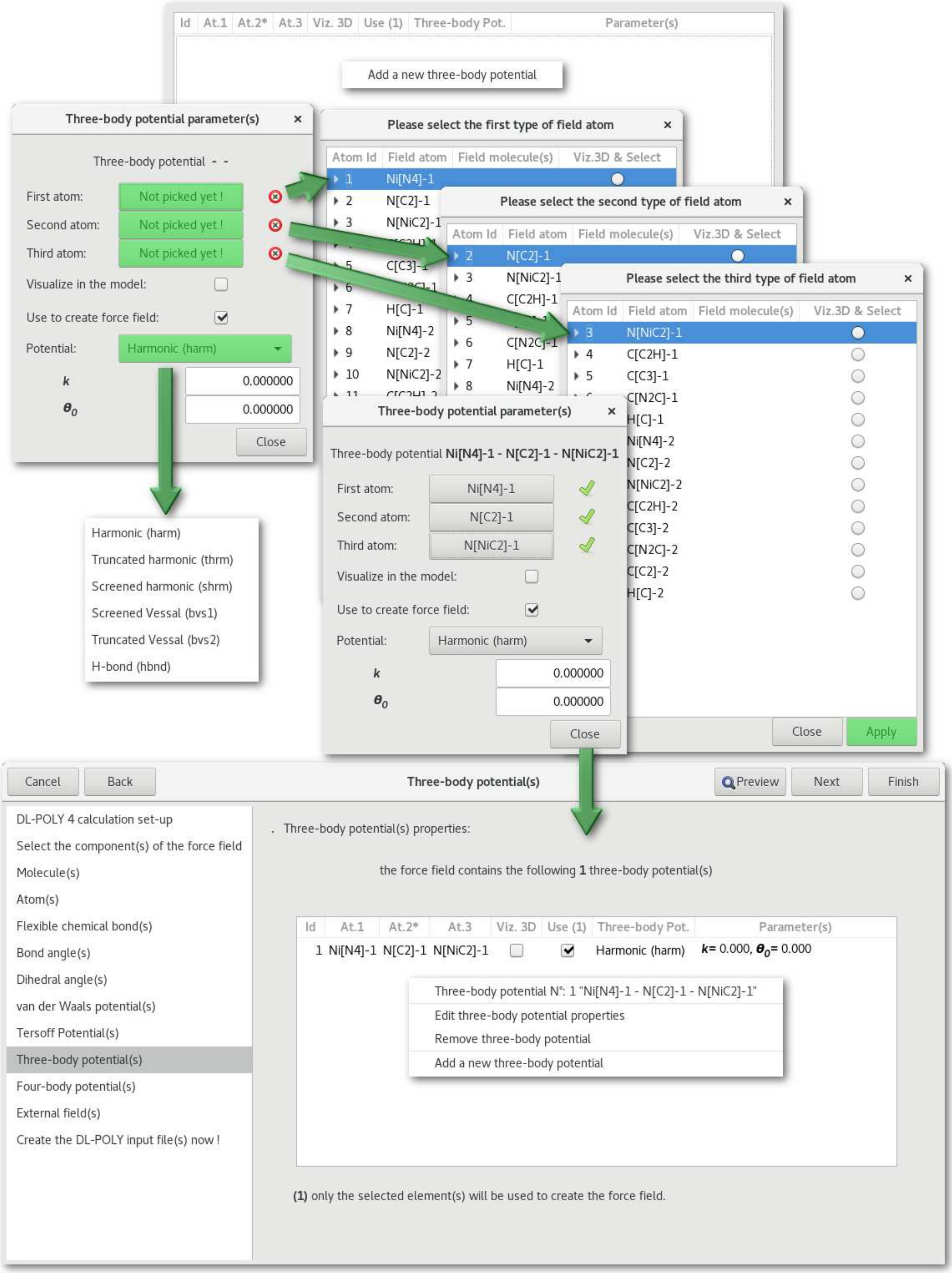
the force field contains the following **1** Tersoff Potential(s)

Id	At.	Viz. 3D	Use (1)	Tersoff Pot.	Parameter(s)
1	Ni[N4]-1	☐	☑	Tersoff (ters)	**A**= 0.000, **a**= 0.000, **B**= 0.000, **b**= 0.000, **R**= 0.000, **S**= 0.000,

(1) only the selected element(s) will be used to create the force field.

Figure 7.30 *"`Tersoff potential(s)`" tab in the "`DL-POLY`" assistant.*

"Three body potential(s)"



Three-body potential parameter(s)

Three-body potential - -

First atom: Not picked yet !

Second atom: Not picked yet !

Third atom: Not picked yet !

Visualize in the model: ☐

Use to create force field: ☑

Potential: Harmonic (harm)

k 0.000000

θ_0 0.000000

Three-body potential parameter(s)

Three-body potential **Ni[N4]-1 - N[C2]-1 - N[NiC2]-1**

First atom: Ni[N4]-1

Second atom: N[C2]-1

Third atom: N[NiC2]-1

Visualize in the model: ☐

Use to create force field: ☑

Potential: Harmonic (harm)

k 0.000000

θ_0 0.000000

. Three-body potential(s) properties:

the force field contains the following **1** three-body potential(s)

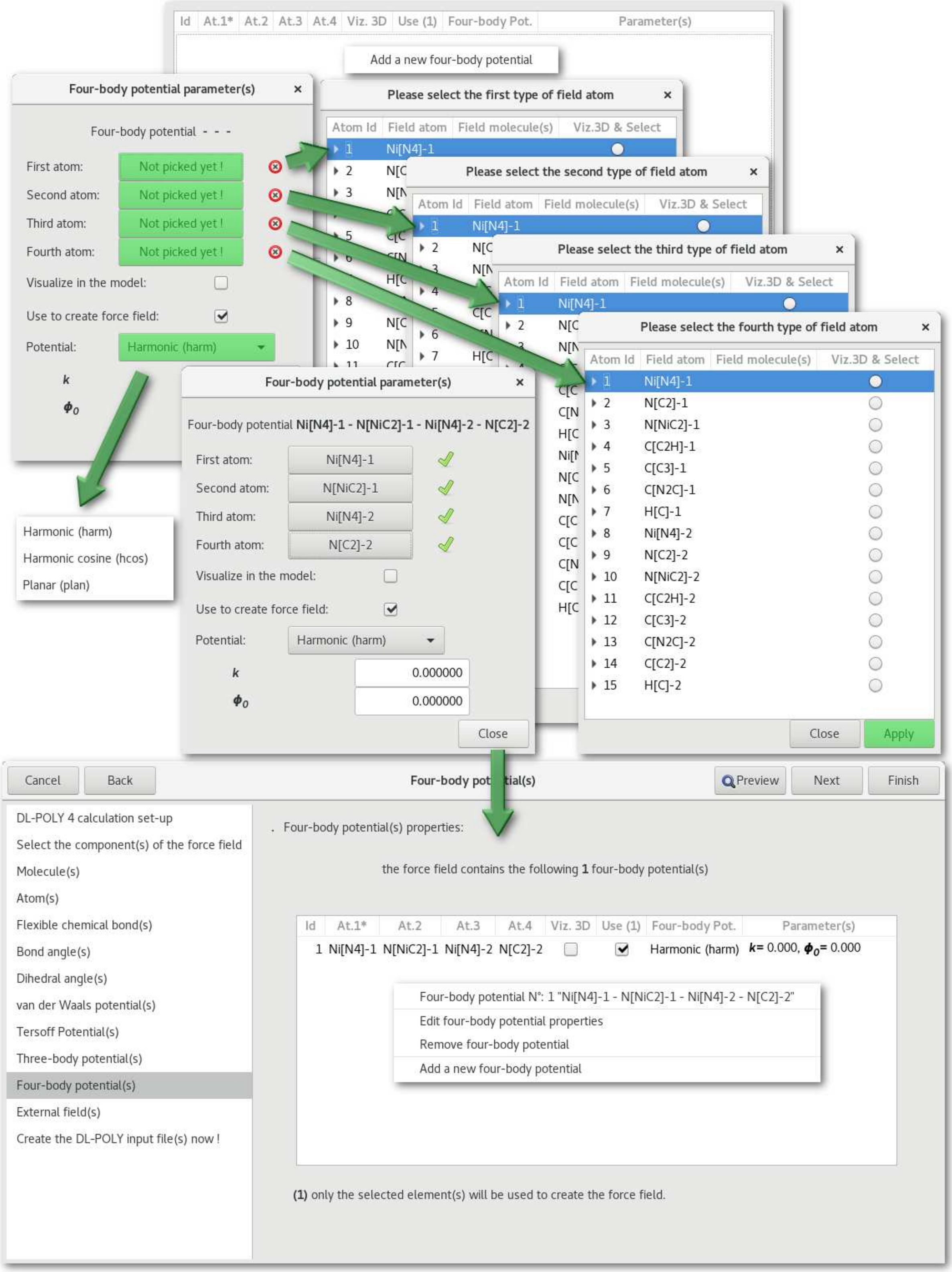
Id	At.1	At.2*	At.3	Viz. 3D	Use (1)	Three-body Pot.	Parameter(s)
1	Ni[N4]-1	N[C2]-1	N[NiC2]-1	☐	☑	Harmonic (harm)	**k**= 0.000, θ_0= 0.000

Three-body potential N°: 1 "Ni[N4]-1 - N[C2]-1 - N[NiC2]-1"

(1) only the selected element(s) will be used to create the force field.

Figure 7.31 *"*`Three potential(s)`*" tab in the "*`DL-POLY`*" assistant.*

"Four body potential(s)"



Four-body potential - - -

First atom: Not picked yet !

Second atom: Not picked yet !

Third atom: Not picked yet !

Fourth atom: Not picked yet !

Visualize in the model: ☐

Use to create force field: ☑

Potential: Harmonic (harm)

Please select the fourth type of field atom

Atom Id	Field atom	Field molecule(s)	Viz.3D & Select
1	Ni[N4]-1		●
2	N[C2]-1		○
3	N[NiC2]-1		○
4	C[C2H]-1		○
5	C[C3]-1		○
6	C[N2C]-1		○
7	H[C]-1		○
8	Ni[N4]-2		○
9	N[C2]-2		○
10	N[NiC2]-2		○
11	C[C2H]-2		○
12	C[C3]-2		○
13	C[N2C]-2		○
14	C[C2]-2		○
15	H[C]-2		○

Four-body potential Ni[N4]-1 - N[NiC2]-1 - Ni[N4]-2 - N[C2]-2

First atom: Ni[N4]-1 ✓

Second atom: N[NiC2]-1 ✓

Third atom: Ni[N4]-2 ✓

Fourth atom: N[C2]-2 ✓

Visualize in the model: ☐

Use to create force field: ☑

Potential: Harmonic (harm)

k 0.000000

ϕ_0 0.000000

Four-body potential(s) properties:

the force field contains the following **1** four-body potential(s)

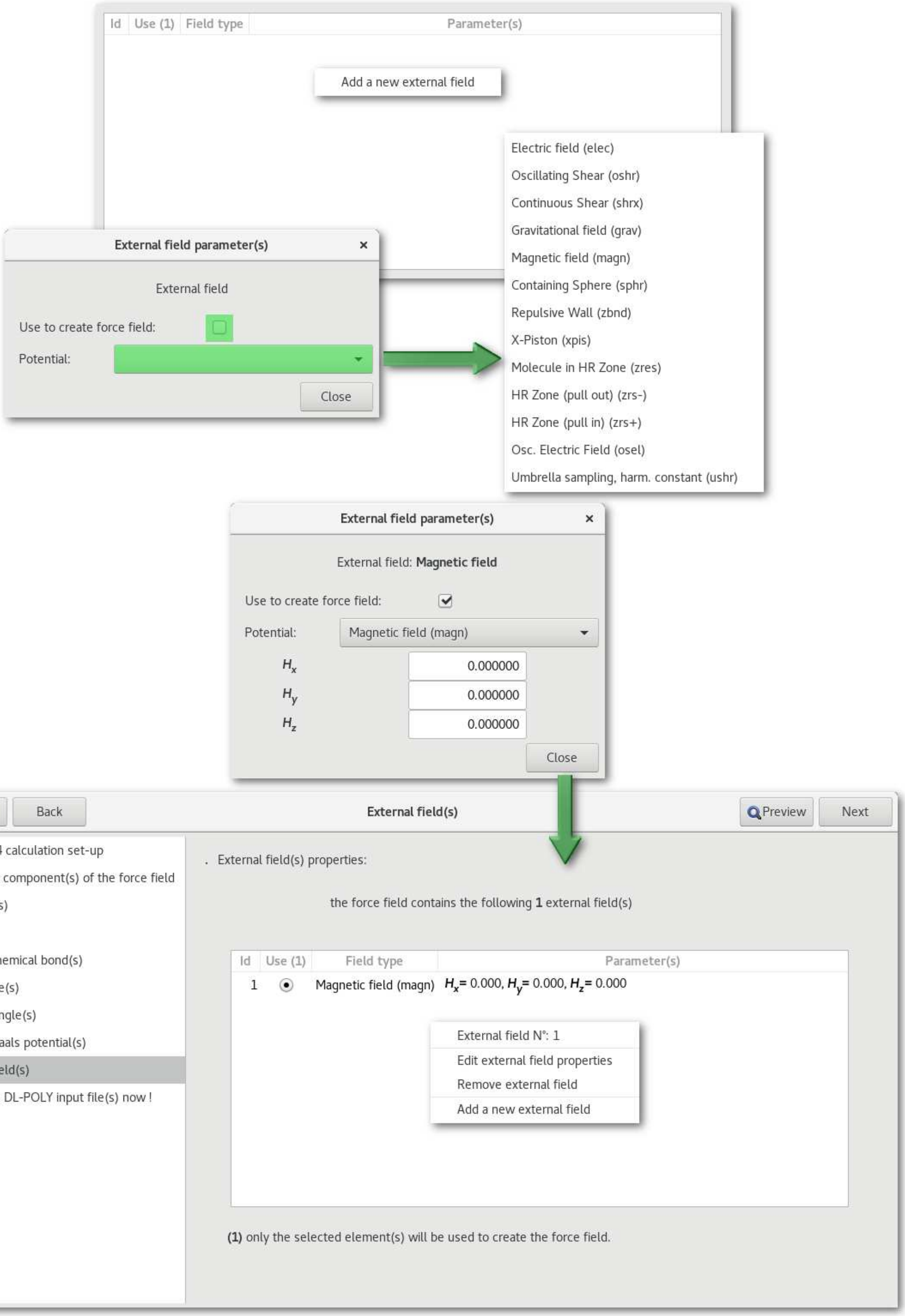
Id	At.1*	At.2	At.3	At.4	Viz. 3D	Use (1)	Four-body Pot.	Parameter(s)
1	Ni[N4]-1	N[NiC2]-1	Ni[N4]-2	N[C2]-2	☐	☑	Harmonic (harm)	**k**= 0.000, ϕ_0= 0.000

Four-body potential N°: 1 "Ni[N4]-1 - N[NiC2]-1 - Ni[N4]-2 - N[C2]-2"

(1) only the selected element(s) will be used to create the force field.

Figure 7.32 *"Four body potential(s)" tab in the "DL-POLY" assistant.*

`"External field(s)"`



External field parameter(s)

External field

Use to create force field: ☐

Potential:

External field parameter(s)

External field: **Magnetic field**

Use to create force field: ☑

Potential: Magnetic field (magn)

H_x 0.000000

H_y 0.000000

H_z 0.000000

External field(s) properties:

the force field contains the following **1** external field(s)

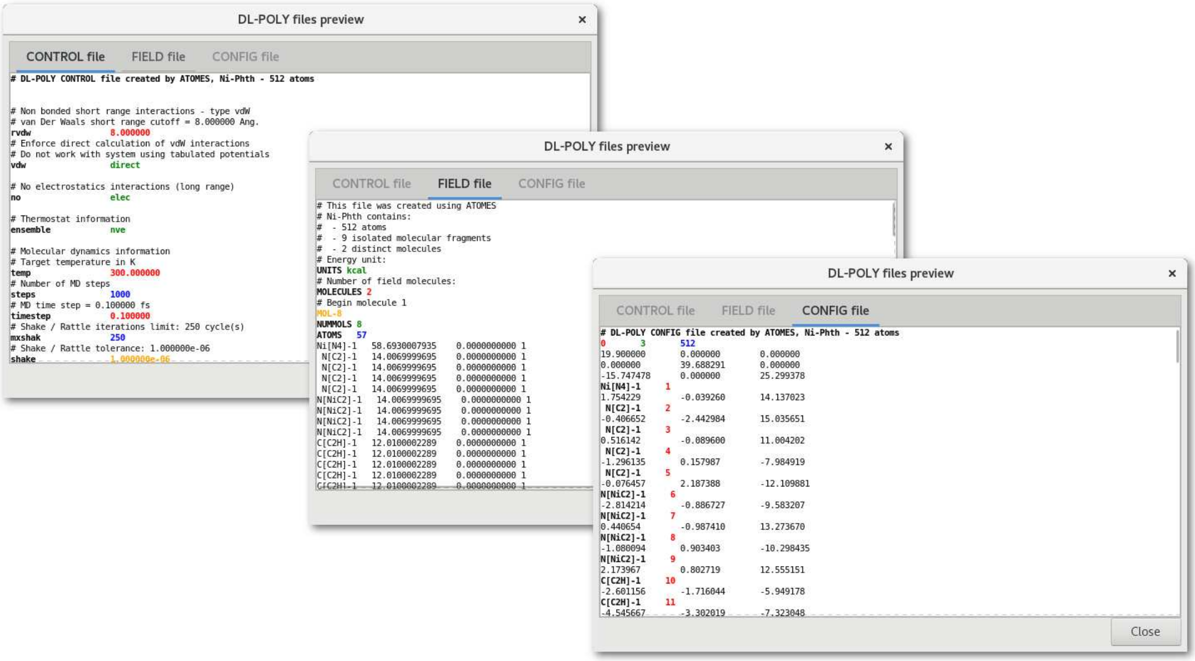
Id	Use (1)	Field type	Parameter(s)
1	●	Magnetic field (magn)	H_x= 0.000, H_y= 0.000, H_z= 0.000

(1) only the selected element(s) will be used to create the force field.

Figure 7.33 *"`External field(s)`" tab in the "`DL-POLY`" assistant.*

7.1.1.4 "`Preview`"

At any time when using the "`DL-POLY`" assistant, the "`Preview`" button allows open the "`DL-POLY files preview`" dialog, to visualize the "`CONTROL`", "`FIELD`" and "`CONFIG`" file(s).



```
# DL-POLY CONTROL file created by ATOMES, Ni-Phth - 512 atoms


# Non bonded short range interactions - type vdW
# van Der Waals short range cutoff = 8.000000 Ang.
rvdw                    8.000000
# Enforce direct calculation of vdW interactions
# Do not work with system using tabulated potentials
vdw                     direct

# No electrostatics interactions (long range)
no                      elec

# Thermostat information
ensemble                nve

# Molecular dynamics information
# Target temperature in K
temp                    300.000000
# Number of MD steps
steps                   1000
# MD time step = 0.100000 fs
timestep                0.100000
# Shake / Rattle iterations limit: 250 cycle(s)
mxshak                  250
# Shake / Rattle tolerance: 1.000000e-06
shake                   1.000000e-06
```

```
# This file was created using ATOMES
# Ni-Phth contains:
#  - 512 atoms
#  - 9 isolated molecular fragments
#  - 2 distinct molecules
# Energy unit:
UNITS kcal
# Number of field molecules:
MOLECULES 2
# Begin molecule 1
MOL-8
NUMMOLS 8
ATOMS   57
Ni[N4]-1   58.6930007935    0.0000000000 1
 N[C2]-1   14.0069999695    0.0000000000 1
 N[C2]-1   14.0069999695    0.0000000000 1
 N[C2]-1   14.0069999695    0.0000000000 1
 N[C2]-1   14.0069999695    0.0000000000 1
N[NiC2]-1   14.0069999695    0.0000000000 1
N[NiC2]-1   14.0069999695    0.0000000000 1
N[NiC2]-1   14.0069999695    0.0000000000 1
N[NiC2]-1   14.0069999695    0.0000000000 1
C[C2H]-1   12.0100002289    0.0000000000 1
C[C2H]-1   12.0100002289    0.0000000000 1
C[C2H]-1   12.0100002289    0.0000000000 1
C[C2H]-1   12.0100002289    0.0000000000 1
C[C2H]-1   12.0100002289    0.0000000000 1
```

```
# DL-POLY CONFIG file created by ATOMES, Ni-Phth - 512 atoms
0       3       512
19.900000       0.000000        0.000000
0.000000        39.688291       0.000000
-15.747478      0.000000        25.299378
Ni[N4]-1     1
1.754229        -0.039260       14.137023
 N[C2]-1     2
-0.406652       -2.442984       15.035651
 N[C2]-1     3
0.516142        -0.089600       11.004202
 N[C2]-1     4
-1.296135       0.157987        -7.984919
 N[C2]-1     5
-0.076457       2.187388        -12.109881
N[NiC2]-1     6
-2.814214       -0.886727       -9.583207
N[NiC2]-1     7
0.440654        -0.987410       13.273670
N[NiC2]-1     8
-1.080094       0.903403        -10.298435
N[NiC2]-1     9
2.173967        0.802719        12.555151
C[C2H]-1     10
-2.601156       -1.716044       -5.949178
C[C2H]-1     11
-4.545667       -3.302019       -7.323048
```

Figure 7.34 *"`DL-POLY files preview`" dialog in the "`DL-POLY`" assistant.*

The "`DL-POLY files preview`" dialog (fig. 7.34) contains a notebook with up to 3 tabs depending on the file(s) to be created. Each tab presents the content of a file, "`CONTROL`", "`FIELD`" or "`CONFIG`", and highlights option(s) and keyword(s) using color(s) and font layout option(s).

7.1.1.5 Finalizing the assistant and file(s) creation

When pressing the "`Apply`" button on the file tab of the assistant, the user is asked to selected a folder. "`CONTROL`", "`FIELD`" and "`CONFIG`" if selected, will be created in the selected directory.

Following the file(s) creation or if the assistant is closed anyway, the "`DL-POLY`" force field data will be preserved. Therefore allowing the re-open the assistant later for further modifications.

All existing force field data can also saved in the **atomes** project and/or workspace files, simply remember to save your work.

7.1.2 LAMMPS

Coming soon

7.2 *Ab-initio MD*

7.2.1 CPMD v4.3.0

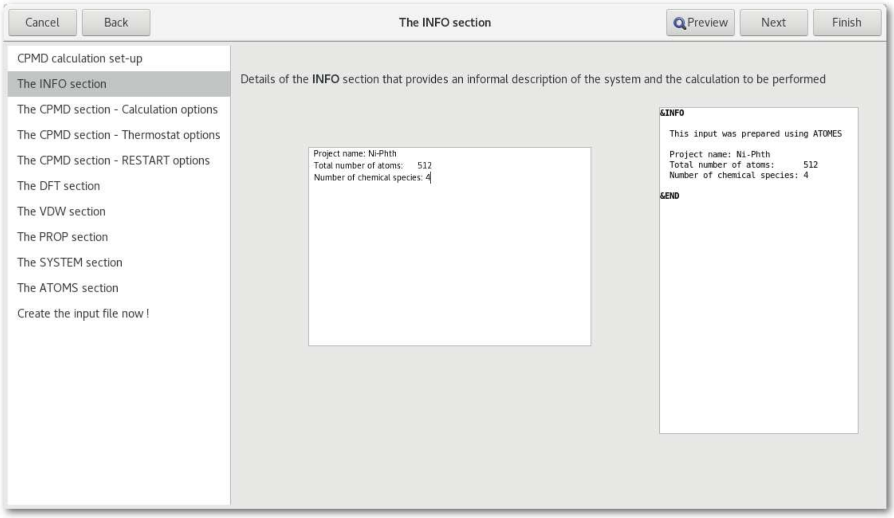
The **atomes** helper for the CPMD calculation offers to prepare input files for **CPMD v4.3.0**. Please note that the CPMD code offers so many calculation options that it is not possible either to provide a description or to offer a comprehensive usage guide for each of these options. Therefore the CPMD calculation assistant only provides help towards basics and / or frequently used calculation options.

In any case if you intent to use the CPMD code please refer to the user manual:

https://www.cpmd.org/wordpress/CPMD/getFile.php?file=manual.pdf

The **atomes** helper for the CPMD calculation provides a step by step interface to configure the different sections of the CPMD input file:

The "`INFO`" section



Details of the **INFO** section that provides an informal description of the system and the calculation to be performed

```
Project name: Ni-Phth
Total number of atoms:    512
Number of chemical species: 4
```

```
&INFO

  This input was prepared using ATOMES

  Project name: Ni-Phth
  Total number of atoms:      512
  Number of chemical species: 4

&END
```

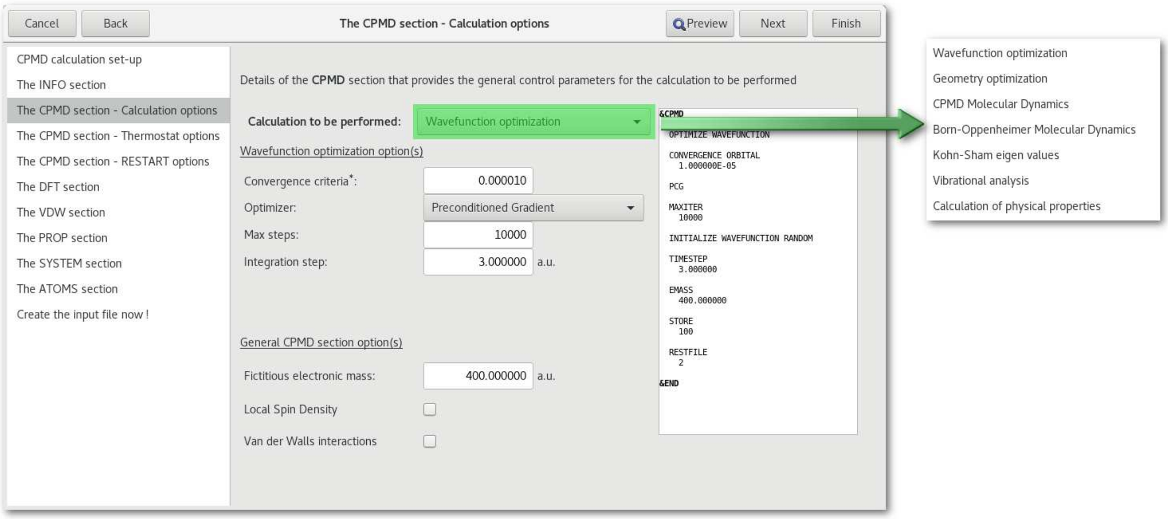
Figure 7.35 *"`INFO section`" tab in the "`CPMD`" assistant.*

The "`CPMD`" section

The creation of the "`CPMD`" section is split over 3 tabs, dedicated respectively to the calculation, thermostat and restart option(s).

"`Calculation options`"

The "`Calculation to be performed`" [Fig. 7.36] combo allows to select the type of job:



The CPMD section - Calculation options

Details of the **CPMD** section that provides the general control parameters for the calculation to be performed

Calculation to be performed: Wavefunction optimization

Wavefunction optimization option(s)

Convergence criteria*: 0.000010
Optimizer: Preconditioned Gradient
Max steps: 10000
Integration step: 3.000000 a.u.

General CPMD section option(s)

Fictitious electronic mass: 400.000000 a.u.
Local Spin Density ☐
Van der Walls interactions ☐

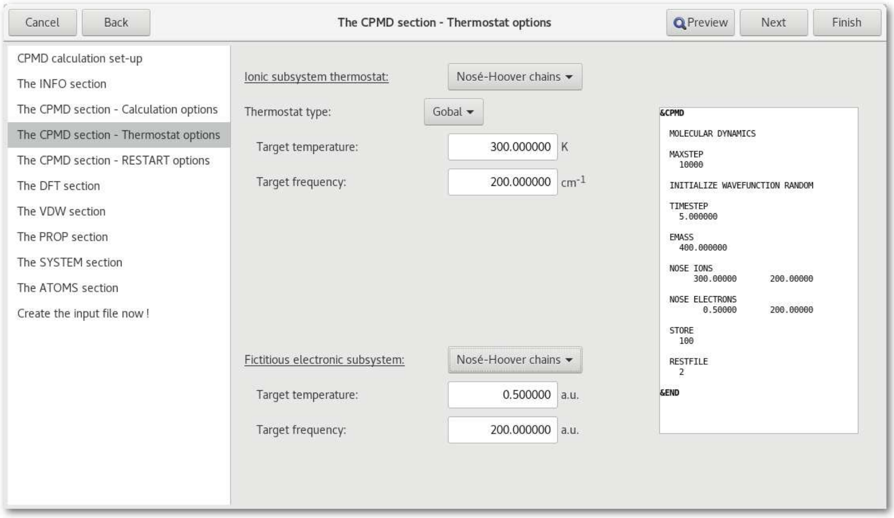
```
&CPMD
  OPTIMIZE WAVEFUNCTION

  CONVERGENCE ORBITAL
    1.000000E-05

  PCG

  MAXITER
    10000

  INITIALIZE WAVEFUNCTION RANDOM

  TIMESTEP
    3.000000

  EMASS
    400.000000

  STORE
    100

  RESTFILE
    2

&END
```

Figure 7.36 *"`CPMD section - Calculation options`" tab in the "`CPMD`" assistant.*

The option(s) directly bellow the combo will change depending on the nature of the calculation, please refer to the CPMD user manual for more information on theses options.

"`Thermostat options`"

If a molecular dynamics calculation is to be performed then the "`CPMD section - Thermostat options`" tab becomes accessible:



Ionic subsystem thermostat: Nosé-Hoover chains

Thermostat type: Gobal

Target temperature: 300.000000 K

Target frequency: 200.000000 cm^{-1}

Fictitious electronic subsystem: Nosé-Hoover chains

Target temperature: 0.500000 a.u.

Target frequency: 200.000000 a.u.

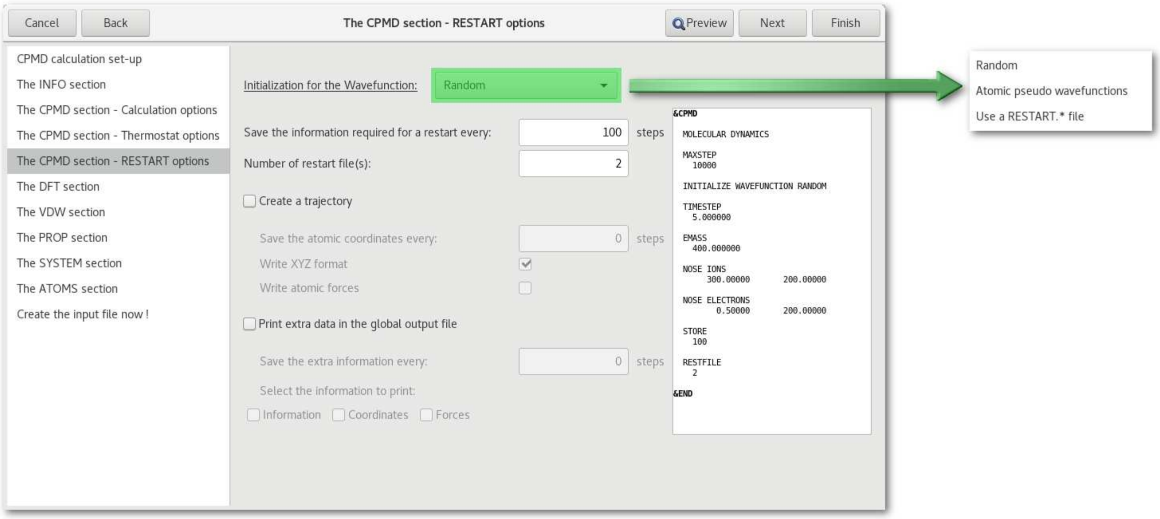
```
&CPMD

 MOLECULAR DYNAMICS

 MAXSTEP
   10000

 INITIALIZE WAVEFUNCTION RANDOM

 TIMESTEP
   5.000000

 EMASS
   400.000000

 NOSE IONS
        300.00000       200.00000

 NOSE ELECTRONS
          0.50000       200.00000

 STORE
   100

 RESTFILE
   2

&END
```

Figure 7.37 *"`CPMD section - Thermostat options`" tab in the "`CPMD`" assistant.*

In order to access the next page of the assistant thermostat(s) must be set up properly. Again for more information please refer to the CPMD user manual.

"`RESTART options`"

The "`CPMD section - Restart options`" tab present options to restart calculation and saving options during the calculation:



Initialization for the Wavefunction: Random

Save the information required for a restart every: 100 steps

Number of restart file(s): 2

☐ Create a trajectory

Save the atomic coordinates every: 0 steps

Write XYZ format ☑

Write atomic forces ☐

☐ Print extra data in the global output file

Save the extra information every: 0 steps

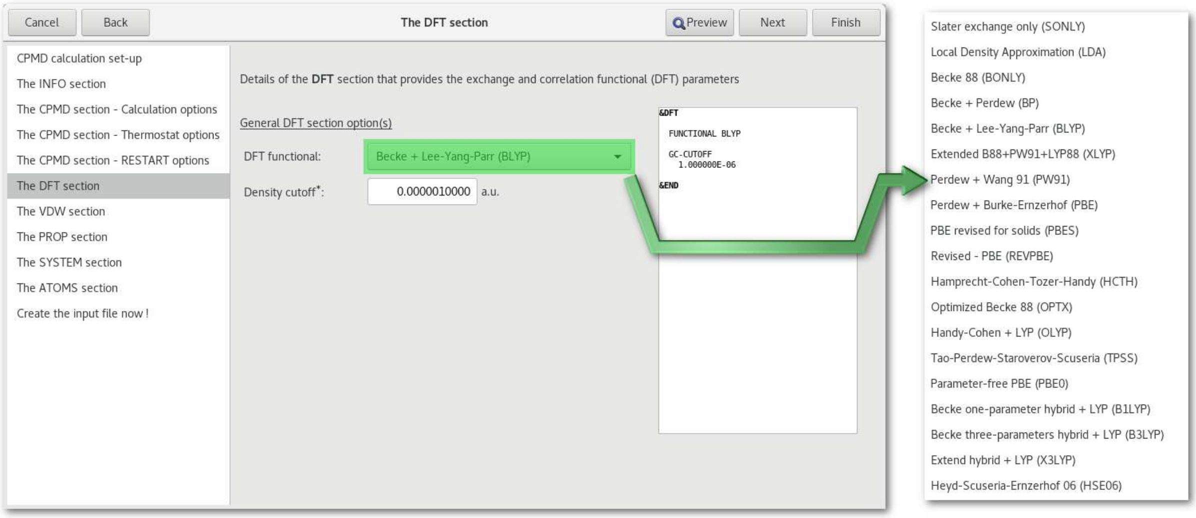
Select the information to print:

☐ Information ☐ Coordinates ☐ Forces

```
&CPMD

 MOLECULAR DYNAMICS

 MAXSTEP
   10000

 INITIALIZE WAVEFUNCTION RANDOM

 TIMESTEP
   5.000000

 EMASS
   400.000000

 NOSE IONS
        300.00000       200.00000

 NOSE ELECTRONS
          0.50000       200.00000

 STORE
   100

 RESTFILE
   2

&END
```

Figure 7.38 *"`CPMD section - Restart options`" tab in the "`CPMD`" assistant.*

The "`DFT`" section



Details of the **DFT** section that provides the exchange and correlation functional (DFT) parameters

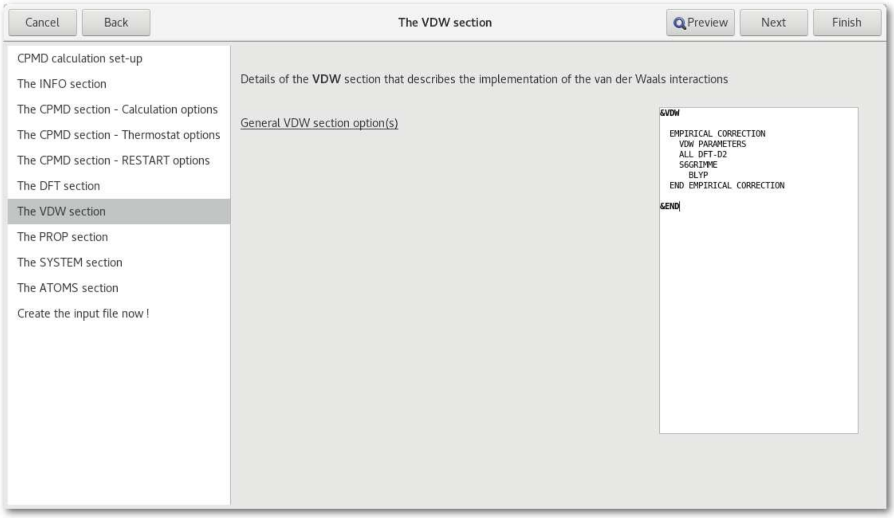
DFT functional: Becke + Lee-Yang-Parr (BLYP)

Density cutoff*: 0.0000010000 a.u.

```
&DFT

  FUNCTIONAL BLYP

  GC-CUTOFF
    1.000000E-06

&END
```

Figure 7.39 *"`DFT section`" tab in the "`CPMD`" assistant.*

The "`VDW`" section



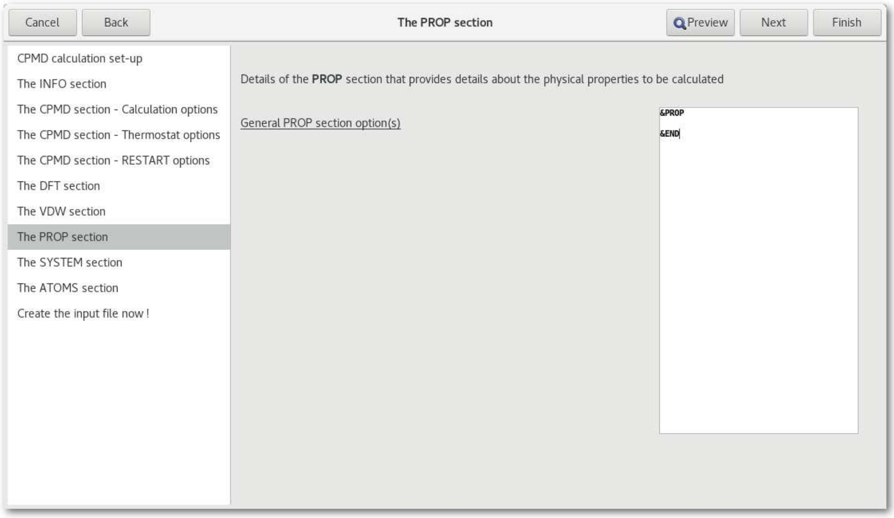
Details of the **VDW** section that describes the implementation of the van der Waals interactions

```
&VDW

  EMPIRICAL CORRECTION
    VDW PARAMETERS
    ALL DFT-D2
    S6GRIMME
      BLYP
  END EMPIRICAL CORRECTION

&END
```

Figure 7.40 *"`VDW section`" tab in the "`CPMD`" assistant.*

Providing that van der Waals interactions are selected in the "`CPMD`" section of the input file, then the "`VDW`" section becomes accessible. However its content is filled automatically based on parameters selected in both the "`CPMD`" and "`DFT`" sections.

The "PROP" section



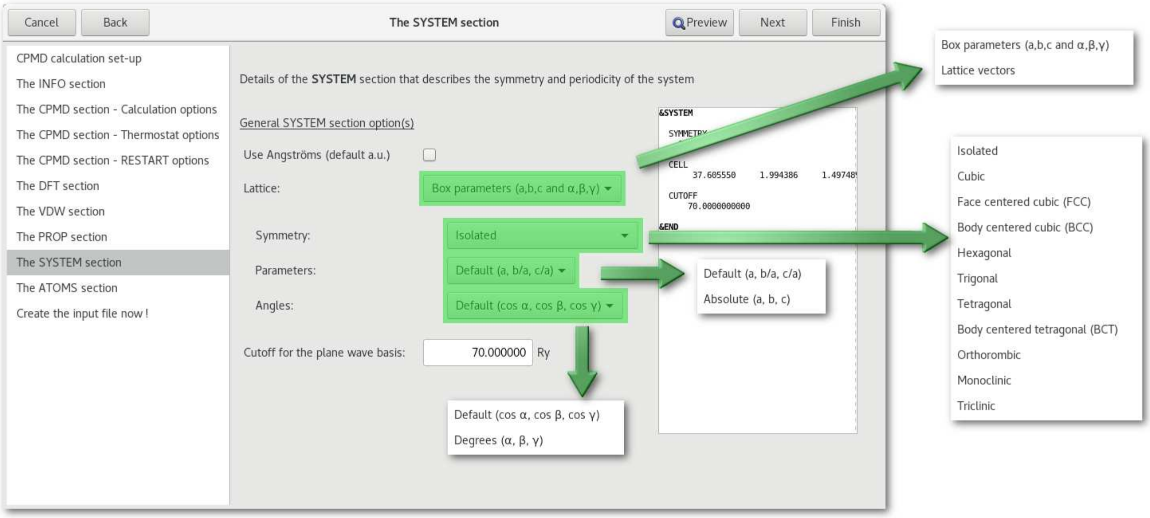
Details of the **PROP** section that provides details about the physical properties to be calculated

```
&PROP

&END
```

Figure 7.41 *"*`PROP section`*" tab in the "*`CPMD`*" assistant.*

Providing that the "`Calculation of physical properties`" is selected in the "`CPMD`" section of the input file, then the "`PROP`" section becomes accessible. However its content is filled automatically based on parameters selected in the "`CPMD`" section.

The "SYSTEM" section



Details of the **SYSTEM** section that describes the symmetry and periodicity of the system

Use Angströms (default a.u.) ☐

Lattice: Box parameters (a,b,c and α,β,γ)

Symmetry: Isolated

Parameters: Default (a, b/a, c/a)

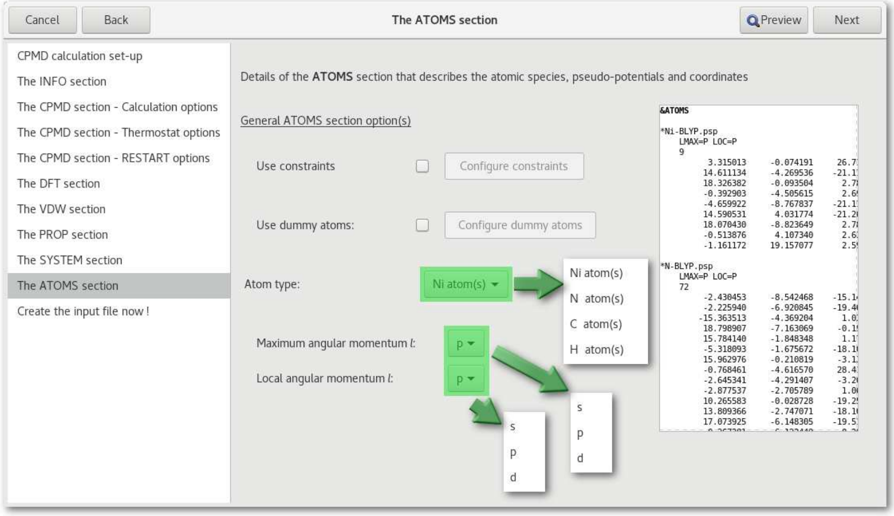
Angles: Default (cos α, cos β, cos γ)

Cutoff for the plane wave basis: 70.000000 Ry

```
&SYSTEM

  SYMMETRY

  CELL
      37.605550     1.994386     1.49748

  CUTOFF
     70.0000000000

&END
```

Figure 7.42 *"*`SYSTEM section`*" tab in the "*`CPMD`*" assistant.*

The "`ATOMS`" section



Details of the **ATOMS** section that describes the atomic species, pseudo-potentials and coordinates

Use constraints ☐

Use dummy atoms: ☐

Atom type: Ni atom(s)

Maximum angular momentum *l*: p

Local angular momentum *l*: p

```
&ATOMS

*Ni-BLYP.psp
    LMAX=P LOC=P
    9
         3.315013     -0.074191     26.7
        14.611134     -4.269536    -21.1
        18.326382     -0.093504      2.7
        -0.392903     -4.505615      2.6
        -4.659922     -8.767837    -21.1
        14.590531      4.031774    -21.2
        18.070430     -8.823649      2.7
        -0.513876      4.107340      2.6
        -1.161172     19.157077      2.5

*N-BLYP.psp
    LMAX=P LOC=P
    72
        -2.430453     -8.542468    -15.1
        -2.225940     -6.920845    -19.4
       -15.363513     -4.369204      1.0
        18.798907     -7.163069     -0.1
        15.784140     -1.848348      1.1
        -5.318093     -1.675672    -18.1
        15.962976     -0.210819     -3.1
        -0.768461     -4.616570     28.4
        -2.645341     -4.291407     -3.2
        -2.877537     -2.705789      1.0
        10.265583     -0.028728    -19.2
        13.809366     -2.747071    -18.1
        17.073925     -6.148305    -19.5
```

Figure 7.43 *"`ATOMS section`" tab in the "`CPMD`" assistant.*

7.2.2 CP2K v9.1

The **atomes** helper for the CP2K calculation offers to prepare input files for **CP2K v9.1**. Please note that the CP2K code offers so many calculation options that it is not possible either to provide a description or to offer a comprehensive usage guide for each of these options. Therefore the CP2K calculation assistant only provides help towards basics and / or frequently used calculation *ab-initio* options.

In any case if you intent to use the CP2K code please refer to the user manual:

https://www.cp2k.org/howto

The **atomes** helper for the CP2K calculation provides a step by step interface to configure the different sections of the CP2K input file(s) for *ab-initio* calculations:

The "`CP2K input structure`" section

The CP2K input can be rather initimidating, you can decide at this stage either to have all input data gathered in a single file, or alternatively split in several, content orientated, files:

The "`GLOBAL`" section

Select the calculation to be performed, and some general options regarding the process. Note that **atomes** provides, when available, basis set(s) and pseudo-potential(s) from the CP2K database. Basis set(s) and pseudopotential(s) will be saved respectively in "`basis.inc`" and "`pseudo.inc`".

The "`FORCE_EVAL`" section

Describe the details of the forces evaluation process.

The "`SUBSYS`" section

The "`MOTION`" section

7.3 Quantum Mechanics and Molecular Mechanics MD

7.3.1 CPMD

Coming soon

7.3.2 CP2K

Coming soon

Appendix

Supported atomic coordinates file formats

The current version of **atomes** can import atomic coordinates in the following formats:

- XYZ [30] *
- Chem3D [31]
- CPMD trajectory [3] * **
- VASP trajectory [32] * ***
- ISAACS Project File [33]
- PDB/ENT (Protein Data Bank) **v3.30**
- CIF (Crystallographic information)
- DL-POLY History file *

Table A.1 *Atomic coordinates file formats read by* **atomes**.

* including NPT trajectories.
** atomic units are assumed in the case of CPMD trajectories.
** and *** require to enter extra parameters through an interactive dialog box:

- Total number of atoms
- Number of chemical species
- Label and number of each atomic species

the input order, label and number of each atomic species will be the one assumed when reading the coordinates from the trajectory file.
atomes can also export atomic coordinates in XYZ or Chem3D format.

Keyboard shortcuts and command line options

B.1 Keyboard shortcuts

- Main window
  - Workspace:

    Ctrl + w : open workspace
    Ctrl + s : save workspace as
    Ctrl + c : close workspace

  - Project:

    Ctrl + n : create new project
    Ctrl + o : open project

  - Misc:

    Ctrl + t : show curve toolboxes
    Ctrl + p : open periodic table
    Ctrl + a : show about dialog
    Ctrl + q : quit

- Curve window:

  Ctrl + a : Autoscale

  Ctrl + c : Close curve window

  Ctrl + e : Open the data plot editing tool box [Fig. 4.6]

  Ctrl + i : Export image

  Ctrl + s : Save / export data

- OpenGL window:
  - Single key shortcuts:
    - Colors:

      a : change atom(s) colormap
      p : change polyhedra(ons) colormap

    - Styles:

      b : change default style to "`Ball and stick`"
      c : change default style to "`Cylinders`"
      d : change default style to "`Dots`"
      s : change default style to "`Spheres`"
      o : change default style to "`Covalent radius`"
      i : change default style to "`Ionic radius`"
      v : change default style to "`van Der Waals radius`"
      r : change default style to "`In cristal radius`"
      w : change default style to "`Wireframe`"

    - Measures:

      m : show all measures for the selection, if pressed:

      - once: display inter-atomic distance(s)
      - twice: display inter-atomic angles
      - a third time: hide measures

    - Misc:

        Esc : exit fullscreen mode
        ␣ : pause / restart spinning

    - Combined keys shortcuts:

        - Mouse mode:

          Alt + a : enter mouse "`Analysis`" mode
          Alt + e : enter mouse "`Edition`" mode

        - Selection:

          Ctrl + a : select / unselect all atoms
          Ctrl + c : copy all selected atom(s)
          Ctrl + n : create new (empty project)

        - Misc:

          Ctrl + l : label / unlabel all atoms
          Ctrl + e : "`Environments configuration`" window [Sec. 5.1.3]
          Ctrl + m : "`Measures`" dialog [Sec. 5.1.4]
          Ctrl + r : "`Recorder`" dialog [Sec. 5.1.6]
          Ctrl + f : enter / exit fullscreen mode

        - Camera motion:

          Shift ⇑ + ↑ : zoom out
          Shift ⇑ + ↓ : zoom in

- OpenGL window **Analysis mode only**

    - Single key shortcuts:

        - Model rotation:

          → : rotate right
          ← : rotate left
          ↑ : rotate up
          ↓ : rotate down

- Combined keys shortcuts:
  - Camera motion:

    Ctrl + → : move camera right
    Ctrl + ← : move camera left
    Ctrl + ↑ : move camera up
    Ctrl + ↓ : move camera down

  - Spinning:

    Ctrl + Shift ⇑ + → : spin right / increase speed r. or reduce speed left
    Ctrl + Shift ⇑ + → : spin left / increase speed left or reduce speed right
    Ctrl + Shift ⇑ + ↑ : spin up / increase speed up or reduce speed down
    Ctrl + Shift ⇑ + ↓ : spin down / increase speed d. or reduce speed up

    Ctrl + s : stop spinning

- OpenGL window: **Edition mode only**
  - Single key shortcuts:
    - Atomic coordinates rotation:

      → : rotate atomic coordinates right
      ← : rotate atomic coordinates left
      ↑ : rotate atomic coordinates up
      ↓ : rotate atomic coordinates down

  - Combined keys shortcuts:
    - Atomic coordinates translation:

      Ctrl + → : translate atomic coordinates right
      Ctrl + ← : translate atomic coordinates left
      Ctrl + ↑ : translate atomic coordinates up
      Ctrl + ↓ : translate atomic coordinates down

B.2 Command line options

atomes can be used from the command line, including using the following options:

- General options:

  "`-h`" or "`-help`": short help.

  "`-v`" or "`-version`": version information.

- File options:

  "`-awf filename`": open **atomes** workspace file.

  "`-apf filename`": open **atomes** project file.

  "`-xyz filename`": open coordinates in XYZ format [30].

  "`-pdb filename`": open coordinates in PDB format.

  "`-ent filename`": open coordinates in PDB format.

  "`-c3d filename`": open coordinates in Chem3D format [31].

  "`-cif filename`": open coordinates in CIF format.

  "`-trj filename`": open CPMD trajectory [3].

  "`-xdatcar filename`": open VASP trajectory [32].

  "`-hist filename`": open DL_POLY history trajectory [1].

  "`-ipf filename`": open ISAACS project file [33].

1. If no file option(s) is (are) provided then **atomes** will try to open the file(s) based on its (their) extension(s) (ex: a file which name end by "`.xyz`" will be assumed to follow the XYZ structure).
2. The structure of "`filename`" is expected to follow the structure introduced with the option (ex: "`-xyz`" for a file that contains coordinates in the XYZ format), but "`filename`" is not required to have the corresponding extention (ex: "`.xyz`").
3. Since **atomes** has a single workspace only a single workspace file can be opened via the command line.

- Examples:

  Open all PDB files in the active directory:

```
user@localhost ~]$ atomes *.pdb
```

  Open a workspace file, and other coordinates files:

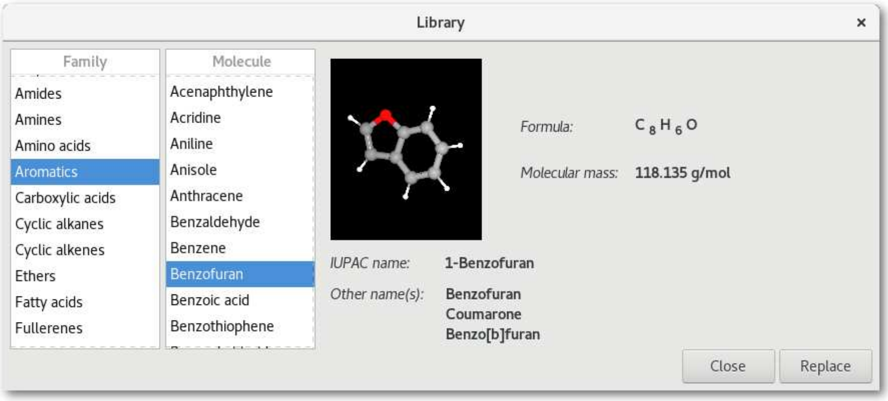
```
user@localhost ~]$ atomes -pdb this.f file.awf -cif that.f *.xyz
```

atomes will parse the command line, detect that a workspace file "`file.awf`" is to be opened and will open it first.
Then the other coordinate files will be opened and added to the workspace:

- As enforced by the "`-pdb`" option, "`this.f`" is supposed to follow the PDB format.
- As enforced by the "`-cif`" option, "`that.f`" is supposed to follow the CIF format.
- All files with the "`.xyz`" extension in the directory will be opened assuming that they follow the XYZ format.

The "`Library`" in atomes

The **atomes** program includes a library with a number of molecules to be used when building or editing atomistic models:



Formula: C_8H_6O

Molecular mass: 118.135 g/mol

IUPAC name: 1-Benzofuran

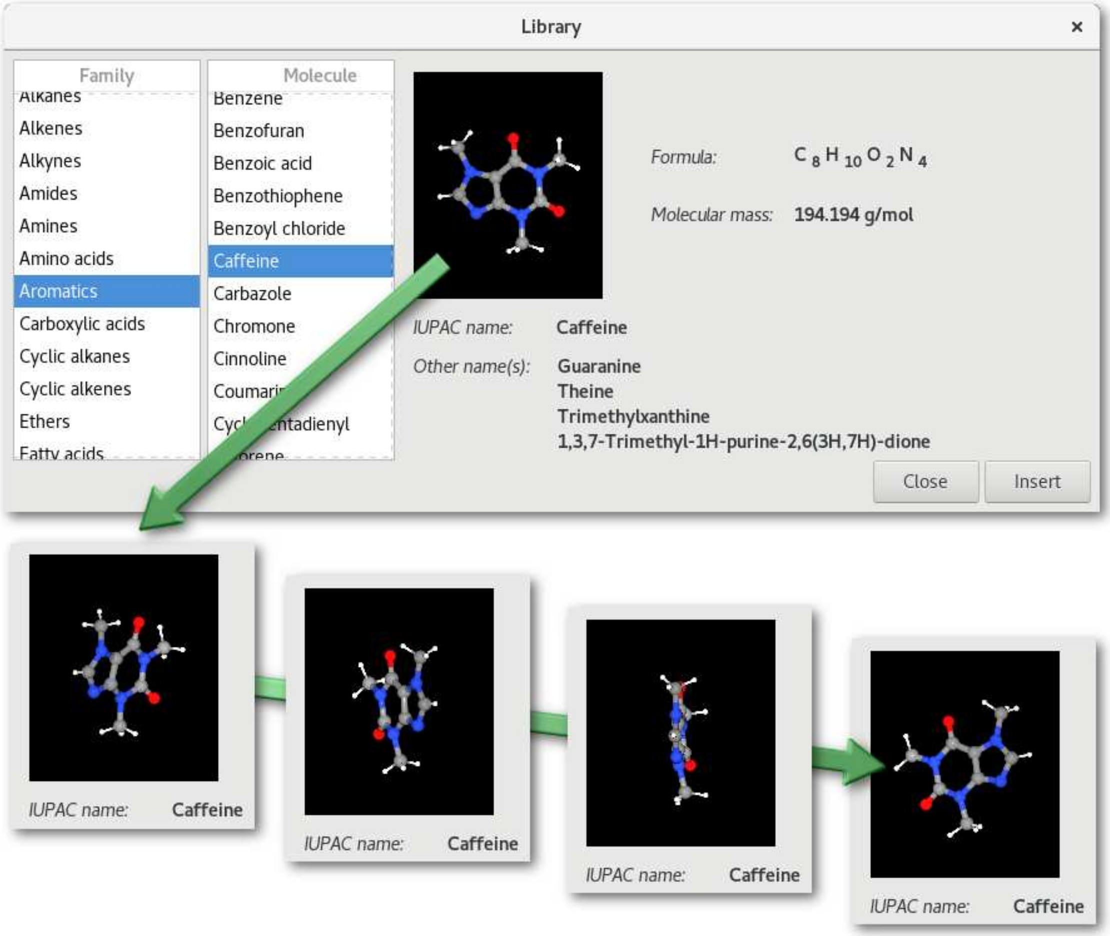
Other name(s): Benzofuran
Coumarone
Benzo[b]furan

Figure C.1 *The "`Library`" dialog of the* **atomes** *program.*

Available molecules can be found in the library by sorted in the following families:

- Misc
- Alcohols
- Aldehydes
- Alkanes
- Alkenes
- Alkynes
- Amides
- Amines
- Amino acids
- Aromatics
- Carboxylic acids
- Cyclic alkanes
- Cyclic alkenes
- Ethers
- Fatty acids
- Fullerenes
- Heterocyclics
- Macrocycles
- Ketones
- Nitriles
- Nucleobases
- Steroids
- Sugars (Linears)
- Sugars (Cyclics)
- Sulfoxides
- Thiols

Each time a new molecule is selected in the tree view on the left side of the window (see figure C.1), then the right side of the "`Library`" dialog is refreshed with the data of the newly selected molecule. The data includes a 3D representation included in an active OpenGL window that allows to rotate the molecule:



Formula: $C_8H_{10}O_2N_4$

Molecular mass: 194.194 g/mol

IUPAC name: Caffeine

Other name(s): Guaranine
Theine
Trimethylxanthine
1,3,7-Trimethyl-1H-purine-2,6(3H,7H)-dione

Figure C.2 *Using the "`Library`" dialog.*

The data files that contain the information regarding each molecule in the library are located in the "`bin/library/molecules`" directory.
To each molecule that appears in the "`Library`" tree view, a file with the "`.sml`" extension can be found in the corresponding family subfolder.
For the example in figure C.2:

- The family is: "`Aromatics`"
- The molecule is: "`Caffeine`"
- The corresponding file is: "`Aromatics/caffeine.sml`".

New files can be added to the library to be found by **atomes** at startup, providing that the new files are added to one of the families of the library. These files must have the "`.sml`" extension, follow the "`XML`" encoding rules, and the following structure:

XIII

The "SCL" "Simple chemical library XML file" format

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- Simple chemical library XML file -->
<scl-xml>
 <class>Aromatics</class>
 <names>
  <library-name>Caffeine</library-name>
  <iupac-name>Caffeine</iupac-name>
  <other-names>
   <name>Guaranine</name>
   <name>Theine</name>
   <name>Trimethylxanthine</name>
   <name>1,3,7-Trimethyl-1H-purine-2,6(3H,7H)-dione</name>
  </other-names>
 </names>
 <chemistry>
  <atoms>24</atoms>
  <species number="4">
   <label id="0" num="8">C</label>
   <label id="1" num="10">H</label>
   <label id="2" num="2">O</label>
   <label id="3" num="4">N</label>
  </species>
 </chemistry>
 <coordinates>
   <atom id="1" sp="0" x="1.785021" y="-0.779129" z="-0.255949"/>
   <atom id="2" sp="0" x="0.401929" y="1.318216" z="-0.016004"/>
   <atom id="3" sp="0" x="-0.733464" y="0.413478" z="0.038347"/>
   <atom id="4" sp="0" x="-0.617909" y="-0.973998" z="-0.109571"/>
   <atom id="5" sp="0" x="-2.772439" y="-0.562269" z="0.209813"/>
   <atom id="6" sp="0" x="0.735608" y="-3.069196" z="-0.210904"/>
   <atom id="7" sp="0" x="-2.730788" y="1.961282" z="0.459758"/>
   <atom id="8" sp="0" x="2.908891" y="1.458603" z="-0.240195"/>
   <atom id="9" sp="1" x="-3.848274" y="-0.720508" z="0.332764"/>
   <atom id="10" sp="1" x="1.561100" y="-3.446348" z="-0.829847"/>
   <atom id="11" sp="1" x="-0.192018" y="-3.562176" z="-0.530166"/>
   <atom id="12" sp="1" x="0.935512" y="-3.340819" z="0.835372"/>
   <atom id="13" sp="1" x="-2.333498" y="2.706064" z="-0.245137"/>
   <atom id="14" sp="1" x="-2.525360" y="2.320312" z="1.478733"/>
   <atom id="15" sp="1" x="-3.818507" y="1.892617" z="0.326144"/>
   <atom id="16" sp="1" x="3.674681" y="0.991531" z="-0.874770"/>
   <atom id="17" sp="1" x="3.303682" y="1.537341" z="0.782105"/>
   <atom id="18" sp="1" x="2.721889" y="2.471199" z="-0.622647"/>
   <atom id="19" sp="2" x="2.892437" y="-1.297551" z="-0.212698"/>
   <atom id="20" sp="2" x="0.363733" y="2.532611" z="0.115710"/>
   <atom id="21" sp="3" x="1.659632" y="0.660920" z="-0.271271"/>
   <atom id="22" sp="3" x="0.612806" y="-1.608906" z="-0.393730"/>
   <atom id="23" sp="3" x="-2.109760" y="0.657267" z="0.234906"/>
   <atom id="24" sp="3" x="-1.874903" y="-1.560540" z="-0.000764"/>
 </coordinates>
</scl-xml>
```

Table C.1 *Example of "`sml`" file in XML format for caffeine.*

Crystal building in atomes

The crystal building process in **atomes** will be briefly presented in the next pages. 2 example cases will be used to illustrate the methodology implemented in the program:

1. The Fd$\bar{3}$m space group, N°227, with the first setting: origin 1.
2. The R$\bar{3}$c space group, N°167, with the second setting: rhombohedral parameters.

The terminology used in the **atomes** program, and therefore used in this manual, is directly taken from the International tables for Crystallography Vol. A. [29]
In the following every single step depends on the considered space group, and corresponds to the way the process is implemented in **atomes**:

1. Determine the origin of the coordinate system.
2. Calculate the inverse transformation matrix.
3. Select the space group extra site positions, if any.
4. Adjust the different symmetrical positions of the first Wyckoff position using 2.
5. Calculate the crystalline positions using 4 and 3.
6. Select the unique position(s) in 5 to build the crystal.
7. Calculate the object position in Cartesian coordinates using 6.
8. Insert object(s) at the appropriate coordinates based on occupancy.

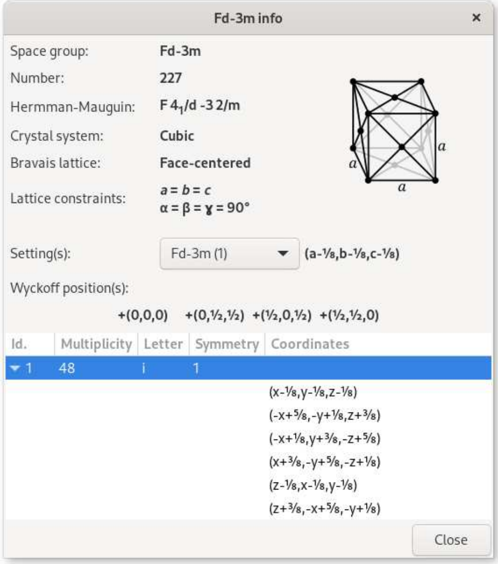
Origin of the coordinate system

The origin of the coordinate system, if any particular, determine how the object fractional coordinates are modified to match the space group criteria before calculating the Cartesian coordinates.

The first step is to build the 4×3 matrix that describe the operation of be performed, the required information is given by the space group setting, the easiest way to use it is on the form of the transformation matrix **P**:
Ex: (**a, b, c**) and can be converted in:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{D.1}$$

(1) Fd$\bar{3}$m space group, N°227, origin 1:



Fd-3m info ×

Space group: Fd-3m
Number: 227
Hermman-Mauguin: F 4₁/d -3 2/m
Crystal system: Cubic
Bravais lattice: Face-centered
Lattice constraints: a = b = c
α = β = γ = 90°

Setting(s): Fd-3m (1) ▾ (a-⅛,b-⅛,c-⅛)

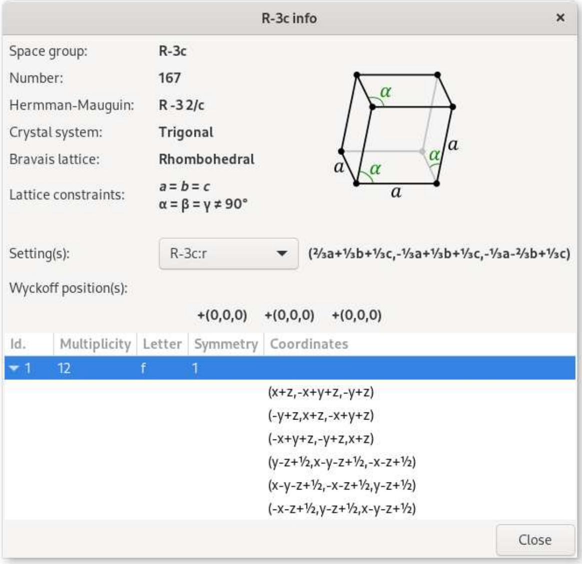
Wyckoff position(s):

+(0,0,0) +(0,½,½) +(½,0,½) +(½,½,0)

Id.	Multiplicity	Letter	Symmetry	Coordinates
▾ 1	48	i	1	
				(x-⅛,y-⅛,z-⅛)
				(-x+⅝,-y+⅛,z+⅜)
				(-x+⅛,y+⅜,-z+⅝)
				(x+⅜,-y+⅝,-z+⅛)
				(z-⅛,x-⅛,y-⅛)
				(z+⅜,-x+⅝,-y+⅛)

($\mathbf{a}$-$\frac{1}{8}$, $\mathbf{b}$-$\frac{1}{8}$, $\mathbf{c}$-$\frac{1}{8}$)

(2) R$\bar{3}$c space group, N°167, second setting:



R-3c info ×

Space group: R-3c
Number: 167
Hermman-Mauguin: R -3 2/c
Crystal system: Trigonal
Bravais lattice: Rhombohedral
Lattice constraints: a = b = c
α = β = γ ≠ 90°

Setting(s): R-3c:r ▾ (⅔a+⅓b+⅓c,-⅓a+⅓b+⅓c,-⅓a-⅔b+⅓c)

Wyckoff position(s):

+(0,0,0) +(0,0,0) +(0,0,0)

Id.	Multiplicity	Letter	Symmetry	Coordinates
▾ 1	12	f	1	
				(x+z,-x+y+z,-y+z)
				(-y+z,x+z,-x+y+z)
				(-x+y+z,-y+z,x+z)
				(y-z+½,x-y-z+½,-x-z+½)
				(x-y-z+½,-x-z+½,y-z+½)
				(-x-z+½,y-z+½,x-y-z+½)

($\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}+\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}+\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}$-$\frac{2}{3}\mathbf{b}+\frac{1}{3}\mathbf{c}$)

The corresponding **P** matrix are:

$$\begin{bmatrix} 1 & 0 & 0 & -\frac{1}{8} \\ 0 & 1 & 0 & -\frac{1}{8} \\ 0 & 0 & 1 & -\frac{1}{8} \end{bmatrix} \qquad \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \end{bmatrix}$$

Inverse transformation matrix

To transform the coordinates to the appropriate system we use the corresponding inverse matrix $\mathbf{P}^{-1}$:

(1) Fd$\bar{3}$m space group, N°227, origin 1: **(2)** R$\bar{3}$c space group, N°167, second setting:

$$\begin{bmatrix} 1 & 0 & 0 & -\frac{1}{8} \\ 0 & 1 & 0 & -\frac{1}{8} \\ 0 & 0 & 1 & -\frac{1}{8} \end{bmatrix} \qquad \begin{bmatrix} 1 & 0 & 1 & 0 \\ -1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \end{bmatrix}$$

The $\mathbf{P}^{-1}$ matrix allows to easily compute the coordinates (x',y',z') of a point (x,y,z) in the appropriate coordinate system using:

$$(x',y',z') = \mathbf{P}^{-1} \times (x,y,z) \tag{D.2}$$

Space group extra site position(s)

The space group extra site position(s) describe translations to be performed on the initial set of Wyckoff position to get the entire list of coordinates.
The list of extra position(s), $E(e_x, e_y, e_z)$, is imported from the space group data file, and is presented on top the Wyckoff positions table of the space group info window:

(1) Fd$\bar{3}$m space group, N°227, origin 1:

$$+(0,0,0)+(0,\tfrac{1}{2},\tfrac{1}{2})+(\tfrac{1}{2},0,\tfrac{1}{2})+(\tfrac{1}{2},\tfrac{1}{2},0)$$

(2) R$\bar{3}$c space group, N°167, second setting:

$$+(0,0,0)+(0,0,0)+(0,0,0)$$

Symmetrical positions using the first Wyckoff position

The first step is to convert the list of coordinates from the first Wyckoff position on the form of matrix **W**:

(1) Fd$\bar{3}$m space group, N°227, origin 1:

(x, y, z)

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

(2) R$\bar{3}$c space group, N°167, second setting:

(x, y, z)

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

The $\mathbf{W'}$ matrix, suitable for the calculation, is calculated using the $\mathbf{P}^{-1}$ matrix for the corresponding space group:

$$\mathbf{W'} = \mathbf{W} \times \mathbf{P}^{-1} \tag{D.3}$$

(1) Fd$\bar{3}$m space group, N°227, origin 1:

$$\begin{bmatrix} 1 & 0 & 0 & -\frac{1}{8} \\ 0 & 1 & 0 & -\frac{1}{8} \\ 0 & 0 & 1 & -\frac{1}{8} \end{bmatrix}$$

(2) R$\bar{3}$c space group, N°167, second setting:

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \end{bmatrix}$$

The results, converted back to standard coordinates, are presented in the Wyckoff positions table of the space group info window:

(1) Fd$\bar{3}$m space group, N°227, origin 1:

$$(x-\tfrac{1}{8}, y-\tfrac{1}{8}, z-\tfrac{1}{8})$$
$$\cdots$$

(2) R$\bar{3}$c space group, N°167, second setting:

$$(x+z, -x+y+z, -y+z)$$
$$\cdots$$

Object position(s)

The first step in getting the final fractional coordinates $F(f_x, f_y, f_z)$ of an object to insert with fractional coordinates given at input $O(o_x, o_y, o_z)$ is to convert its coordinates to the proper coordinates system $O'(o'_x, o'_y, o'_z)$:

$$O'(o'_x, o'_y, o'_z) = \mathbf{P} \times O(o_x, o_y, o_z) \tag{D.4}$$

Then for a particular Wyckoff position $\mathbf{W'}$ and extra site position $E(x,y,z)$, the final fractional coordinates $F(f_x,f_y,f_z)$ are calculated by:

$$F(f_x,f_y,f_z) = E(e_x,e_y,e_z) + \mathbf{W'} \times O'(o'_x,o'_y,o'_z) \tag{D.5}$$

Removing duplicate position(s)

Since one of the goal in **atomes** is to build crystal structure of super-structure to work with, all crystalline positions cannot be conserved and duplicate positions (same positions using the periodic boundary conditions) must be removed.
When final positions $F(f_x,f_y,f_z)$ are calculated duplicates are removed on the fly. The first final position with a unique set of coordinates $F(f_x,f_y,f_z)$ is preserved while the others will be ignored. Duplicates are identical set of atomic coordinates, that can be found because of the symmetrical properties of the space group.
In **atomes** a duplicate position $F_b(b_x,b_y,b_z)$ will be removed if $F_a(a_x,a_y,a_z)$ has already been found and providing that:

$$\begin{array}{rl} & \Big[a_x = b_x \ \textbf{or}\ abs(a_x-b_x) = n, n \text{ integer}\Big] \\ \textbf{and} & \Big[a_y = b_y \ \textbf{or}\ abs(a_y-b_y) = n, n \text{ integer}\Big] \\ \textbf{and} & \Big[a_z = b_z \ \textbf{or}\ abs(a_z-b_z) = n, n \text{ integer}\Big] \end{array}$$

Calculate the object final position(s) in Cartesian coordinates

After the construction/selection process Cartesian coordinates $C(c_x,c_y,c_z)$ of an object with fractional coordinates $F(f_x,f_y,f_z)$ are calculated using:

$$C(c_x,c_y,c_z) = \mathbf{FtC} \times F(f_x,f_y,f_z) \tag{D.6}$$

with **FtC** the fractional to Cartesian conversion matrix is defined by:

$$\begin{bmatrix} \mathbf{a} & \mathbf{b}\cos\gamma & \mathbf{c}\cos\beta \\ 0 & \mathbf{b}\sin\gamma & \mathbf{c}\omega \\ 0 & 0 & \frac{\Omega}{\mathbf{ab}\sin\gamma} \end{bmatrix} \tag{D.7}$$

where ω and Ω are respectively:

$$\omega = \frac{\cos\alpha - \cos\beta\cos\gamma}{\sin\gamma} \tag{D.8}$$

and:

$$\Omega = \mathbf{abc}\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma} \tag{D.9}$$

a, b, c and α, β, γ are the lattice parameters provided at input.

Occupancy

The only thing left to do after that it to select which set of coordinates are to be occupied among the list prepared in the previous steps. Depending on the occupancy defined at input **atomes** does the following:

- If the occupancy is equal to 1.0: all coordinates are to be occupied and no particular selection is performed.
- If the occupancy is < 1.0, then the following options are possible to handle occupancy:
  1. "`Random for the initial cell only`": sites are filled randomly in the initial cell only, then the initial cell is simply replicated.
  2. "`Random cell by cell`": sites are filled randomly for each cell, cell by cell separately.
  3. "`Completely random`": sites are filled randomly for the entire network, the final crystal is considered as whole.
  4. "`Successively`": sites are filled successively, all object(s) A are inserted (for the first $n(A)$ positions), then all object(s) B are inserted (for the next $n(B)$ positions) ...
  5. "`Alternatively`": sites are filled alternatively: object A is inserted on the first position, object B is inserted on the second position, object A on the third position, object B on the fourth position ... and so on.

  For 1, 2, 4 and 5 the number of object(s) by cell is constant, but it can vary for 3. For 4 and 5 the order of the positions to be filled is the order they are found in during the previous steps.

Final check: distance(s) between inserted objects

Finally the last calculation performed by **atomes** when creating the crystal is distance check between the object(s) be inserted. Note that this check performed, if and only if, no *overlapping* is allowed.
If any distance d_{ab} between 2 objects a and b, is found to be *too small* the following can happen:

1. If $d_{ab} < 0.5$ Å then a warning message will pop-up and ask for the user confirmation to continue, or not, to build the crystal.
2. If the user decides to build the crystal anyway and if $d_{ab} = 0.0$ then for fail safe reasons object b is removed from the list to build.

The "SGL" "Space group info XML file" format

The data files that contain the information regarding each of the 230 space groups are located in the "`bin/library/space_groups`" directory.

In this folder to each space group corresponds a file with a name following the construction:

`"space group number"-"space group name"."sgl"`

For the Fd$\bar{3}$m space group, the corresponding file is "`227-Fd-3m.sgl`".
These files must have the "`.sgl`" extension, follow the "`XML`" encoding rules, and the following structure:

```xml
<?xml version="1.0" encoding="UTF-8"?>
<!-- Space group info XML file -->
<sg-xml>
  <space-group>R-3c</space-group>
  <sg-num>167</sg-num>
  <hm-symbol>R -3 2/c</hm-symbol>
  <bravais>Trigonal</bravais>
  <settings num="2">
    <set name="R_-3_c_:h" x="a" y="b" z="c">
      <points num="3">
        <pt x="0" y="0" z="0"/>
        <pt x="2/3" y="1/3" z="1/3"/>
        <pt x="1/3" y="2/3" z="2/3"/>
      </points>
    </set>
    <set name="R_-3_c_:r" x="2/3a+1/3b+1/3c" y="-1/3a+1/3b+1/3c" z="-1/3a-2/3b+1/3c">
      <points num="3">
        <pt x="0" y="0" z="0"/>
        <pt x="0" y="0" z="0"/>
        <pt x="0" y="0" z="0"/>
      </points>
    </set>
  </settings>
  <wyckoff num="6">
    <wyck id="1" mul="12" let="f" site="1">
      <pos x="x" y="y" z="z"/>
      <pos x="-y" y="x-y" z="z"/>
      <pos x="-x+y" y="-x" z="z"/>
      <pos x="y" y="x" z="-z+1/2"/>
      <pos x="x-y" y="-y" z="-z+1/2"/>
      <pos x="-x" y="-x+y" z="-z+1/2"/>
      <pos x="-x" y="-y" z="-z"/>
      <pos x="y" y="-x+y" z="-z"/>
      <pos x="x-y" y="x" z="-z"/>
      <pos x="-y" y="-x" z="z+1/2"/>
      <pos x="-x+y" y="y" z="z+1/2"/>
      <pos x="x" y="x-y" z="z+1/2"/>
    </wyck>
    <wyck id="2" mul="6" let="e" site=".2">
      <pos x="x" y="0" z="1/4"/>
      <pos x="0" y="x" z="1/4"/>
      <pos x="-x" y="-x" z="1/4"/>
      <pos x="-x" y="0" z="3/4"/>
      <pos x="0" y="-x" z="3/4"/>
      <pos x="x" y="x" z="3/4"/>
    </wyck>
    <wyck id="3" mul="6" let="d" site="-1">
      <pos x="1/2" y="0" z="0"/>
      <pos x="0" y="1/2" z="0"/>
      <pos x="1/2" y="1/2" z="0"/>
      <pos x="0" y="1/2" z="1/2"/>
      <pos x="1/2" y="0" z="1/2"/>
      <pos x="1/2" y="1/2" z="1/2"/>
    </wyck>
    <wyck id="4" mul="4" let="c" site="3.">
      <pos x="0" y="0" z="z"/>
      <pos x="0" y="0" z="-z+1/2"/>
      <pos x="0" y="0" z="-z"/>
      <pos x="0" y="0" z="z+1/2"/>
    </wyck>
    <wyck id="5" mul="2" let="b" site="-3.">
      <pos x="0" y="0" z="0"/>
      <pos x="0" y="0" z="1/2"/>
    </wyck>
    <wyck id="6" mul="2" let="a" site="32">
      <pos x="0" y="0" z="1/4"/>
      <pos x="0" y="0" z="3/4"/>
    </wyck>
  </wyckoff>
</sg-xml>
```

Table D.1 *Example of the "`167-R-3c.sgl`" file in XML format for the R$\bar{3}$c space group.*

The physics in atomes

E.1 The periodic boundary conditions

Taking into account the finite size of model/simulation box is crucial to compute correctly many of the structural characteristics (e.g. ring statistics) of the system being studied.
The importance of the finite size of model box can be illustrated using a 1 dm^3 edged cube of water (1 L) at room temperature. This cube contains approximately 3.3×10^{25} water molecules, each of them can be considered as a sphere having a diameter of 2.8 Å. Following this scheme surface interactions can affect up to 10 layers of spheres (water molecules) far from the surface of the model cubic box. In this case the number of water molecules exposed to the surface is about 2×10^{19}, which is a small fraction of the total number of molecules in the model.
Currently structure models often contain somewhere from 1 thousand to several thousands of molecules/atoms. As a result a very substantial fraction of them will be influenced by the finite size of the simulation/model box. The problems is solved by applying the so-called **P**eriodic **B**oundary **C**onditions "PBC" which means surrounding the simulation box with its translational images in the 3 directions of space, as illustrated below.

Users of **atomes** should take special care that their model boxes are inherently periodic so that when the periodic boundary conditions are applied the structural characteristics computed are not compromised.

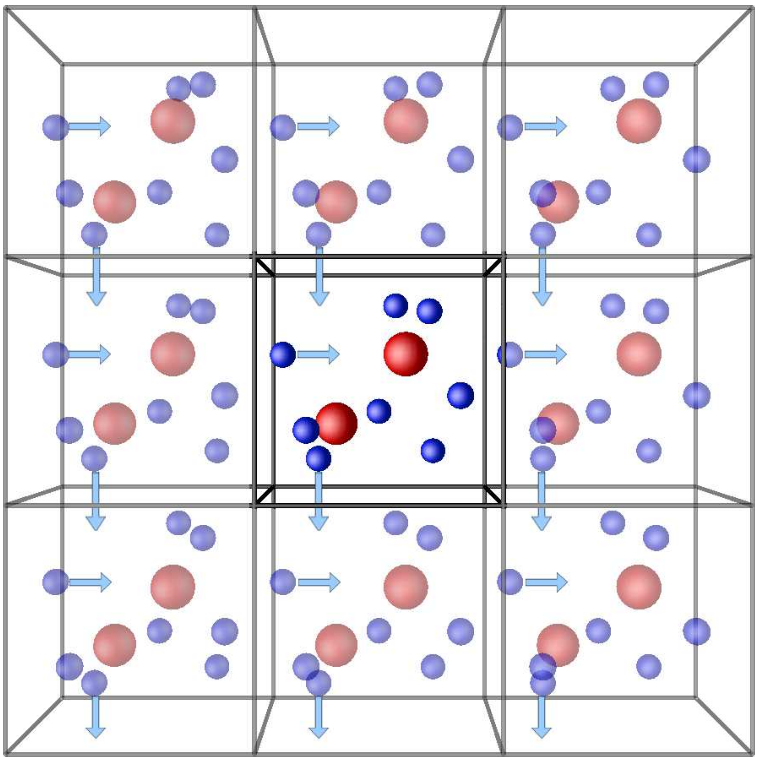


Figure E.1 *Schematic representation of the idea of periodic boundary conditions.*

Figure E.1 illustrates the principle of the periodic boundary conditions that can be used[1] in **atomes**: a particle which goes out from the simulation box by one side is reintroduced in the box by the opposite side (in the 3 dimensions of space).

When PBC are used the maximum inter-atomic distance r_{max} which is taken into account in the calculations, depends on the lattice parameters:

$$r_{max} \simeq \frac{L \times \sqrt{3}}{2} \qquad \text{with } L = \text{box size} \tag{E.1}$$

The surface/finite model size effects would therefore be small, if any. In general, the larger the simulation box and the number of molecules/atoms in it, the smaller the surface/size effects will be.

---

[1] Please note that the use of PBC is not mandatory, isolated molecules can be studied using **atomes**

E.2 Radial distribution functions

The Radial Distribution Function, R.D.F. , g(r), also called pair distribution function or pair correlation function, is an important structural characteristic, therefore computed by **atomes**.

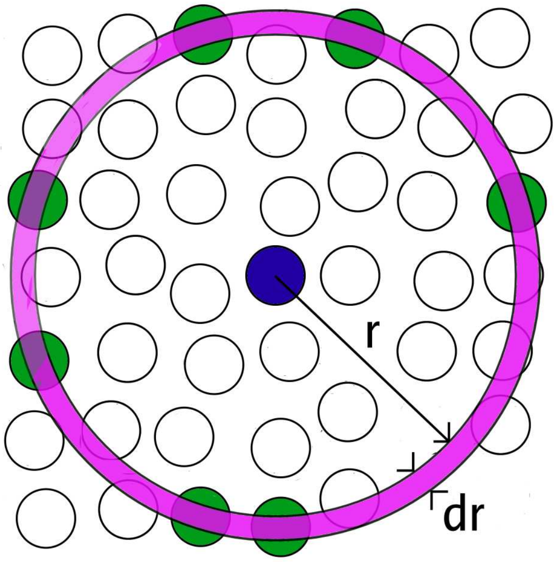


Figure E.2 *Space discretization for the evaluation of the radial distribution function.*

Considering a homogeneous distribution of the atoms/molecules in space, the $g(r)$ represents the probability to find an atom in a shell dr at the distance r of another atom chosen as a reference point [Fig. E.2]. By dividing the physical space/model volume into shells dr [Fig. E.2] it is possible to compute the number of atoms $dn(r)$ at a distance between r and $r+dr$ from a given atom:

$$dn(r) = \frac{N}{V} g(r)\, 4\pi\, r^2\, dr \tag{E.2}$$

where N represents the total number of atoms, V the model volume and where $g(r)$ is the radial distribution function. In this notation the volume of the shell of thickness dr is approximated:

$$\left(V_{\text{shell}} = \frac{4}{3}\pi(r+dr)^3 - \frac{4}{3}\pi r^3 \simeq 4\pi\, r^2\, dr\right) \tag{E.3}$$

When more than one chemical species are present the so-called partial radial distribution functions $g_{\alpha\beta}(r)$ may be computed :

$$g_{\alpha\beta}(r) = \frac{dn_{\alpha\beta}(r)}{4\pi r^2\, dr\, \rho_\alpha} \qquad \text{with} \qquad \rho_\alpha = \frac{N_\alpha}{V} = \frac{N \times c_\alpha}{V} \tag{E.4}$$

where c_α represents the concentration of atomic species α.

These functions give the density probability for an atom of the α species to have a neighbor of the β species at a given distance r. The example features GeS_2 glass.

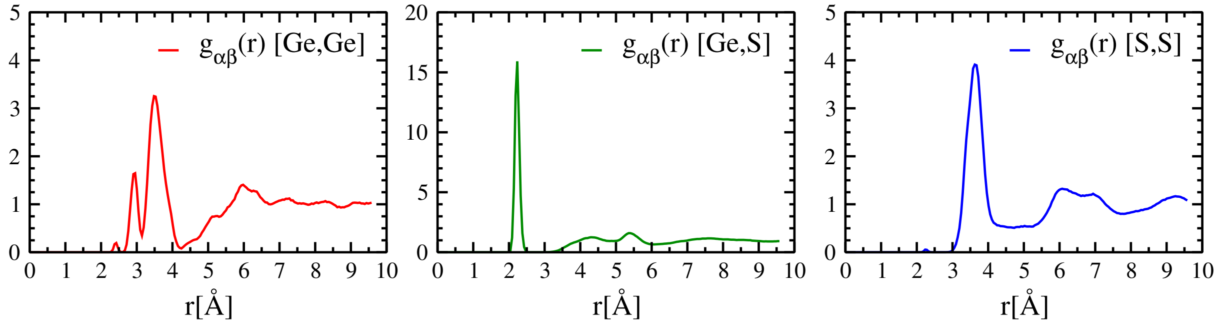


Figure E.3 *Partial radial distribution functions of glassy GeS_2 at 300 K.*

Figure E.3 shows the partial radial distribution functions for GeS_2 glass at 300 K. The total RDF of a system is a weighted sum of the respective partial RDFs, with the weights depend on the relative concentration and x-ray/neutron scattering amplitudes of the chemical species involved.
It is also possible to use the reduced $\mathbf{G}_{\alpha\beta}(r)$ partial distribution functions defined as:

$$\mathbf{G}_{\alpha\beta}(r) = 4\pi r \rho_0 \left(g_{\alpha\beta}(r) - 1 \right) \tag{E.5}$$

atomes gives access to:

- The partial $g_{\alpha\beta}(r)$ and $\mathbf{G}_{\alpha\beta}(r)$ distribution functions, and more see [Eq.E.14].
- The corresponding $dn_{\alpha\beta}(r)$ integrated number of neighbors.

Also two methods are available to compute the radial distribution functions:

- The standard real space calculation typical to analyze 3-dimensional models
- The experiment-like calculation using the Fourier transform of the structure factor obtained using the Debye equation (see section E.3 for details).

E.3 Neutrons and X-rays scattering

Model static structure factors $S(q)$ may be compared to experimental scattering data and that is why are useful structural characteristics computed by **atomes**Thereafter we describe the theoretical background of $S(q)$s computed by **atomes**

E.3.1 Total scattering - Debye approach

Neutron or X-ray scattering static structure factor $S(q)$ is defined as:

$$S(q) = \frac{1}{N}\sum_{j,k} b_j b_k \left\langle e^{iq[\mathbf{r}_j - \mathbf{r}_k]} \right\rangle \tag{E.6}$$

where b_j and $\mathbf{r}_j$ represent respectively the neutron or X-ray scattering length, and the position of the atom j. N is the total number of atoms in the system studied.
To take into account the inherent/volume averaging of scattering experiments it is necessary to sum all possible orientations of the wave vector q compared to the vector $\mathbf{r}_j - \mathbf{r}_k$. This average on the orientations of the q vector leads to the famous Debye's equation:

$$S(q) \;=\; \frac{1}{N}\sum_{j,k} b_j b_k \frac{\sin(q|\mathbf{r}_j - \mathbf{r}_k|)}{q|\mathbf{r}_j - \mathbf{r}_k|} \tag{E.7}$$

Nevertheless the instantaneous individual atomic contributions introduced by this equation E.7 are not easy to interpret. It is more interesting to express these contributions using the formalism of radial distribution functions [Sec. E.2].
In order to achieve this goal it is first necessary to split the self-atomic contribution ($j = k$), from the contribution between distinct atoms:

$$S(q) \;=\; \sum_j c_j b_j^2 \;+\; \underbrace{\frac{1}{N}\sum_{j \neq k} b_j b_k \frac{\sin(q|\mathbf{r}_j - \mathbf{r}_k|)}{q|\mathbf{r}_j - \mathbf{r}_k|}}_{I(q)} \qquad \text{with} \qquad c_j = \frac{N_j}{N} \tag{E.8}$$

where $4\pi\,\sum_j c_j b_j^2$ represents the total scattering cross section of the material.
The function $I(q)$ which describes the interaction between distinct atoms is related to the radial distribution functions through a Fourier transformation:

$$I(q) \;=\; 4\pi\rho \int_0^{\infty} dr\, r^2\, \frac{\sin qr}{qr}\, G(r) \tag{E.9}$$

where the function $G(r)$ is defined using the partial radial distribution functions [Eq. E.4]:

$$G(r) \;=\; \sum_{\alpha,\beta} c_\alpha b_\alpha\, c_\beta b_\beta\, (g_{\alpha\beta}(r) - 1) \tag{E.10}$$

where $c_\alpha = \frac{N_\alpha}{N}$ and b_α represents the neutron or X-ray scattering length of species α.
$G(r)$ approaches - $-\sum_{\alpha,\beta} c_\alpha b_\alpha\, c_\beta b_\beta$ for $r = 0$, and 0 for $r \to \infty$.

Usually the self-contributions are subtracted from equation E.8 and the structure factor is normalized using the relation:

$$S(q) - 1 = \frac{I(q)}{\langle b^2 \rangle} \quad \text{with} \quad \langle b^2 \rangle = \left(\sum_{\alpha} c_\alpha b_\alpha \right)^2 \tag{E.11}$$

It is therefore possible to write the structure factor [Eq. E.7] in a more standard way:

$$S(q) = 1 + 4\pi\rho \int_0^\infty dr\, r^2 \frac{\sin qr}{qr} (\mathbf{g}(r) - 1) \tag{E.12}$$

where $\mathbf{g}(r)$ (the radial distribution function) is defined as:

$$\mathbf{g}(r) = \frac{\displaystyle\sum_{\alpha,\beta} c_\alpha b_\alpha \, c_\beta b_\beta \, g_{\alpha\beta}(r)}{\langle b^2 \rangle} \tag{E.13}$$

In the case of a single atomic species system the normalization allows to obtain values of $S(q)$ and $\mathbf{g}(r)$ which are independent of the scattering factor/length and therefore independent of the measurement technique. In most cases, however, the total $S(q)$ and $\mathbf{g}(r)$ are combinations of the partial functions weighted using the scattering factor and therefore depend on the measurement technique (Neutron, X-rays ...) used or simulated.

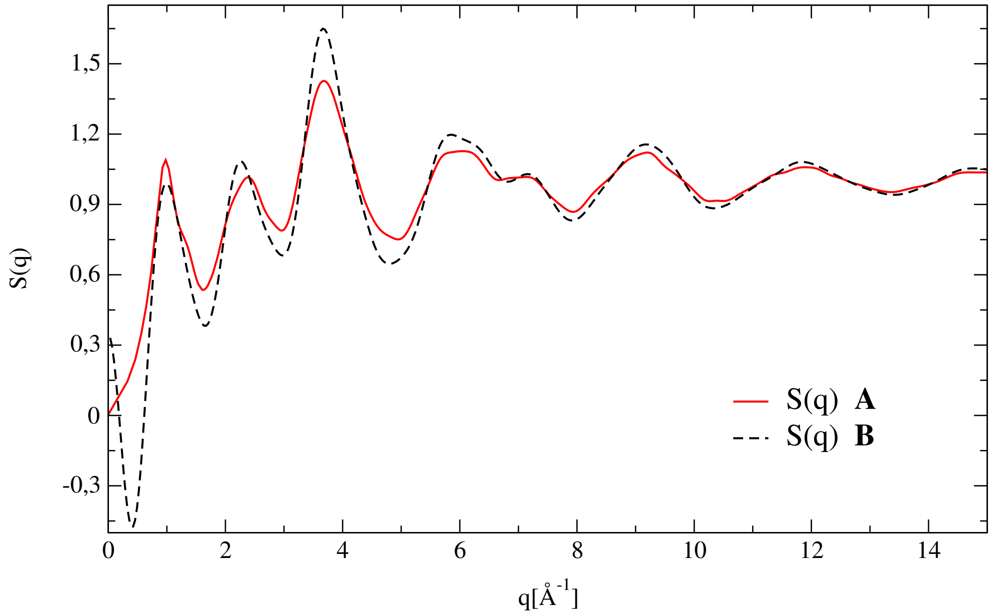


Figure E.4 *Total neutron structure factor for glassy GeS_2 at 300 K -* **A** *Evaluation using the atomic correlations [Eq. E.7],* **B** *Evaluation using the pair correlation functions [Eq. E.12].*

Figure E.4 presents a comparison between the calculations of the total neutron structure factor done using the Debye relation [Eq. E.7] and the pair correlation functions

[Eq. E.12]. The material studied is a sample of glassy GeS_2 at 300 K obtained using ab-initio molecular dynamics. In several cases the structure factor $S(q)$ and the radial distribution function $\mathbf{g}(r)$ [Eq. E.13] can be compared to experimental data. To simplify the comparison **atomes** computes several radial distribution functions used in practice such as $G(r)$ defined [Eq. E.10], the differential correlation function $D(r)$, $\mathbf{G}(r)$, and the total correlation function $T(r)$ defined by:

$$\begin{aligned} D(r) &= 4\pi r\rho\, G(r) \\ \mathbf{G}(r) &= \frac{D(r)}{\langle b^2 \rangle} \\ T(r) &= D(r) + 4\pi r\rho\, \langle b^2 \rangle \end{aligned} \tag{E.14}$$

$\mathbf{g}(r)$ equals zero for $r = 0$ and approaches 1 for $r \to \infty$.
$D(r)$ equals zero for $r = 0$ and approaches 0 for $r \to \infty$.
$\mathbf{G}(r)$ equals zero for $r = 0$ and approaches 0 for $r \to \infty$.
$T(r)$ equals zero for $r = 0$ and approaches ∞ for $r \to \infty$.

This set of functions for a model of GeS_2 glass (at 300 K) obtained using ab-initio molecular dynamics is presented in figure E.5.

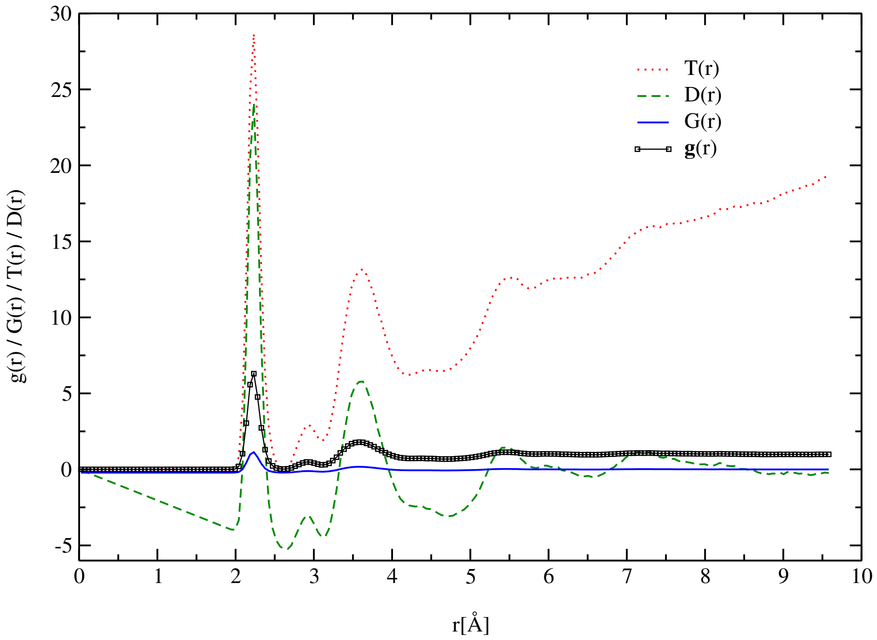


Figure E.5 *Example of various distribution functions neutron-weighted in glassy* GeS_2 *at 300 K.*

atomes can compute, for the case of **x-rays** and/or **neutrons**, the following functions:

- $S(q)$ and $Q(q) = q[S(q) - 1.0]$ [12, 13] computed using the Debye equation
- $S(q)$ and $Q(q) = q[S(q) - 1.0]$ [12, 13] computed using the Fourier transform of $\mathbf{g}(r)$
- $\mathbf{g}(r)$, $\mathbf{G}(r)$, $D(r)$ and $T(r)$ computed using the standard real space calculation
- $\mathbf{g}(r)$, $\mathbf{G}(r)$, $D(r)$ and $T(r)$ computed using the Fourier transform of Debye $S(q)$

E.3.2 Partial structure factors

There are a few, somewhat different definitions of partials $S(q)$ used in practice, and computed by **atomes**

E.3.2.1 Faber-Ziman definition/formalism

One way used to define the partial structure factors has been proposed by Faber and Ziman [14]. In this approach the structure factor is represented by the correlations between the different chemical species. To describe the correlation between the α and the β chemical species the partial structure factor $S_{\alpha\beta}^{FZ}(q)$ is defined by:

$$S_{\alpha\beta}^{FZ}(q) = 1 + 4\pi\rho \int_0^\infty dr\, r^2 \frac{\sin qr}{qr} \left(g_{\alpha\beta}(r) - 1\right) \tag{E.15}$$

where the $g_{\alpha\beta}(r)$ are the partial radial distribution functions [Eq. E.4].
The total structure factor is then obtained by the relation:

$$S(q) = \sum_{\alpha,\beta} c_\alpha b_\alpha\, c_\beta b_\beta \left[S_{\alpha\beta}^{FZ}(q) - 1\right] \tag{E.16}$$

E.3.2.2 Ashcroft-Langreth definition/formalism

In a similar approach, based on the correlation between the chemical species, and developed by Ashcroft and Langreth [15, 16, 17], the partial structure factors $S_{\alpha\beta}^{AL}(q)$ are defined by:

$$S_{\alpha\beta}^{AL}(q) = \delta_{\alpha\beta} + 4\pi\rho\left(c_\alpha c_\beta\right)^{1/2} \int_0^\infty dr\, r^2 \frac{\sin qr}{qr} \left(g_{\alpha\beta}(r) - 1\right) \tag{E.17}$$

where $\delta_{\alpha\beta}$ is the Kronecker delta, $c_\alpha = \frac{N_\alpha}{N}$, and the $g_{\alpha\beta}(r)$ are the partial radial distribution functions [Eq. E.4].
Then the total structure factor can be calculated using:

$$S(q) = \frac{\sum_{\alpha,\beta} b_\alpha b_\beta \left(c_\alpha c_\beta\right)^{1/2} \left[S_{\alpha\beta}^{AL}(q) + 1\right]}{\sum_\alpha c_\alpha b_\alpha^2} \tag{E.18}$$

E.3.2.3 Bhatia-Thornton definition/formalism

In this approach, used in the case of binary systems AB$_x$ [18] only, the total structure factor $S(q)$ can be express as the weighted sum of 3 partial structure factors:

$$S(q) = \frac{\langle b\rangle^2 S_{NN}(q) + 2\langle b\rangle(b_\text{A} - b_\text{B})S_{NC}(q) + (b_\text{A} - b_\text{B})^2 S_{CC}(q) - (c_\text{A}b_\text{A}^2 + c_\text{B}b_\text{B}^2)}{\langle b\rangle^2} + 1 \tag{E.19}$$

where $\langle b\rangle = c_\text{A}b_\text{A} + c_\text{B}b_\text{B}$, with c_A and b_A representing respectively the concentration and the scattering length of species A.
$S_{NN}(q)$, $S_{NC}(q)$ and $S_{CC}(q)$ represent combinations of the partial structure factors calculated using the Faber-Ziman formalism and weighted using the concentrations of the 2 chemical species:

$$S_{NN}(q) = \sum_{\text{A}=1}^{2}\sum_{\text{B}=1}^{2} c_\text{A}c_\text{B}S_\text{AB}^{FZ}(q) \tag{E.20}$$

$$S_{NC}(q) = c_\text{A}c_\text{B} \times \left[\, c_\text{A} \times \left(S_\text{AA}^{FZ}(q) - S_\text{AB}^{FZ}(q)\right) \;-\; c_\text{B} \times \left(S_\text{BB}^{FZ}(q) - S_\text{AB}^{FZ}(q)\right)\,\right] \tag{E.21}$$

$$S_{CC}(q) = c_\text{A}c_\text{B} \times \left[1 + c_\text{A}c_\text{B} \times \left[\sum_{\text{A}=1}^{2}\sum_{\text{B}\neq\text{A}}^{2}\left(S_\text{AA}^{FZ}(q) - S_\text{AB}^{FZ}(q)\right)\right]\right] \tag{E.22}$$

- $S_{NN}(q)$ is the Number-Number partial structure factor.
  Its Fourier transform allows to obtain a global description of the structure of the solid, ie. of the distribution of the experimental scattering centers, or atomic nuclei, positions. The nature of the chemical species spread in the scattering centers is not considered. Furthermore if $b_\text{A} = b_\text{B}$ then $S_{NN}(q) = S(q)$.

- $S_{CC}(q)$ is the Concentration-Concentration partial structure factor.
  Its Fourier transform allows to obtain an idea of the distribution of the chemical species over the scattering centers described using the $S_{NN}(q)$. Therefore the $S_{CC}(q)$ describes the chemical order in the material. In the case of an ideal binary mixture of 2 chemical species A and B[2], $S_{CC}(q)$ is constant and equal to c_Ac_B. In the case of an ordered chemical mixture (chemical species with distinct diameters, and with heteropolar and homopolar chemical bonds) it is possible to link the variations of the $S_{CC}(q)$ to the product of the concentrations of the 2 chemical species of the mixture:
  - $S_{CC}(q) = c_Ac_B$: random distribution.
  - $S_{CC}(q) > c_Ac_B$: homopolar atomic correlations (A-A, B-B) preferred.
  - $S_{CC}(q) < c_Ac_B$: heteropolar atomic correlations (A-B) preferred.
  - $\langle b\rangle = 0$: $S_{CC}(q) = S(q)$.

---

[2] Particles that can be described using spheres of the same diameter and occupying the same molar volume, subject to the same thermal constrains, in a mixture where the substitution energy of a particle by another is equal to zero.

- $S_{NC}(q)$ is the Number-Concentration partial structure factor.
  Its Fourier transform allows to obtain a correlation between the scattering centers and their occupation by a given chemical species. The more the chemical species related partial structure factors are different ($S_{AA}(q) \neq S_{BB}(q)$) and the more the oscillations are important in the $S_{NC}(q)$. In the case of an ideal mixture $S_{NC}(q) = 0$, and all the information about the structure of the system is given by the $S_{NN}(q)$.

If we consider the binary mixture as an ionic mixture then it is possible to calculate the Charge-Charge $S_{ZZ}(q)$ and the Number-Charge $S_{NZ}(q)$ partial structure factors using the Concentration-Concentration $S_{CC}(q)$ and the Number-Concentration $S_{NC}(q)$:

$$S_{ZZ}(q) = \frac{S_{CC}(q)}{c_A c_B} \qquad \textit{and} \qquad S_{NZ}(q) = \frac{S_{NC}(q)}{c_B/Z_A} \tag{E.23}$$

c_A and Z_A represent the concentration and the charge of the chemical species A, the global neutrality of the system must be respected therefore $c_A Z_A + c_B Z_B = 0$.

Figure E.6 illustrates, and allows to compare, the partial structure factors of glassy GeS$_2$ at 300 K calculated in the different formalism Faber-Ziman [14], Ashcroft-Langreth [15, 16, 17], and Bhatia-Thornton [18].

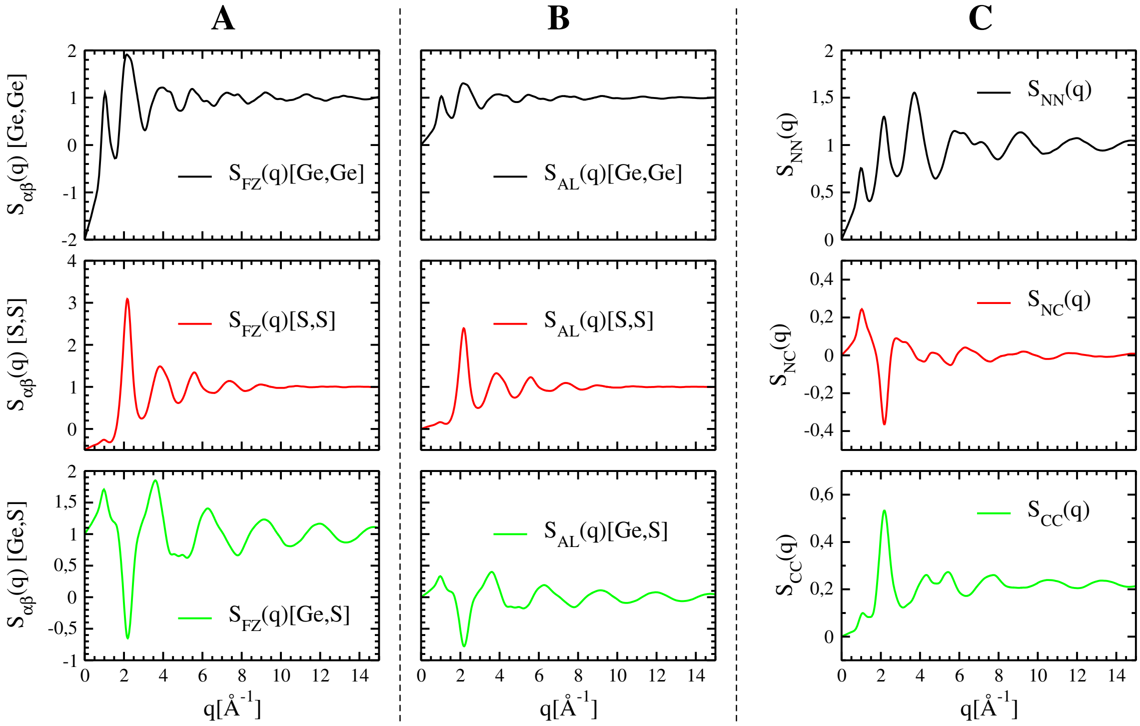


Figure E.6 *Partial structure factors of glassy GeS$_2$ at 300 K.* **A** *Faber-Ziman [14],* **B** *Ashcroft-Langreth [15, 16, 17] and* **C** *Bhatia-Thornton [18].*

atomes can compute all types of partial structure factors: Faber-Ziman $S^{FZ}_{\alpha\beta}(q)$, Ashcroft-Langreth $S^{AL}_{\alpha\beta}(q)$ and Bhatia-Thornton $S_{NN}(q)$, $S_{NC}(q)$, $S_{CC}(q)$ and $S_{ZZ}(q)$.

E.4 Local atomic coordination properties

Several properties related to the atomic bonds and angles between them can be computed using **atomes**. The existence or the absence of a bond between two atoms i of species α and j of species β is determined by the analysis of the partial $g_{\alpha\beta}(r)$ and total $g(r)$ radial distribution functions. Precisely **atomes** will consider that a bond exists if the interatomic distance D_{ij} is smaller than both the cutoff given to describe the maximum distance for first neighbor atoms between the species α and β, $Rcut_{\alpha\beta}$ (often the first minimum of $g_{\alpha\beta}(r)$), and the first minimum of the total radial distribution function, $Rcut_{tot}$.

atomes allows the user to specify both $Rcut_{\alpha\beta}$ and $Rcut_{tot}$ to choose an appropriate description of the atomic bonds in the system under study. When atomic bonds in a model are defined properly other structural characteristics can be evaluated, as follows:

E.4.1 Average first coordination numbers

atomes computes total as well as partials coordination numbers.

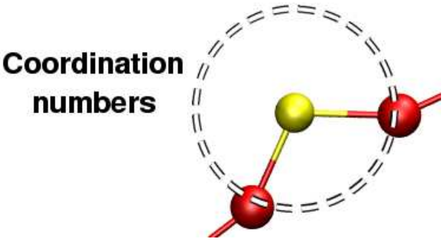


Figure E.7 *Coordination numbers.*

E.4.2 Individual atomic neighbor analysis

atomes computes the fraction of each type of coordination spheres in the model. The presence of of structural defects can lead to a wide number of local environments, figure E.8 illustrates the different coordination spheres found in a GeS_2 glass.

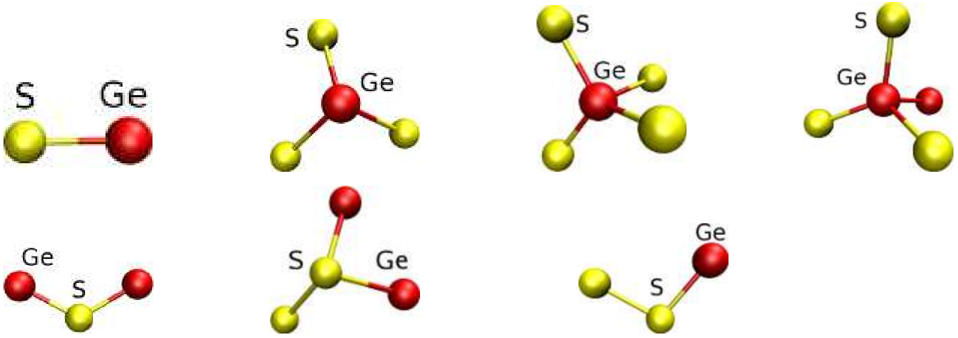


Figure E.8 *Illustration of several coordination spheres that can be found in glassy GeS_2.*

E.4.3 Proportion of tetrahedral links and units in the structure model

Often the structure of a material is represented using building blocks. One of the the most frequently occurring building blocks are tetrahedra. Figure E.9 shows a model of GeS_2 materials using GeS_4 tetrahedra as building blocks.

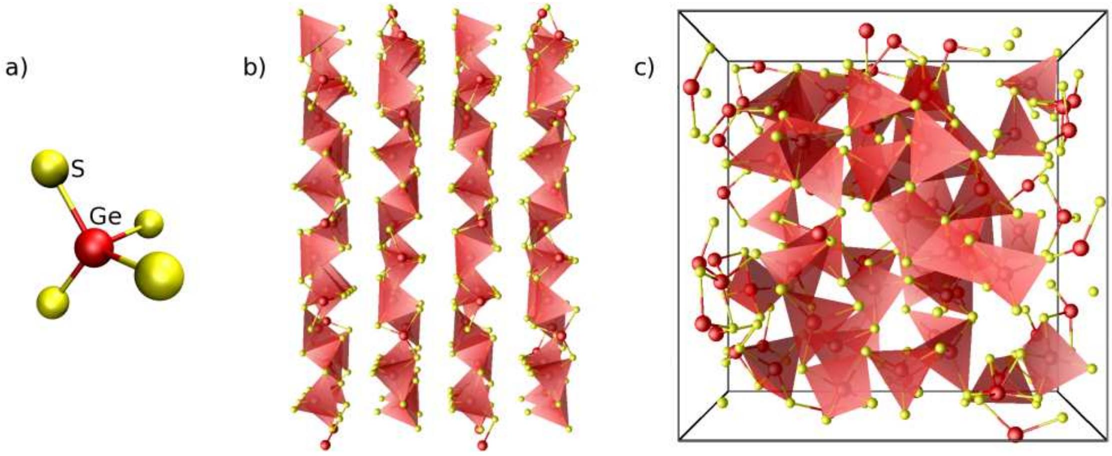


Figure E.9 *Illustration of the presence of GeS_4 tetrahedra in the GeS_2 material's family. a) GeS_4 tetrahedra, representations b) of the α-GeS_2 crystal and c) of the GeS_2 glass using tetrahedra.*

atomes computes the fraction of the different tetrahedra in materials, the distinction between these tetrahedra being made on the nature of the connection between each of them. Tetrahedra can be linked either by corners or edges [Fig. E.10], **atomes** computes the fraction of atoms forming tetrahedra as well as to the fraction of linked tetrahedra.

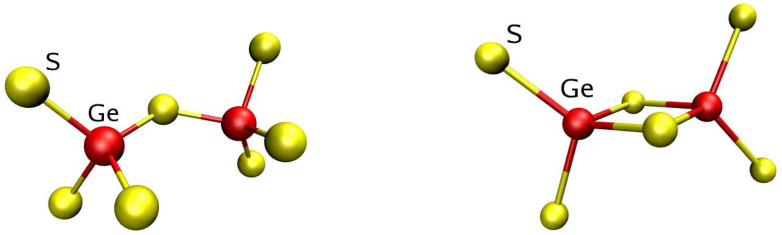


Figure E.10 *Corner sharing (left) and edge sharing (right) tetrahedra.*

E.4.4 Distribution of bond lengths for the first coordination spheres

atomes gives access to the bond length distribution between first neighbor atoms [Fig. E.11]:

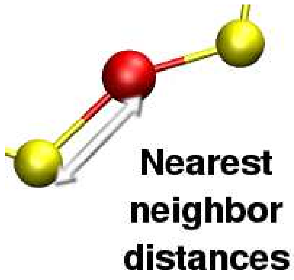


Figure E.11 *Nearest neighbor distances distribution.*

E.4.5 Angles distributions

atomes also computes the distributions of bond angles and dihedral angles [Fig. E.12]:

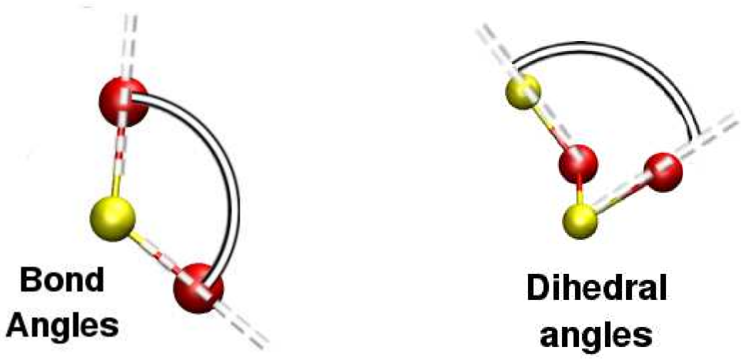


Figure E.12 *Bond angles (left) and diehdral angles (right).*

E.5 Ring statistics

The analysis of the topology of network-type structure models (liquid, crystalline or amorphous systems) is often based on the part of the structural information which can be represented in the graph theory using nodes for the atoms and links for the bonds. The absence or the existence of a link between two nodes is determined by the analysis of the total and partial radial distribution functions of the system.

In such a network a series of nodes and links connected sequentially without overlap is called a path. Following this definition a ring is therefore simply a closed path. If we study thoroughly a specific node of this network we see that this node can be involved in numerous rings. Each of these rings is characterized by its size and can be classified based upon the relations between the nodes and the links which constitute it.

E.5.1 Size of the rings

There are two possibilities for the numbering of rings. On the one hand, one can use the total number of nodes of the ring, therefore a N-membered ring is a ring containing N nodes. One the other hand, one can use the number of *network forming* nodes (ex: Si atoms in SiO_2 and Ge atoms in GeS_2 which are the atoms of highest coordination in these materials) an N-membered ring is therefore a ring containing 2×N nodes. For crystals and SiO_2-like glasses the second definition is usually applied. Nevertheless the first method has to be used in the case of chalcogenide liquids and glasses in order to count rings with homopolar bonds (ex: Ge-Ge and S-S bonds in GeS_2) - See section E.5.5 for further details.

From a theoretical point of view it is possible to obtain an estimate for the ring of maximum size that could exist in a network. This theoretical maximum size will depend on the properties of the system studied as well as on the definition of a ring.

E.5.2 Definitions

E.5.2.1 King's shortest paths criterion

The first way to define a ring has been given by Shirley V. King [19] (and later by Franzblau [20]). In order to study the connectivity of glassy SiO_2 she defines a ring as the shortest path between two of the nearest neighbors of a given node [Fig. E.13].

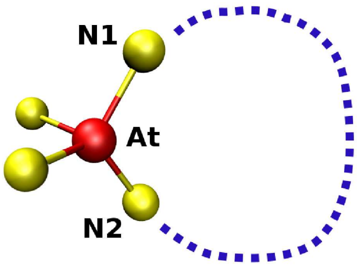


Figure E.13 *King's criterion in the ring statistics: a ring represents the shortest path between two of the nearest neighbors (**N1** and **N2**) of a given node (**At**).*

In the case of the King's criterion one can calculate the maximum number of different ring sizes, $NS_{max}(KSP)$, which can be found using the atom **At** to initiate the search:

$$NS_{max}(KSP) \; = \; \frac{Nc(\mathbf{At}) \times (Nc(\mathbf{At}) - 1)}{2} \tag{E.24}$$

where $N_c(\mathbf{At})$ is the number of neighbors of atom **At**. $NS_{max}(KSP)$ represents the number of ring sizes found if all couples of neighbors of atom **At** are connected together with paths of different sizes.
It is also possible to calculate the theoretical maximum size, $TMS(KSP)$, of a King's shortest path ring in the network using:

$$TMS(KSP) \; = 2 \times (D_{max} - 2) \times (Nc_{max} - 2) + 2 \times D_{max} \tag{E.25}$$

where D_{max} is the longest distance, in number of chemical bonds, separating two atoms in the network, and Nc_{max} represents the average number of neighbors of the chemical species of higher coordination. If used when looking for rings, periodic boundary conditions have to be taken into account to calculate D_{max}. The relation [Eq. E.25] is illustrated in figure E.16-2).

E.5.2.2 Guttman's shortest paths criterion

A later definition of ring was proposed by Guttman [21], who defines a ring as the shortest path which comes back to a given node (or atom) from one of its nearest neighbors [Fig. E.14].

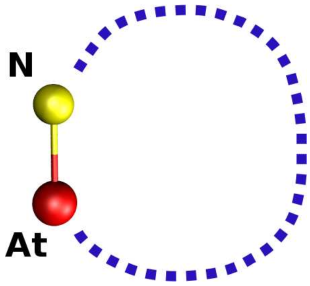


Figure E.14 *Guttman's criterion in the ring statistics: a ring represents the shortest path which comes back to a given node (**At**) from one of its nearest neighbors (**N**).*

Differences between the King and the Guttman's shortest paths criteria are illustrated in figure E.15.
Like for the King's criterion, with the Guttman's criterion one can calculate the maximum number of different ring sizes, $NS_{max}(GSP)$, which can be found using the atom **At** to initiate the search:

$$NS_{max}(GSP) = N_c(\mathbf{At}) - 1 \tag{E.26}$$

where $N_c(\mathbf{At})$ is the number of neighbors of atom **At**. $NS_{max}(GSP)$ represents the number of ring sizes found if the neighbors of atom **At** are connected together with paths of different sizes.

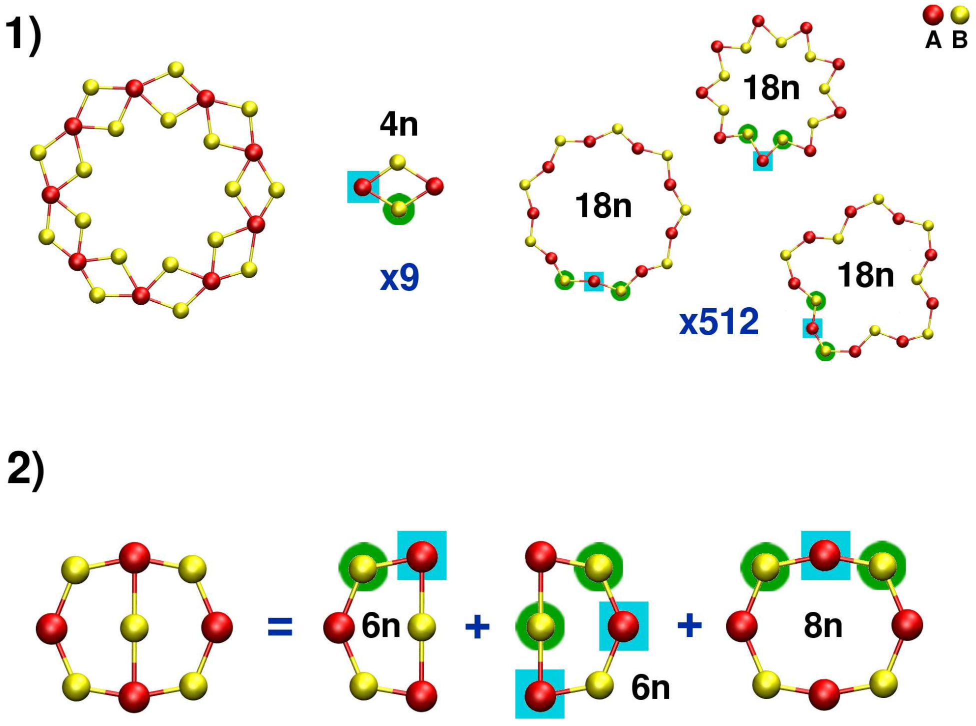


Figure E.15 *Differences between the King and the Guttman shortest paths criteria for the ring statistics in an* AB_2 *system. In these two examples the search is initiated from chemical species A (blue square). The nearest neighbor(s) of chemical species B (green circles) are used to continue the analysis. 1) In the first example only rings with 4 nodes are found using the Guttman's criterion, whereas rings with 18 nodes are also found using the King's criterion (*2^9 *rings with 18 nodes). 2) In the second example the King's shortest path criterion allows to find the ring with 8 nodes ignored by the Guttman's criterion which is only able to find the rings with 6 nodes.*

It is also possible to calculate the **T**heoretical **M**aximum **S**ize, $TMS(GSP)$, of a Guttman's ring in the network using:

$$TMS(GSP) = 2 \times D_{max} \tag{E.27}$$

where D_{max} represents the longest distance, in number of chemical bonds, separating two atoms in the network. If used when looking for rings, periodic boundary conditions have to be taken into account to calculate D_{max}. The relation [Eq. E.27] is illustrated in figure E.16-1.

Since the introduction of the King's and the Guttman's criteria other definitions of rings have been proposed. These definitions are based on the properties of the rings to be decomposed into the sum of smaller rings.

E.5.2.3 The primitive rings criterion

A ring is primitive [22, 23] (or Irreducible [24]) if it can not be decomposed into two smaller rings [Fig. E.17].

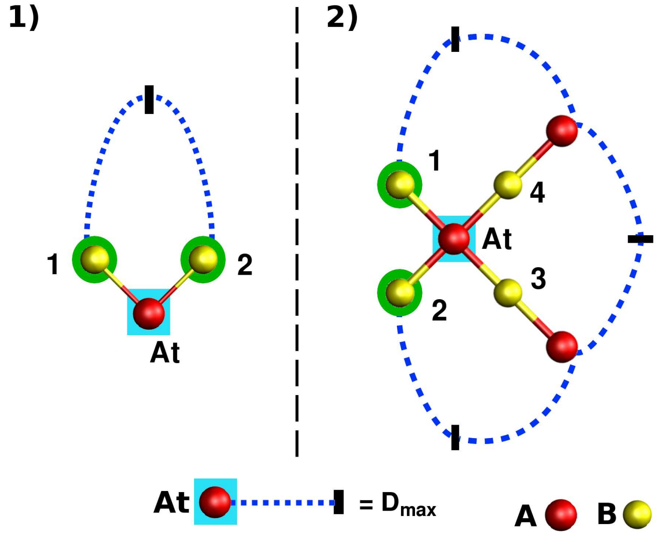


Figure E.16 *Theoretical maximum size of the rings for an* AB_2 *system (*$Nc_{max} = Nc_A = 4$*) and using: 1) the Guttman's criterion, 2) the King's criterion. The theoretical maximum size represent the longest distance between two nearest neighbors 1 and 2 (green circles) of the atom* **At** *used to initiate the search (blue square).*

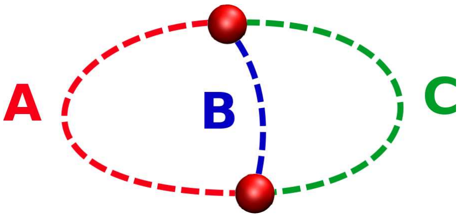


Figure E.17 *Primitive rings in the ring statistics: the 'AC' ring defined by the sum of the A and the C paths is primitive only if there is no B path shorter than A and shorter than C which allows to decompose the 'AC' ring into two smaller rings 'AB' and 'AC'.*

The primitive rings analysis between the paths in figure E.17 may lead to 3 results depending on the relations between the paths A, B, and C:

- If paths A, B, and C have the same length: A = B = C then the rings 'AB', 'AC' and 'BC' are primitives.
- If the relation between the paths is like ? =? <? (ex: A = B < C) then 1 smaller ring ('AB') and 2 bigger rings ('AC' and 'BC') exist. None of these rings can be decomposed into the sum of two smaller rings therefore the 3 rings are again primitives.
- If the relation between the path is like ? <? =? (ex: A < B = C) or ? <? <? (ex: A < B < C) then a shortest path exists (A). It will be possible to decompose the ring ('BC') built without this shortest path into the sum of 2 smaller rings ('AB' and 'AC'), therefore this ring will not be primitive.

E.5.2.4 The strong rings criterion

The strong rings [22, 23] are defined by extending the definition of primitive rings. A ring is strong if it can not be decomposed into a sum of smaller rings whatever this sum is, ie. whatever the number of paths in the decomposition is.

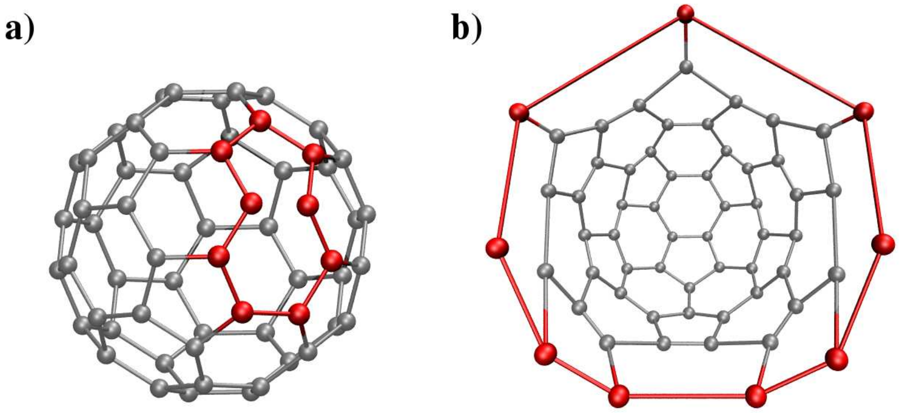


Figure E.18 *Strong rings in the ring statistics:* **a)** *the 9-carbon-atoms ring created after breaking a C-C bond in a Buckminster fulleren molecule is a counterexample of strong ring;* **b)** *the combination of shortest rings, 11 5-carbon-atoms rings and 19 6-carbon-atoms rings, appears easily after the deformation of the* C_{60} *molecule.*

By definition the strong rings are also primitives, therefore to search for strong rings can be summed as to find the strong rings among the primitive rings. This technique is limited to relatively simple cases, like crystals or structures such as the one illustrated in figure E.18. On the one hand the CPU time needed to complete such an analysis for amorphous systems is very important. On the other hand it is not possible to search for strong rings using the same search depth than for other types of rings. The strong ring analysis is indeed diverging which makes it very complex to implement for amorphous materials.

In the case of primitive rings like in the case of strong rings, there is no theoretical maximum size of rings in the network.

E.5.3 Description of a network using ring statistics - existing tools

Ring statistics are mainly used to obtain a snapshot of the connectivity of a network. Thereby the better the snapshot will be, the better the description and the understanding of the properties of the material will be. In the literature many papers present studies of materials using ring statistics. In these studies either the number of **R**ings per **N**ode 'R_N' [34, 35] or the number of **R**ings per **C**ell 'R_C' [36, 37, 38] are given as a result of the analysis. The first (R_N) is calculated for one node by counting all the rings corresponding to the property we are looking for (King's, Guttman's, primitive or strong ring criterion). The second (R_C) is calculated by counting all the different rings corresponding at least once (at least for one node) to the property we are looking for (King's, shortest path, primitive or strong ring criterion). The values of R_N and R_C are often reduced to the number of nodes of the networks. Furthermore the results are presented according to each size of rings.
An example is proposed with a very simple network illustrated in figure E.19.

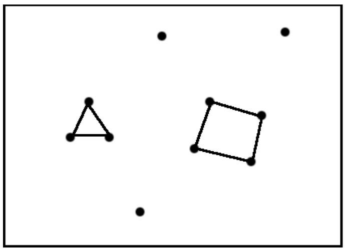


Figure E.19 *A very simple network.*

This network is composed of 10 nodes, arbitrary of the same chemical species, and 7 bonds. Furthermore it is clear that in this network there are 1 ring with 3 nodes and 1 ring with 4 nodes.
It is easy to calculate R_N and R_C for the network in figure E.19 (n = number of nodes):

n	$R_N(n)$
3	1/10
4	1/10

n	$R_C(n)$
3	3/10
4	4/10

Table E.1 *R_N and R_C for the network in figure E.19*

In the literature the values of R_N and R_C are usually given separately [34, 35, 36, 37, 38]. Nevertheless these two properties are not sufficient in order to describe a network using rings. A simple example is proposed in figure E.20.

The two networks [Fig. E.20-a] and [Fig. E.20-b] do have very similar compositions with 10 nodes and 7 links but they are clearly different. Nevertheless the previous definitions of rings per cell and rings per node even taken together will lead to the same description for these two different networks [Tab. E.2].

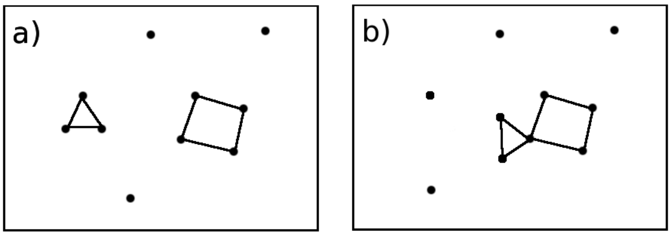


Figure E.20 *Two simple networks having very close compositions: 10 nodes and 7 links.*

n	$R_N(n)$
3	1/10
4	1/10

n	$R_C(n)$
3	3/10
4	4/10

Table E.2 *R_N and R_C calculated for the networks illustrated in figure E.20.*

In both cases a) and b) there are 1 ring with 3 nodes and 1 ring with 4 nodes. It has to be noticed that these two rings have properties which correspond to each of the definitions introduced previously (King, Guttman, primitive and strong).
Thus none of these definitions is able to help to distinguish between these two networks. Therefore even though these simple networks are different, the previous definitions lead to the same description.

Thereby it is justified to wonder about the interpretation of the data presented in the literature for amorphous systems with a much higher complexity.

E.5.4 Rings and connectivity: the R.I.N.G.S. method implemented in atomes

In the **atomes** program the results of the ring statistics analysis are outputted following the new R.I.N.G.S. method [25, 39], this method is presented in the next pages.

The first goal of ring statistics is to give a faithful description of the connectivity of a network and to allow to compare this information with others obtained for already existing structures. It is therefore important to find a guideline which allows to establish a distinction and then a comparison between networks studied using ring statistics. We propose thereafter a new method to achieve this goal. First of all we noticed fundamental points that must be considered to get a reliable and transferable method:

1. *The results must be reduced to the* **total** *number of nodes in the network.*
   The nature of the nodes used to initiate the analysis when looking for rings will have a significant influence, therefore it is essential to reduce the results to a value for one node. Otherwise it would be impossible to compare the results to the ones obtained for systems made of nodes (particles) of different number and/or

nature.

2. *Different networks must be distinguishable whatever the method used to define a ring.* Indeed it is essential for the result of the analysis to be trustworthy independently of the method used to define a ring (King, Guttman, primitives, strong). Furthermore this will allow to compare the results of these different ring statistics.

E.5.4.1 Number of rings per cell 'R_C'

We have already introduced this value, which is the first and the easiest way to compare networks using ring statistics.

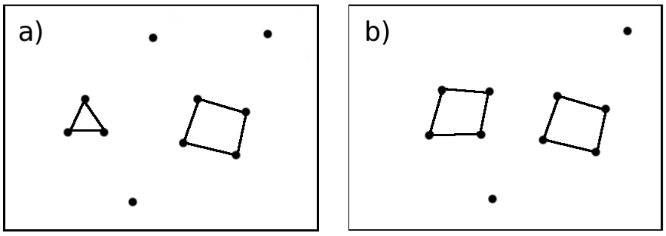


Figure E.21 *The first comparison element: the total number of rings in the network.*

n	$R_C(n)$
3	1/10
4	1/10

n	$R_C(n)$
3	0/10
4	2/10

Table E.3 *Number of rings in the simple networks represented in figure E.21.*

In the most simple cases, such as the one represented in figure E.21, the networks can be distinguished using only the number of rings [Tab. E.3]. Nevertheless in most of the cases other information are needed to describe accurately the connectivity of the networks.

E.5.4.2 Description of the connectivity: difference between rings and nodes

The second information needed to investigate the properties of a network using rings is the evaluation of the connectivity between rings. Indeed the distribution of the ring sizes gives a first information on the connectivity, nevertheless it can not be exactly evaluated unless one studies how the rings are connected. The impact of the relations between rings, already presented in figure E.20, has been illustrated in detail in figure E.22. Figure E.22 represents the different possibilities to combine 2 rings with 6 nodes and 1 ring with 4 nodes in a network composed of 16 nodes.

Among the 9 networks presented in figure E.22 none can be distinguished using the R_C value [Tab. E.4].

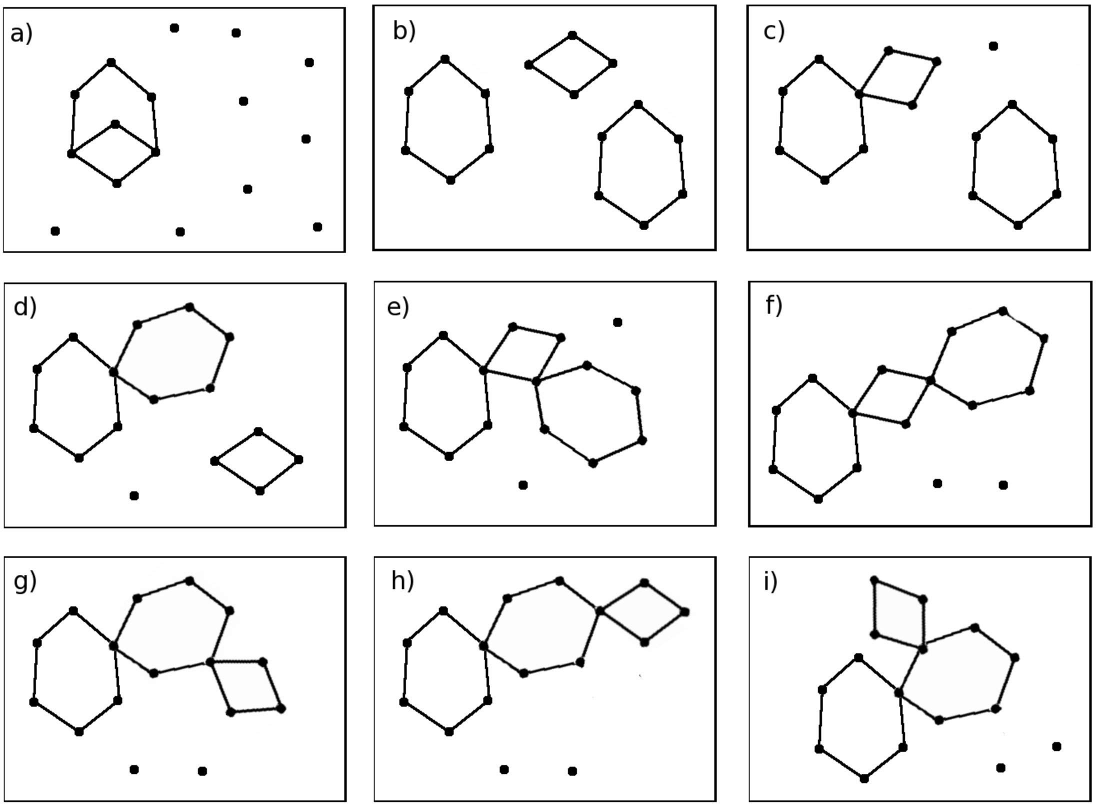


Figure E.22 *The 9 different networks with 16 nodes, composed of 2 rings with 6 nodes and 1 ring with 4 nodes.*

n	$R_C(n)$
4	1/16
6	2/16

Table E.4 *Number of rings for the different networks presented in figure E.22.*

Furthermore it is not possible to distinguish these networks using the R_N value.
It seems possible to isolate the case a) [Tab. E.5] from the other cases b) → i) [Tab. E.5]. Nevertheless the results obtained using the primitive rings criterion are similar for all cases a) → i) [Tab. E.5], this is in contradiction with the second statement [2] proposed in our method.

Before introducing parameters able to distinguish the configurations presented in figure E.22 it is important to wonder about the number of cases to distinguish. From the point of view of the connectivity of the rings, configurations a), b), c) and d) are clearly different. Nevertheless following the same approach configurations e) and f) on the one hand and configurations g), h) and i) on the other hand are identical. A schematic representation [Fig. E.23] is sufficient to illustrate the similarity of the relations between these networks. The difference between each of these networks does

Case a)	$R_N(n)$	
n	King / Guttman.	Primitive / Strong.
4	4/16	**4/16**
6	10/16	**12/16**

Cases b) → i)	$R_N(n)$
n	All criteria.
4	**4/16**
6	**12/16**

Table E.5 *Number of rings per node for the networks presented in figure E.22.*

not appear in the connectivity of the rings but in the connectivity of the particles.

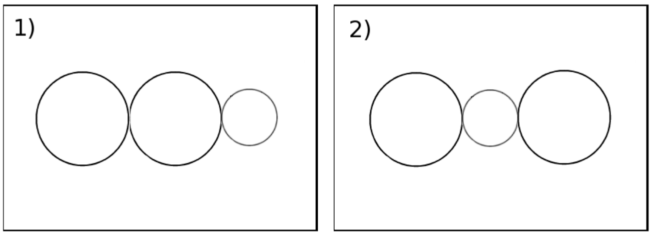


Figure E.23 *Schematic representation of cases g) → i) (1) and e) → f) (2) illustrated in figure E.22.*

Thus among the networks illustrated in figure E.22 six dispositions of the rings have to be distinguished (a, b, c, d, e, g). The proportions of particles involved, or not involved, in the construction of rings will become an important question.

The new tool defined in our method is able to describe accurately the information still missing on the connectivity. It is a square symmetric matrix of size $(R-r+1)\times(R-r+1)$, where R and r represent respectively the bigger and the smaller size of a ring found when analyzing the network: we have called this matrix the connectivity matrix [Tab. E.6].

$$C_{mat} = \begin{bmatrix} P_N(r) & P_N(r+1,r) & \cdots & P_N(R,r) \\ P_N(r,r+1) & \ddots & & P_N(R,r+1) \\ \vdots & & \ddots & \vdots \\ P_N(r,R) & \cdots & \cdots & P_N(R) \end{bmatrix}$$

Table E.6 *General connectivity matrix.*

The diagonal elements $P_N(i)$ of this matrix represent the **P**roportion of **N**odes at the

origin of at least one ring of size i. And the non-diagonal elements $P_N(i,j)$ represent the **P**roportion of **N**odes at the origin of ring(s) of size i and j.
The matrix elements have a value ranging between 0 and 1. The lowest and non equal to 0 is of the form $\frac{1}{Nn}$, the highest and non equal to 1 is of the form $\frac{Nn-1}{Nn}$, where Nn represents the number of nodes in the network.

	King / Guttman.	Primitive / Strong.
Cas a)	$\begin{bmatrix} 4/16 & 2/16 \\ 2/16 & 5/16 \end{bmatrix}$	$\begin{bmatrix} 4/16 & 4/16 \\ 4/16 & 7/16 \end{bmatrix}$
	All criteria.	
Case b)	$\begin{bmatrix} 4/16 & 0/16 \\ 0/16 & 12/16 \end{bmatrix}$	
Case c)	$\begin{bmatrix} 4/16 & 1/16 \\ 1/16 & 12/16 \end{bmatrix}$	
Case d)	$\begin{bmatrix} 4/16 & 0/16 \\ 0/16 & 11/16 \end{bmatrix}$	
Case e) → f)	$\begin{bmatrix} 4/16 & 2/16 \\ 2/16 & 12/16 \end{bmatrix}$	
Case g) → i)	$\begin{bmatrix} 4/16 & 1/16 \\ 1/16 & 11/16 \end{bmatrix}$	
n= ring with n nodes	$\begin{bmatrix} n4 & n6/n4 \\ n4/n6 & n6 \end{bmatrix}$	

Table E.7 *General connectivity matrix for the networks represented in figure E.22 and studied using the different definitions of rings.*

The connectivity matrix of the configurations illustrated in figure E.22 are presented in table E.7. We see that this matrix allows to distinguish each network whatever the way used to define a ring is. This matrix remains simple for small systems (crystalline or amorphous) or when using a small maximum ring size for the analysis. Nevertheless its reading can be considerably altered when analysing amorphous systems with a high maximum ring size for the analysis.

To simplify the reading and the interpretation of the data contained in this matrix for more complex systems, we chose a similar approach to extract information on the connectivity between the rings. As a first step we decided to evaluate only the diagonal elements $P_N(n)$ of the general connectivity matrix. Indeed these values allow us to obtain a better view of the connectivity than the standard R_N value.

	$P_N(n)$	
n	King / Guttman.	Primitive / Strong.
Case a)		
4	4/16	4/16
6	5/16	7/16

	$P_N(n)$
n	All criteria.
Case b) → c)	
4	4/16
6	12/16
Case d)	
4	4/16
6	11/16
Case e) → f)	
4	4/16
6	12/16
Case g) → i)	
4	4/16
6	11/16

Table E.8 *$P_N(n)$ - Proportion of nodes at the origin of at least one ring of size n for the networks in figure E.22.*

It is clear [Tab. E.8] that using $P_N(n)$ improves the separation between the networks illustrated in figure E.22. Nevertheless $P_N(n)$ does not allow to distinguish each of them. We notice that the distinction between networks is improved [Tab. E.8] in particular when compared to the one obtain with $R_N(n)$ [Tab. E.5].

Therefore in a second step we chose to calculate two properties whose definitions are very similar to the one of $P_N(n)$. The first, named $P_{N_{\text{max}}}(n)$, represents the proportion of nodes for which the rings with n nodes are the longest closed paths found using these nodes to initiate the search. The second named, $P_{N_{\text{min}}}(n)$, represents the proportion of nodes for which the rings with n nodes are the shortest closed paths found using these nodes to initiate the search.
The terms *longest* and *shortest path* must be considered carefully to avoid any confusion with the terms used in section E.5.2 to define the rings. For one node it is possible to find several rings whose properties correspond to the definitions proposed previously (King's, Guttman's, primitive or strong ring criterion). These rings are solutions found when looking for rings using this particular node to initiate the analysis. In order to calculate $P_{N_{\text{max}}}(n)$ and $P_{N_{\text{min}}}(n)$ the longest and the shortest path have to be determined among these different solutions.
$P_{N_{\text{max}}}(n)$ and $P_{N_{\text{min}}}(n)$ have values ranging between 0 and $P_N(n)$. The lowest and non equal to 0 is of the form $\frac{1}{Nn}$, the highest and non equal to 1 is of the form $\frac{Nn-1}{Nn}$, where Nn represents the total number of nodes in the network. For the minimum ring size, s_{min}, existing in the network or found during the search, $P_{N_{min}}(s_{min}) = P_N(s_{min})$. In the same way for the maximum ring size, s_{max}, existing in the network or found during the search, $P_{N_{max}}(s_{max}) = P_N(s_{max})$.

To clarify these information it is possible to normalize $P_{N_{\text{max}}}(n)$ and $P_{N_{\text{min}}}(n)$ by $P_N(n)$. By reducing these values we obtain, for each size of rings, values independent of the total number of nodes Nn of the system. Then for a considered ring size the values only refer to the number of nodes where the search returns rings of this size:

$$P_{max}(n) = \frac{P_{N_{max}}(n)}{P_N(n)} \quad \text{and} \quad P_{min}(n) = \frac{P_{N_{min}}(n)}{P_N(n)}$$

The normalized terms $P_{\text{max}}(n)$ and $P_{\text{min}}(n)$ have values ranging between 0 and 1. The lowest and non equal to 0 is of the form $\frac{1}{Nn}$, the highest and non equal to 1 is of the form $\frac{Nn-1}{Nn}$. For the minimum ring size, s_{min}, existing in the network or found during the search, $P_{min}(s_{min}) = 1$. In the same way for the maximum ring size, s_{max}, existing in the network or found during the search, $P_{max}(s_{max}) = 1$.
$P_{\text{max}}(n)$ and $P_{\text{min}}(n)$ give complementary information to the ones obtained with $R_C(n)$ and $P_N(n)$ in order to distinguish and compare networks using ring statistics. We can illustrate this result by presenting the complete information obtained with this method [Tab. E.9] for the networks represented in figure E.22.
$P_{\text{max}}(n)$ and $P_{\text{min}}(n)$ give information about the connectivity of the rings with each other as a function of their size. If a ring of size n is found using a particular node to initiate the search, $P_{\text{max}}(n)$ gives the probability that this ring is the longest ring which can be found using this node to initiate the search. At the opposite, $P_{\text{min}}(n)$ gives the probability that this ring is the shortest ring which can be found using this node to initiate the search.
Thereafter we will use the terms 'connectivity profile' to designate the results of a ring statistics analysis. This profile is related to the definition of rings used in the search and is made of the 4 values defined in our method: $R_C(n)$, $P_N(n)$, $P_{\text{max}}(n)$ and $P_{\text{min}}(n)$.

King / Guttman.

n	$R_C(n)$	$P_N(n)$	$P_{\max}(n)$	$P_{\min}(n)$
Case a)				
4	1/16	4/16	0.5	1.0
6	2/16	5/16	1.0	0.6

Primitive / Strong.

n	$R_C(n)$	$P_N(n)$	$P_{\max}(n)$	$P_{\min}(n)$
Case a)				
4	1/16	4/16	0.5	1.0
6	2/16	7/16	1.0	3/7

All criteria.

n	$R_C(n)$	$P_N(n)$	$P_{\max}(n)$	$P_{\min}(n)$
Case b)				
4	1/16	4/16	1.0	1.0
6	2/16	12/16	1.0	1.0
Case c)				
4	1/16	4/16	0.75	1.0
6	2/16	12/16	1.0	11/12
Case d)				
4	1/16	4/16	1.0	1.0
6	2/16	11/16	1.0	1.0
Case e) → f)				
4	1/16	4/16	0.5	1.0
6	2/16	12/16	1.0	10/12
Case g) → i)				
4	1/16	4/16	0.75	1.0
6	2/16	11/16	1.0	10/11

Table E.9 *Connectivity profiles results of the ring statistics for the networks presented in figure E.22.*

The **atomes** program provides access to the connectivity profile of the system under study and allows to choose the study the connectivity using all the different methods used to define a ring. Thus King's rings, Guttman's rings, Primitive rings as well as Strong rings analysis are available.

E.5.5 Bond defects in ring statistics

E.5.5.1 ABAB and BABA rings

The ring statistics of amorphous networks are often focused on finding rings made of a succession of atoms with an alternation of chemical species, called ABAB rings. The most common examples come from the alternation of Si and O atoms (in silica polymorphs) or Ge and S (in GeS_2 polymorphs). These solids are usually built with tetrahedra (SiO_4 or GeS_4) therefore we study the network distribution of tetrahedra.
The ideal technique to setup the analysis of such systems is to choose the atoms of highest coordination to initiate the search, respectively Si in SiO_2 and Ge in GeS_2. In most cases all rings can be found using this method. Nevertheless we can demonstrate that some solutions, so some rings, can be ignored by this analysis. This is highlighted in figure E.24 which represents a cluster of atoms isolated from an AB_2 amorphous network.

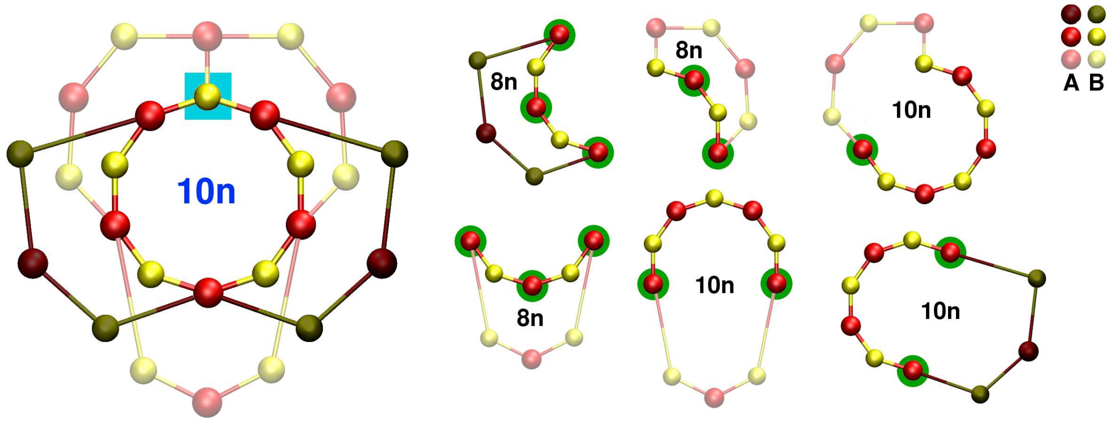


Figure E.24 *Cluster of atoms isolated from an AB_2 amorphous network. A bond defect is located on an atom of the chemical species B (blue square). When looking for King's shortest paths [S. E.5.2.1] using the chemical species A to initiate the search the central ring with 10 nodes is ignored. However among the solutions of the analysis (with the initial nodes circled in green) other rings with 10 nodes are found in the network.*

We can see that this piece of network is characterized by a bond defect. An atom of the B species appears to be over-coordinated by three atoms of the A species. When looking for rings, using the King's criterion [S. E.5.2.1] and initiating the search using the A atoms, the central ring with 10 nodes is ignored. Nevertheless other rings with 10 nodes are found and stored as solutions of the analysis. In order to find the central ring the search has to be initiated from the overcoordinated B atom.
By analogy with the terminology ABAB this ring can be called a BABA ring. Indeed the alternation of chemical species is well respected. Therefore it is legitimate to question the relevance of the analysis without this result. In other words we have to check out if this BABA ring is, or not, an ABAB ring.
The properties of this ring meet the definition and can therefore improve the description

of the connectivity of the network. This kind of coordination defect [Fig. E.24] is uncommon in vitreous silica [34, 40], nevertheless it is frequent in chalcogenide glasses [41, 42].

E.5.5.2 Homopolar bonds

In amorphous materials the homopolar bond defects can have a significant influence on the ring statistics. This is true in particular for AB_2 chalcogenide glasses. Figure E.25 illustrates standard cases that may be encountered when looking for rings in an AB_2 system which contains homopolar bonds.

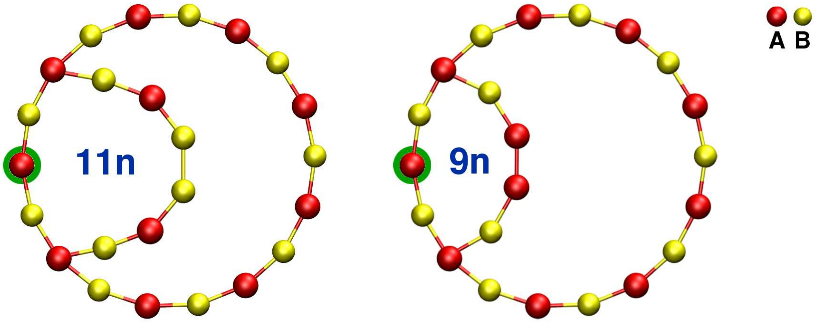


Figure E.25 *Illustration of the influence of homopolar bonds in ABAB rings: in both examples the smallest rings found when initiating the search using the circled nodes (green color) contain an homopolar bond A-A or B-B.*

The smallest rings found when initiating the search using the circled nodes (green color) are not ABAB rings. Therefore their size must be given using the total number of nodes. In figure E.25 the smallest rings are a ring with 9 nodes and a ring with 11 nodes containing respectively an A-A and a B-B homopolar bond. These rings are significantly smaller than the shortest ABAB ring with 18 nodes that may be found when looking for rings using the same green-circled nodes to initiate the analysis [Fig. E.25].

The **atomes** program provides options to take into account or avoid A-B-A-B rings as well as homopolar bonds.

E.5.6 Number of rings not found and that "potentially exist"

One of the first information it is possible to extract from ring statistics, except the number of rings, is the number of rings not found by the analysis. Indeed calculation times do strongly depend on the maximum search depth, ie. the maximum size of a ring. To carry out the analysis this value has to be chosen to get the best possible compromise between CPU time and quality of the description.
Nevertheless whatever this limiting value is, some rings of a size bigger than the maximum search depth may not be found by the analysis. In the King E.5.2.1 and the Guttman's criteria E.5.2.2 it is possible to evaluate the number of "potentially not

found" rings or rings that "potentially exist".
Thus for a given atom **At** we can consider that a closed path exists and is not found:

1. If the atom **At** has at least 2 nearest neighbors
2. If no closed path is found:
    - a- Starting from one neighbor to go back on the considered atom **At** (Guttman's criterion)
    - b- Between one couple of neighbors of the atom **At** (King's criterion)
3. If the 2 nearest neighbors of the atom **At** have at least 2 nearest neighbors (to avoid non bridging atoms)

Thus if during the analysis these 3 conditions are full filled (1, 2-a, 3 for the Guttman's criterion, and 1, 2-b, 3 for the King's criterion) then we can say that this analysis has potentially missed a ring between the neighbors of atom **At**. The smaller this number of "potentially" missed rings will be the better this analysis will be and the better the description of the connectivity of the material studied will be. The term "potentially" has been chosen because the method only allows to avoid first neighbor non bridging atoms.

Following this method **atomes** gives access to the number of rings that "potentially exist" and not found during the analysis.

E.6 Chain statistics

To get information on the connectivity of a material one can also rely on chain statistics. The idea of this calculation is to look for path between 2 atoms A and B, respecting the following rules:

- Total coordination for A (α) must be $\neq 2$
- Total coordination for B (β) must be $\neq 2$
- Total coordination for all atom(s) between A and B must be equal to 2.

Chains are then litteraly succession of atoms isolated from the rest of the material. **atomes** offers several options to enforce specific definition of a chain for the search:

- Total coordination for A and B can be restricted to 1: searching for chains would mean searching for isolated 1 dimensional (on a coordination point of view) structures in the material.
- The chemistry of the atoms in the chain(s) can be considered:
  - Only searching for AAAA ($\alpha\alpha\alpha\alpha$) chains (homopolar bonds exclusively).
  - Excluding homopolar bonds from the search (heteropolar bonds exclusively).
  - Only searching for ABAB ($\alpha\beta\alpha\beta$) chains (perfect alternate of heteropolar bonds.

E.7 Invariants of spherical harmonics as atomic order parameters

Invariants formed from bond spherical harmonics allow to obtain quantitative information on the local atomic symmetries in materials. The analysis starts by associating a set of spherical harmonics with every bond linking an atom to its nearest neighbors. For a given bond defined by a vector $\vec{r}$ a spherical harmonic may be defined as:

$$Q_{lm}(\vec{r}) \;=\; Y_{lm}\langle\theta(\vec{r}),\psi(\vec{r})\rangle \tag{E.28}$$

where $Y_{lm}(\theta,\psi)$ is the spherical harmonic associated to the bond, θ and ψ are the angular components of the spherical coordinates of the bond which Cartesian coordinates are defined by $\vec{r}$.

Because the Q_{lm} for a given l can be scrambled by changing to a rotated coordinate system, it is important to consider rotational invariant combinations, such as [26, 43]:

$$Q_l \;=\; \left[\frac{4\pi}{2l+1}\sum_{m=-l}^{l}\left|\bar{Q}_{lm}\right|^2\right]^{1/2} \tag{E.29}$$

where $\bar{Q}_{lm}$ is defined by:

$$\bar{Q}_{lm} = \langle Q_{lm}(\vec{r}) \rangle \tag{E.30}$$

and represents an average of the $Y_{lm}(\theta, \psi)$ over all $\vec{r}$ vectors in the system whether these vectors belong to the same atomic configuration or not. Just as the angular momentum quantum number, l, is a characteristic quantity of the 'shape' of an atomic orbital, the quantity Q_l is a rotationally invariant characteristic value of the shape/symmetry of a given local atomic configuration (if the average is not taken on all bonds of the system but only within a given configuration) or an average of such values for a set of configurations. Thus it is possible to compare Q_l's computed for well known crystal structures (e.g. FCC, HFC ...) and some local atomic configurations in a material's model. The results of the comparison gives information for the presence/absence of a particular local atomic symmetry.

atomes allows to compute the average Q_l's for each chemical species as well as the average Q_l's for a user specified local atomic coordination.

E.8 Mean square displacement of atoms

Atoms in solids, liquids and gases move constantly at any given temperature, i.e. they are subject to a "thermal" displacement from their average positions. This displacement is particularly important in the case of a liquids. Atomic displacement does not follow a simple trajectory: "collisions" with other atoms render atomic trajectories quite complex shaped in space.

The trajectory followed by an atom in a liquid resembles that of a pedestrian random walk. Mathematically this represents a sequence of steps done one after another where each step follows a random direction which does not depend on the one of the previous step (Markov's chain of events).

In the case of a one-dimensional system (straight line) the displacement of the atom will therefore be either a forward step (+) or a backward step (-). Furthermore it will be impossible to predict one or the other direction (forward or backward) since they have an equal probability to occur.

One can conclude that the distance an atom may travel is close to zero. Nevertheless if we choose not to sum the displacements themselves (+/-) but the square of these displacements then we will end up with a non-zero, positive quantity of the total squared distance traveled. Consequently this allows to obtain a better evaluation of the real (square) distance traveled by an atom.

The **M**ean **S**quare **D**isplacement MSD is defined by the relation:

$$MSD(t) = \langle \mathbf{r}^2(t) \rangle = \left\langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \right\rangle \tag{E.31}$$

where $\mathbf{r}_i$(t) is the position of the atom i at the time t, and the $\rangle$ $\langle$ represent an average on the time steps and/or the particles.

However, during the analysis of the results of molecular dynamics simulations it is important to subtract the drift of the center of mass of the simulation box:

$$MSD(t) = \left\langle |\mathbf{r}_i(t) - \mathbf{r}_i(0) - [\mathbf{r}_{cm}(t) - \mathbf{r}_{cm}(0)]|^2 \right\rangle \tag{E.32}$$

where $\mathbf{r}_{cm}$(t) represents the position of the center of mass of the system at the time t. The MSD also contains information on the diffusion of atoms. If the system is solid (frozen) then MSD "saturate", and the kinetic energy is not sufficient enough to reach a diffusive behavior. Nevertheless if the system is not frozen (e.g. liquid) then the MSD will grow linearly in time. In such a case it is possible to investigate the behavior of the system looking at the slope of the MSD. The slope of the MSD or the so called diffusion constant D is defined by:

$$D = \lim_{t \to \infty} \frac{1}{6t} \langle \mathbf{r}^2(t) \rangle \tag{E.33}$$

atomes provides access to the several MSD related functions:

- MSD for each chemical species with autocorrelation on all the dynamics
- MSD for each chemical species without autocorrelation on all the dynamics (step by step)
- Directional MSD (x, y, z, xy, xz, yz) for each chemical species with autocorrelation on all the dynamics
- Directional MSD (x, y, z, xy, xz, yz) for each chemical species without autocorrelation on all the dynamics (step by step)
- Drift of the center of mass (x, y, z)
- Correction applied to correct the drift of the center of mass in equation [Eq. E.32] (x, y, z)

The chemical properties database in atomes

A database of chemical/physical properties is included in the **atomes** program, this appendix presents these properties (atomic radii, x-ray and neutron scattering lengths) as well as the references of the articles from which this information was obtained. Note that the data presented in this appendix is available for download on the web site of the program:

https://atomes.ipcms.fr

F.1 Atomic radii

F.1.1 Covalent radii

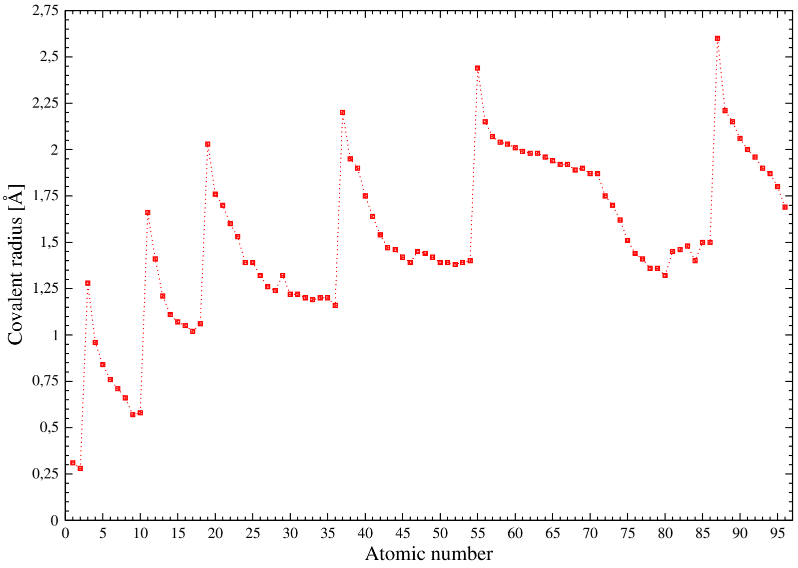


Figure F.1 *Covalent radii used in the* **atomes** *program.*

Figure F.1 presents the covalent radii used in **atomes** see [44] for details.

F.1.2 Ionic radii

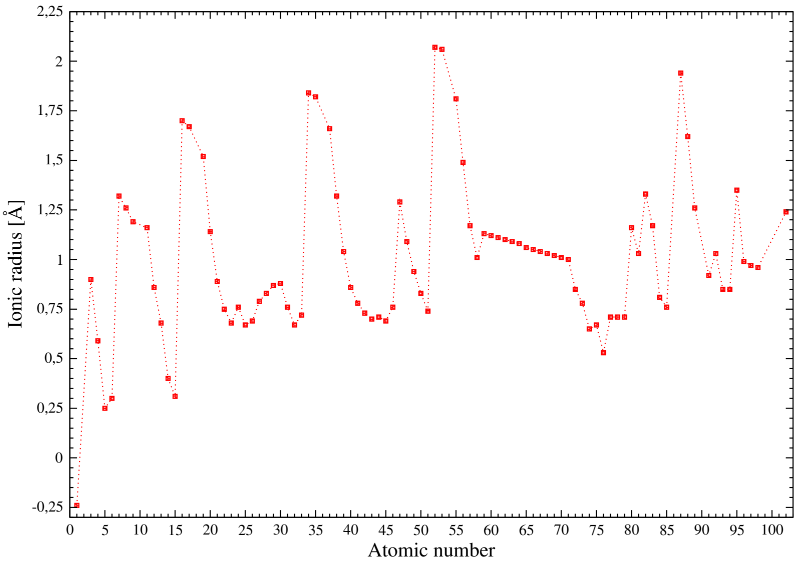


Figure F.2 *Ionic radii used in the* **atomes** *program.*

Figure F.2 presents the ionic radii used in **atomes** see [45] for details.

F.1.3 VDW radii

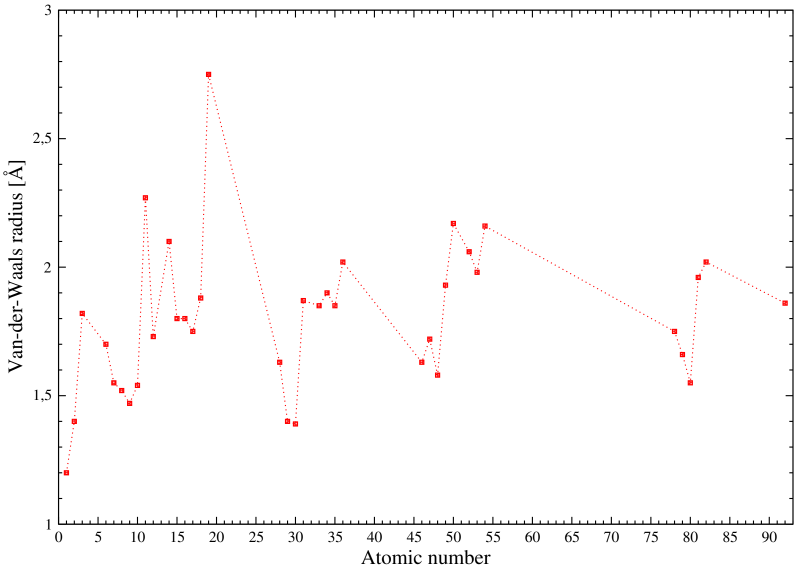


Figure F.3 *Van Der Waals radii used in the* **atomes** *program.*

Figure F.3 presents the Van Der Waals radii used in **atomes** see [46] for details.

F.1.4 Shannon radii in crystal

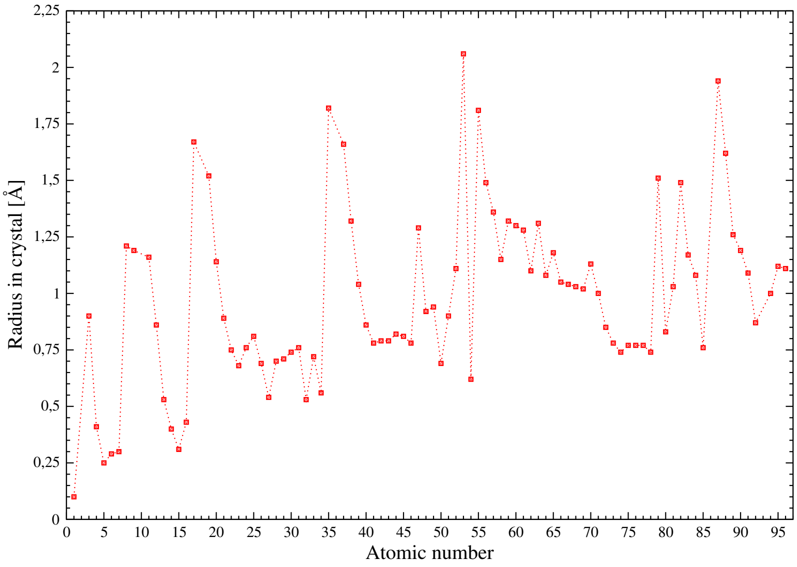


Figure F.4 *Shannon radii in crystals used in the* **atomes** *program.*

Figure F.4 presents the Shannon radii in crystals used in **atomes** see [47, 48] for details.

F.2 Neutron scattering lenghts

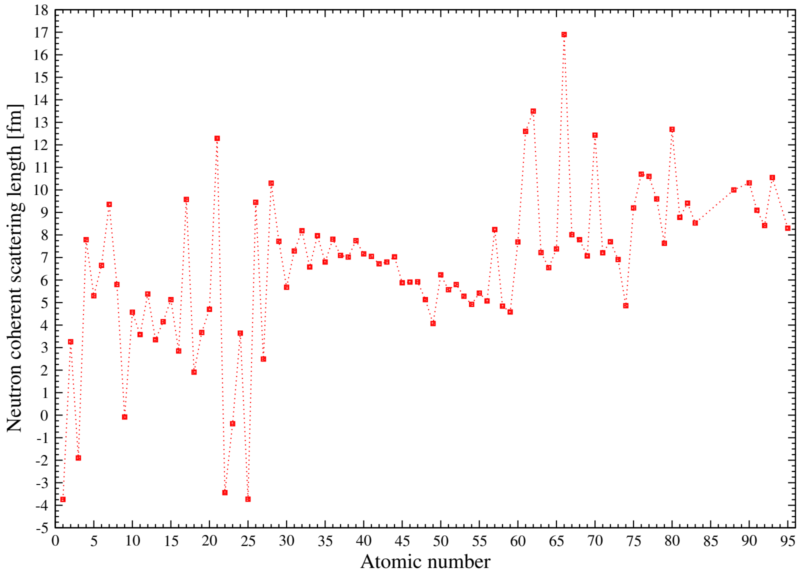


Figure F.5 *Neutron scattering lengths used in the* **atomes** *program.*

Figure F.5 presents the neutron scattering lengths used in **atomes** see [49, 50] for details.

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