

# Reference manuals

Nemesis

Petr Kulhanek

[kulhanek@chemi.muni.cz](mailto:kulhanek@chemi.muni.cz)

National Center for Biomolecular Research, Faculty of Science  
Masaryk University, Kotlářská 2, CZ-61137 Brno

# Nemesis

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# Nemesis

## Starting the program:

```
$ module add nemesis  
$ nemesis
```

## Mouse:

Left mouse button	selection
Middle mouse button	rotation
Right mouse button	translation
Scroll wheel	zoom

## Modifiers:

Shift	XZ -> Y moves
Ctrl	toggles between secondary and primary manipulator

# Nemesis - Build Project

The screenshot shows the Nemesis Molecular Modelling Package interface. The main window is titled "Project 1 : NEMESIS - Molecular Modelling Package". The interface is divided into several panels:

- Structures panel:** Contains a table with columns "Name", "SID", and "Ato". The table has one entry: "Structure 1" with "SID" 1. A blue arrow points from the text "layers" to the "SID" column.
- Build panel:** Contains chemical symbols for atoms (C, F, O, N, Cl, Br, S, I) and bond types (single, double, triple). A blue arrow points from the text "molecule construction/editing" to the "Cl" symbol. Below the symbols are buttons for "Delete atom", "Make bond", "Break bond", and "Delete bond". The "Optimize" button is circled in red, with a blue arrow pointing from the text "geometry optimization using a force field" to it.
- Profile objects panel:** Contains a table with columns "Name" and "Ty". The table has four entries: "Light 1" (Light), "Background 1" (Backgro), "Standard Model 1" (Standar), and "Freezed Atoms 1" (Freezec). A blue arrow points from the text "graphic models" to this panel.
- Geometry panel:** Contains buttons for "Position", "Distance", "Angle", and "Torsion". A blue arrow points from the text "geometry measurement" to this panel.

At the bottom of the interface, there are buttons for "Restrain", "Property", and "Label".

**Force field settings for optimization:** menu Geometry-> Optimizer Setup

# Geometry optimization visualization

- 1) Project: Trajectory
- 2) File-> Import Trajectory as -> Gaussian Geometry Optimization

The screenshot shows the NEMESIS Molecular Modelling Package interface. The main window displays a 3D ball-and-stick model of an ethane molecule. The 'Trajectories' panel on the left lists 'Trajectory 1 Structure 1'. A blue arrow labeled 'double click' points from this entry to a 'Trajectory' dialog box. This dialog box has tabs for 'Basic', 'Play', 'Segments', 'Filters', and 'Referenced by'. It contains a table with the following data:

SI	Name	Snapshots	Type
1	ethan	6	Gaussian Geometry O

A second blue arrow labeled 'double click' points from the 'ethan' entry in the table to a 'Gaussian Geometry Optimization' dialog box. This dialog box has tabs for 'Basic', 'Energy', and 'Info'. The 'Energy' tab is active and displays a table with the following data:

ID	Energy [a.u.]	Relative Energy [kca
1	-0.028617175	0.00
2	-0.028893932	-0.17
3	-0.028929498	-0.20
4	-0.028931879	-0.20
5	-0.028934299	-0.20
6	-0.028935040	-0.20

At the bottom of the interface, a blue oval highlights a set of playback controls (stop, play, next, previous, etc.), with the text 'optimization process' written below it.

# Vibration visualization

- 1) Project: Trajectory
- 2) File-> Import Trajectory as -> Gaussian Vibrations

The screenshot shows the Nemesis Molecular Modelling Package interface. The main window displays a 3D ball-and-stick model of a molecule. A blue arrow points from the 'Trajectory 1 Structure 1' entry in the 'Trajectories' panel to the 'Trajectory' dialog box. Inside this dialog, a table lists vibrations, and a blue arrow points from the 'ethan\_freq' entry to the 'Gaussian Vibrations' dialog box. In the 'Gaussian Vibrations' dialog, a blue oval highlights the 'Vibrations' tab, which contains a table of 24 vibrations. A blue arrow points from the 'start the animation' text to the play button in the bottom toolbar.

double click

double click

choose a vibration

start the animation

ID	Frequency	IR Intensity	Scale
1	224.6	0.0	
2	878.2	0.0	
3	878.2	0.0	
4	1120.0	0.0	
5	1120.0	0.0	
6	1137.8	0.0	
7	1359.3	0.0	
8	1408.2	0.0	
9	1408.2	0.0	
10	1443.6	0.0	
11	1443.6	0.0	
12	1443.6	0.0	
13	1443.6	0.0	
14	1443.6	0.0	
15	1443.6	0.0	
16	1443.6	0.0	
17	1443.6	0.0	
18	1443.6	0.0	
19	1443.6	0.0	
20	1443.6	0.0	
21	1443.6	0.0	
22	1443.6	0.0	
23	1443.6	0.0	
24	1443.6	0.0	