

# C7800

# Počítačová chemie a molekulové modelování I - cvičení

Referenční manuál - Nemesis

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# Nemesis

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# Nemesis

## Spuštění programu:

\$ module add nemesis

\$ nemesis

## Myš:

Levé tlačítko                      selekce

Prostřední tlačítko              rotace

Levé tlačítko                      posun

Kolečko                              zoom

## Modifikátory:

Shift                                  XZ -> Y pohyby

Ctrl                                    přepíná mezi sekundárním a primárním manipulátorem

# 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 first row is "Structure 1" with "SID" 1. A blue arrow points to this row with the label "vrstvy".
- Build panel:** Contains various chemical symbols and buttons. A blue arrow points to the "O=" symbol with the label "stavba/editace molekuly". The "Optimize" button is circled in red, with a blue arrow pointing to it from the label "optimalizace geometrie pomocí silového pole".
- Profile objects panel:** Contains a table with columns "Name" and "Ty". The first row is "Light 1" with "Ty" "Light". A blue arrow points to this row with the label "grafické modely".
- Geometry panel:** Contains buttons for "Position", "Distance", "Angle", and "Torsion". A blue arrow points to this panel with the label "měření geometrie".

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

Nastavení silového pole pro optimalizaci: menu Geometry-> Optimizer Setup

# Vizualizace optimalizace geometrie

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

The screenshot displays the NEMESIS Molecular Modelling Package interface. The main window shows a 3D ball-and-stick model of an ethane molecule. A blue arrow labeled "dvojklik" (double-click) points from the "Trajectory 1 Structure 1" entry in the "Trajectories" panel to the "Trajectory" dialog box. Another blue arrow labeled "dvojklik" points from the "Trajectory" dialog box to the "Gaussian Geometry Optimization" dialog box. The "Gaussian Geometry Optimization" dialog box has the "Energy" tab selected, showing a table of energy values for six snapshots.

ID	Energy [a.u.]	Relative Energy [kcal]
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 a blue arrow pointing to it from the text "průběh optimalizace" (optimization process).

průběh optimalizace

# Vizualizace vibrací

- 1) Projekt: 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. The Trajectories panel on the left shows 'Trajectory 1 Structure 1'. A blue arrow labeled 'dvojklik' (double-click) points from this entry to the Trajectory window. The Trajectory window shows a table with columns 'SI', 'Name', 'Snapshots', and 'Type'. The first row is '1 ethan\_freq 180 Gaussian Vibratic'. A second blue arrow labeled 'dvojklik' points from this row to the Gaussian Vibrations dialog box. The dialog box has a 'Basic' tab and a table with columns 'ID', 'Frequency', and 'IR Intensity'. The first five rows are highlighted with a blue oval, and a blue arrow labeled 'zvolíme vibraci' (we select vibrations) points to this oval. Below the table, there are fields for 'Number of vibrations: 24' and 'Active vibrations: 0', and buttons 'Activate imaginary' and 'Deactivate all'. A third blue arrow labeled 'spustíme animaci' (we start the animation) points from the dialog box to the animation controls at the bottom of the interface, which include a play button and a stop button, both circled in blue.

SI	Name	Snapshots	Type
1	ethan_freq	180	Gaussian Vibratic

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	