

Referenční manuály

Nemesis

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Nemesis

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Spuštění programu:

\$ module add nemesis

\$ nemesis

Myš:

Levé tlačítko	selekce
Prostřední tlačítko	rotace
Pravé 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:** Located on the right, it has tabs for "Basic" and "General". Under "General", there are buttons for building molecules: C=C, C≡, =C=, F-, Cl-, Br-, I-, O=, O-, S=, S-, N=, N=, N-, N-. A blue arrow points to the Cl- button with the label "stavba/editace molekuly". Below these are buttons for "Delete atom", "Make bond", "Break bond", and "Delete bond". 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:** Located at the bottom left, it shows a list of objects: "Light 1" (Light), "Background 1" (Backgro), "Standard Model 1" (Standar), and "Freezed Atoms 1" (Freezec). A blue arrow points to this panel with the label "grafické modely".
- Geometry panel:** Located at the bottom right, it has tabs 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

Project 1 : NEMESIS - Molecular Modelling Package

en 9:01 PM Petr Kulhanek

Number of trajectories: 1

Active Profile: Profile 1

Profile objects

Name	Type
Light 1	Light
Background 1	Background
Standard Model 1	Standard
Frozen Atoms 1	Frozen

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průběh optimalizace

Vizualizace vibrací

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

The screenshot shows the Nemesis software interface. The main window displays a 3D molecular model of ethane. 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 dialog box. The Trajectory dialog box shows a table with columns 'SI', 'Name', 'Snapshots', and 'Type'. The first row is '1 ethan_freq 180 Gaussian Vibratic'. A blue arrow labeled 'dvojklik' points from this row to the Gaussian Vibrations dialog box. The Gaussian Vibrations dialog box has a 'Vibrations' tab with a table of vibrational modes. The first six rows are circled in orange, with a blue arrow labeled 'zvolíme vibraci' (we select vibrations) pointing to them. Below the table are fields for 'Number of vibrations: 24' and 'Active vibrations: 0', and buttons 'Activate imaginary' and 'Deactivate all'. A blue arrow labeled 'spustíme animaci' (we start the animation) points from the 'Activate imaginary' button to the animation controls at the bottom of the interface, which include a play button and a stop button, both circled in orange.

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	