

TSM

Modelování molekulárních struktur

Referenční manuál - Nemesis

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Nemesis

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 "Cl-" symbol with the label "stavba/editace molekuly". The "Optimize" button is circled in red, with a blue arrow pointing to it and 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

Project 1 : NEMESIS - Molecular Modelling Package

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

dvojklik

dvojklik

SI	Name	Snapshots	Type
1	ethan	6	Gaussian Geometry Optimization

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

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' 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 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 10 rows are highlighted in orange, and a blue arrow labeled 'zvolíme vibraci' points to this selection. Below the table, there are fields for 'Number of vibrations: 24' and 'Active vibrations: 0', and buttons 'Activate imaginary' and 'Deactivate all'. A blue arrow labeled 'spustíme animaci' points from the dialog box to the animation controls at the bottom of the interface, which include a play button and a stop button.

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	