Visualizing molecular structures for analysis of NMR spectra

Start in ChemDraw

- 1. Make a molecule in ChemDraw
- 2. Select it
- 3. Copy to clipboard in SMILES format: Edit:Copy As:SMILES

Load a molecule in Avogadro and optimize geometry

Avogadro manuals are here: https://avogadro.cc/docs/

- 1. Start a new document: File: New
- 2. Build:Insert:SMILES
- 3. Paste from clipboard (Cmd-V or Ctrl-V), click OK
- 4. Set view parameters: Display Settings, check Ball and Stick
- 5. Right-click to deselect the atoms
- 6. Optimize molecular geometry by energy minimization: Extensions:Optimize Geometry

Parameters of geometry optimization are set in Extensions: Molecular Mechanics: Setup force field. For more details on force fields and optimization see https://avogadro.cc/docs/optimizing-geometry/molecular-mechanics/

Distance measurements in Avogadro

- 1. Rotate the molecule to see both atoms of interest with Select Tool
- 2. Press Click to Measure button in the toolbar
- 3. Click first atom, click second atom
- 4. Read the distance on the bottom of the screen
- 5. Clicking on the same atom again removes it from the selection

From:

https://pydio.campus.nd.edu/docs/ - NMR

Permanent link:

https://pydio.campus.nd.edu/docs/doku.php?id=visualization_of_molecules&rev=1748819947

Last update: 2025/06/02 00:19

