

# Reference manuals

Avogadro

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# Avogadro

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[http://avogadro.openmolecules.net/wiki/Main\\_Page](http://avogadro.openmolecules.net/wiki/Main_Page)

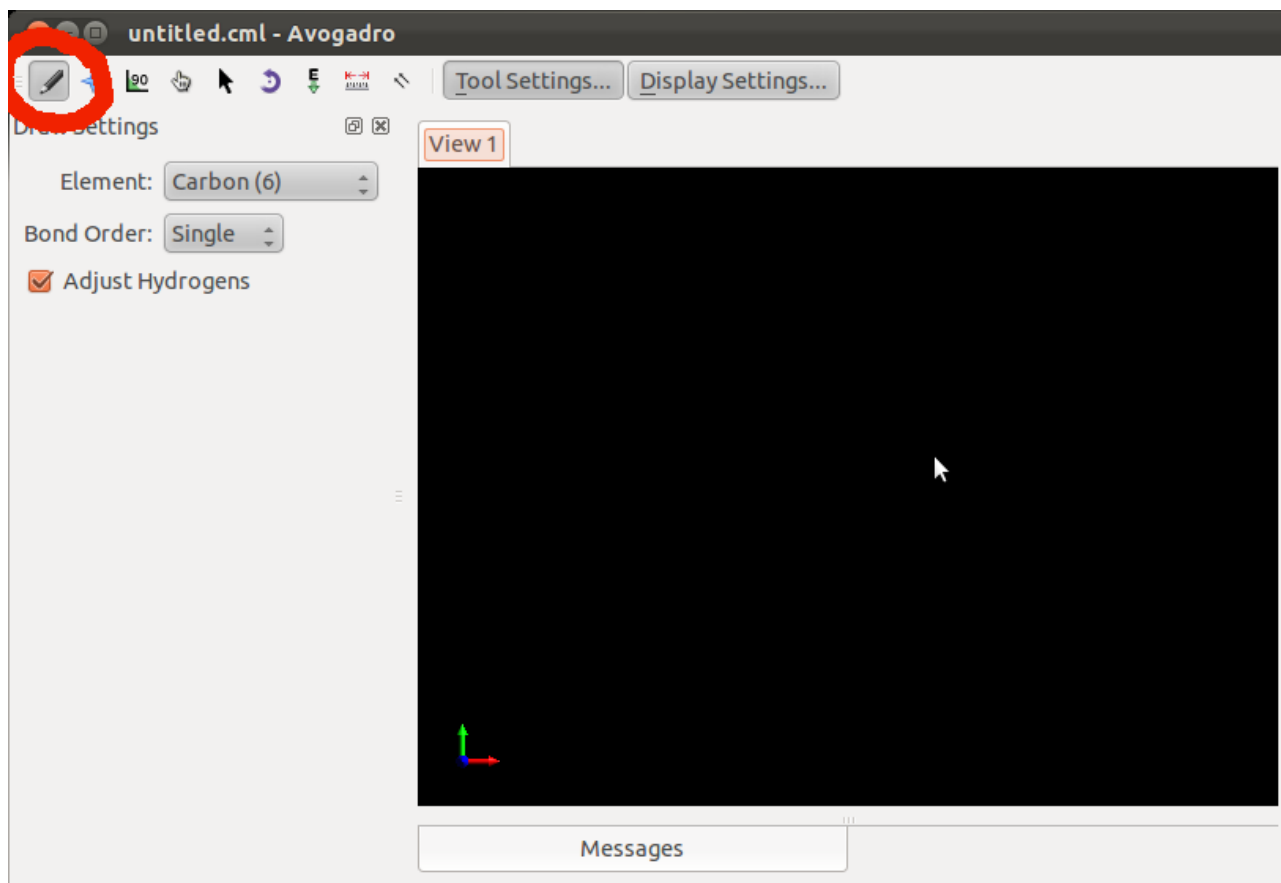
Program for construction and visualization of molecules. Freely available for MS Windows and Linux.

Functionality overview: <https://www.youtube.com/watch?v=xdmLoBILmq5>

# Building a model

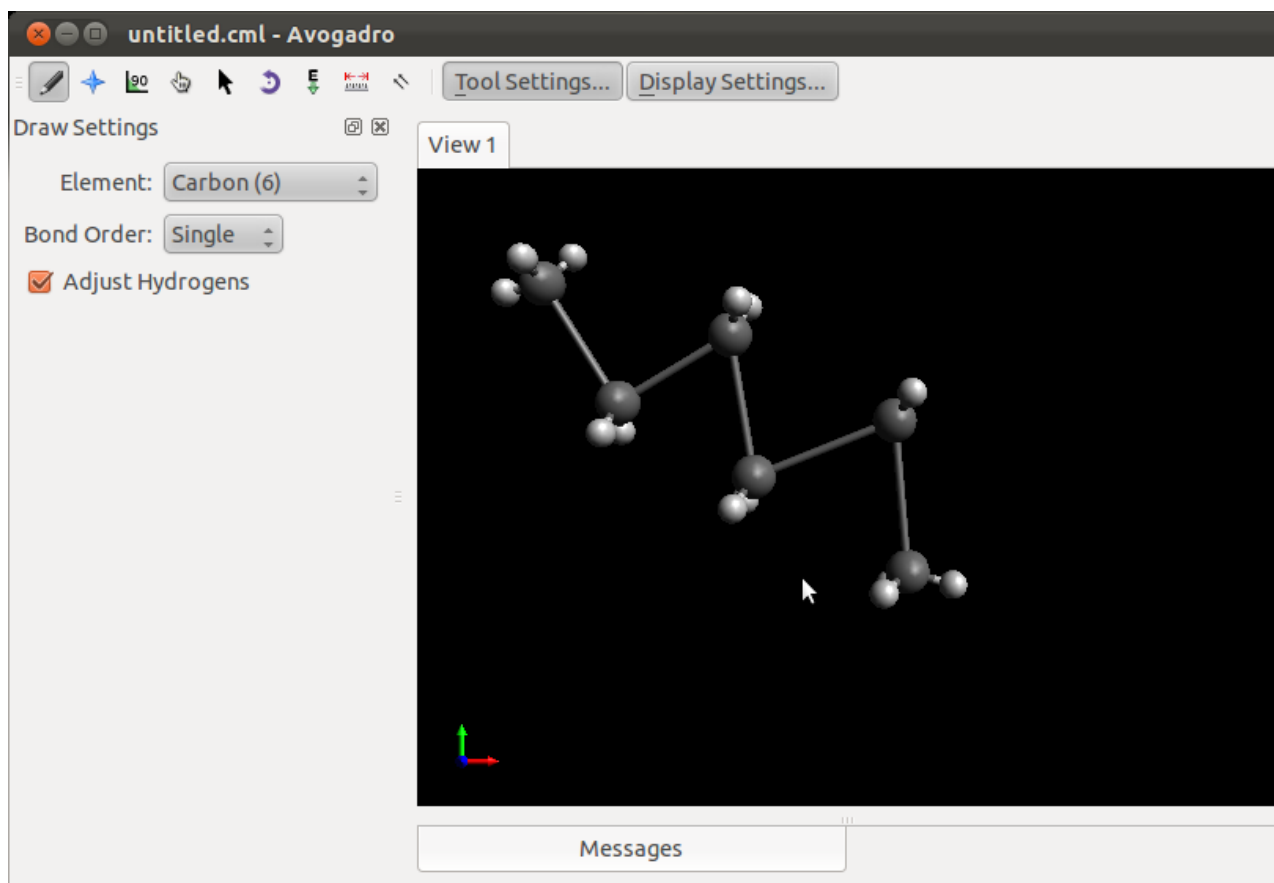
# Building a model

You can use the **Avogadro** program to build a 3D model of the reactant and the product. It is a freely distributed program that can be used both under the MS Windows operating system and under Linux clones (e.g., Ubuntu).



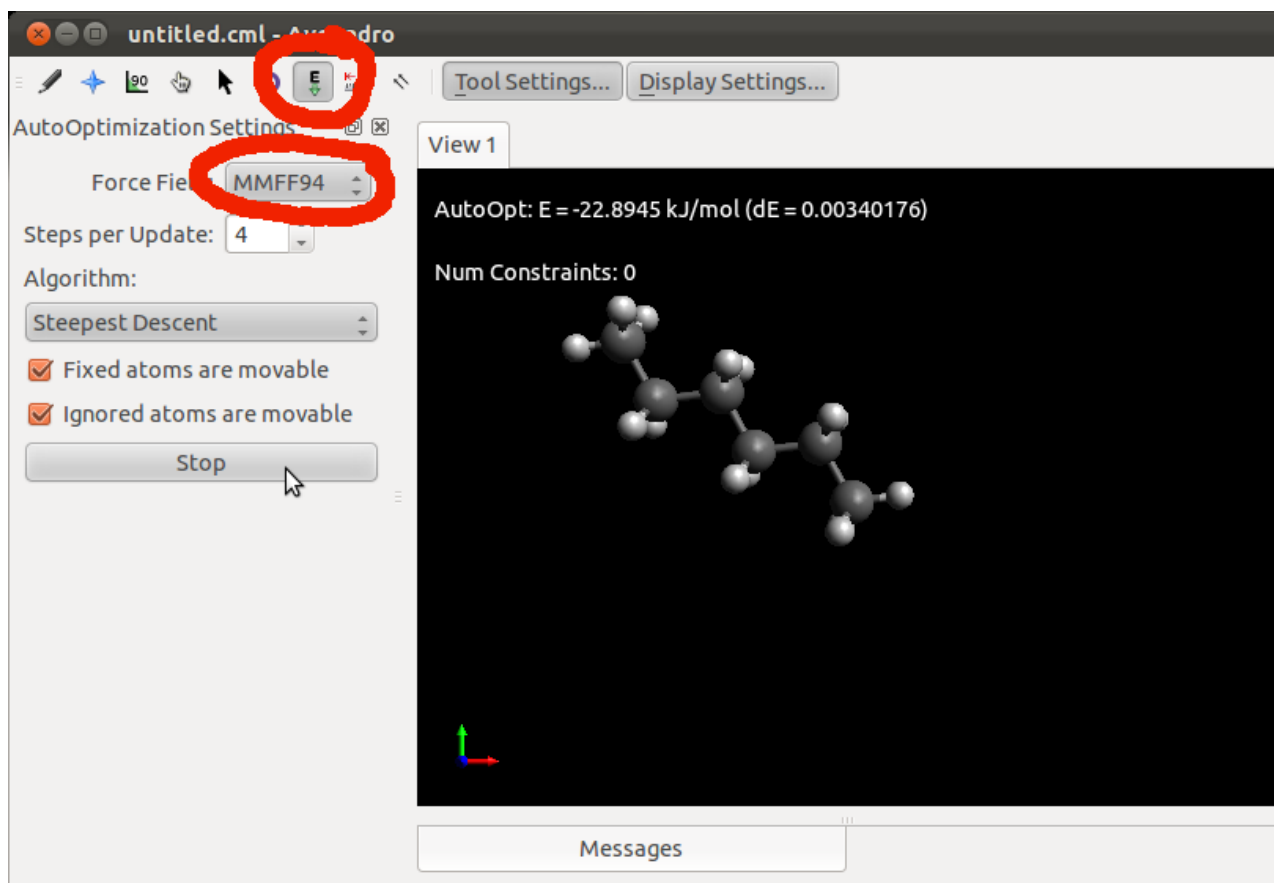
# Model draft

When building a molecule, the bond lengths, angles and other parameters of the molecule are not optimal. This is due to the way structures are edited in the Avogadro program. The draft model must therefore be modified by optimizing the geometry before further use.



# Model optimization

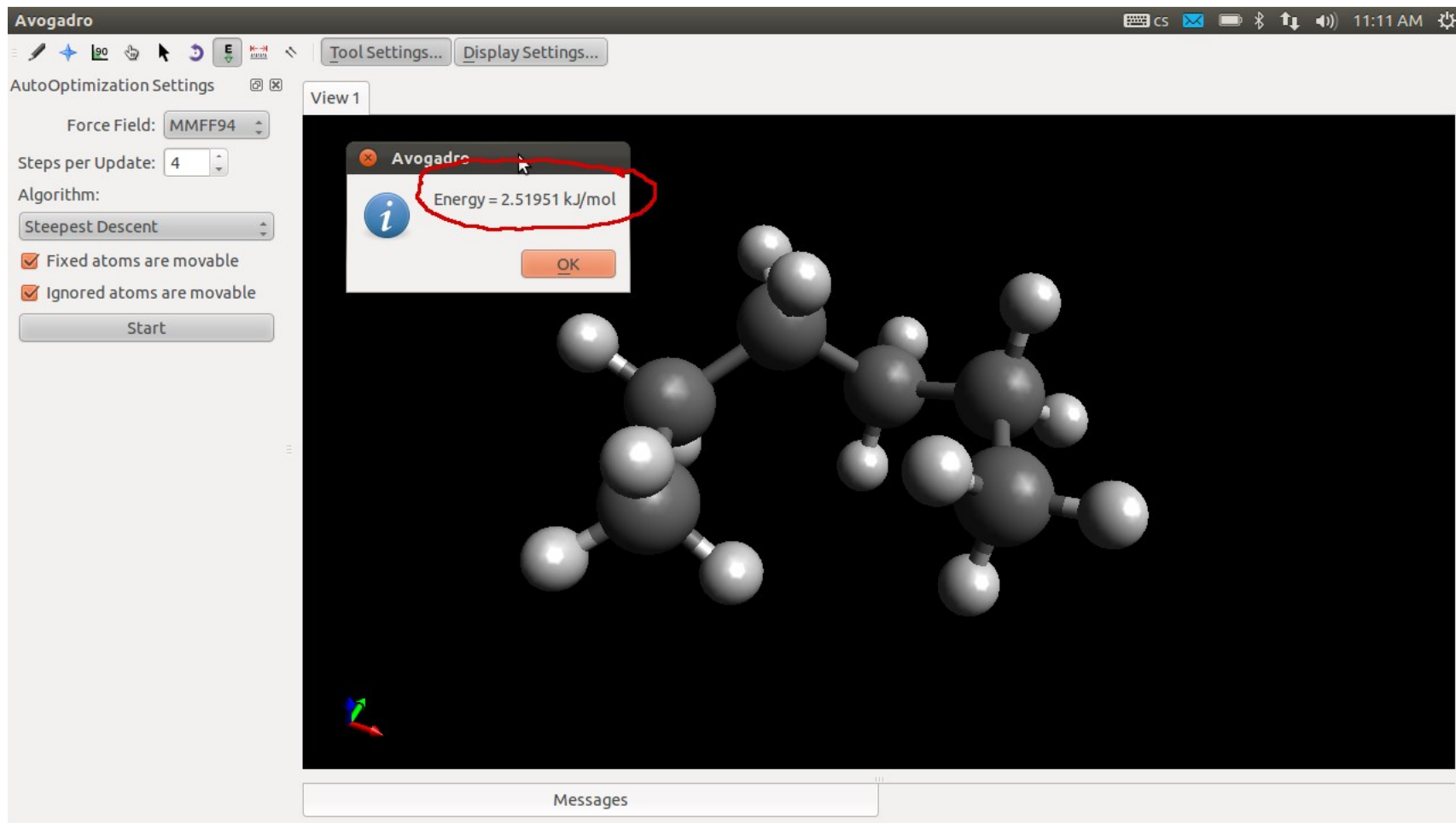
The program uses molecular mechanics (MM) methods to optimize geometry. For it to function properly, you must correctly define bond orders in the structure. Because MM is an empirical method, you must also choose the type of parameterization. In our case, we will use the force field MMFF94.



# Searching for the global minimum

# Finding the most stable geometry, I

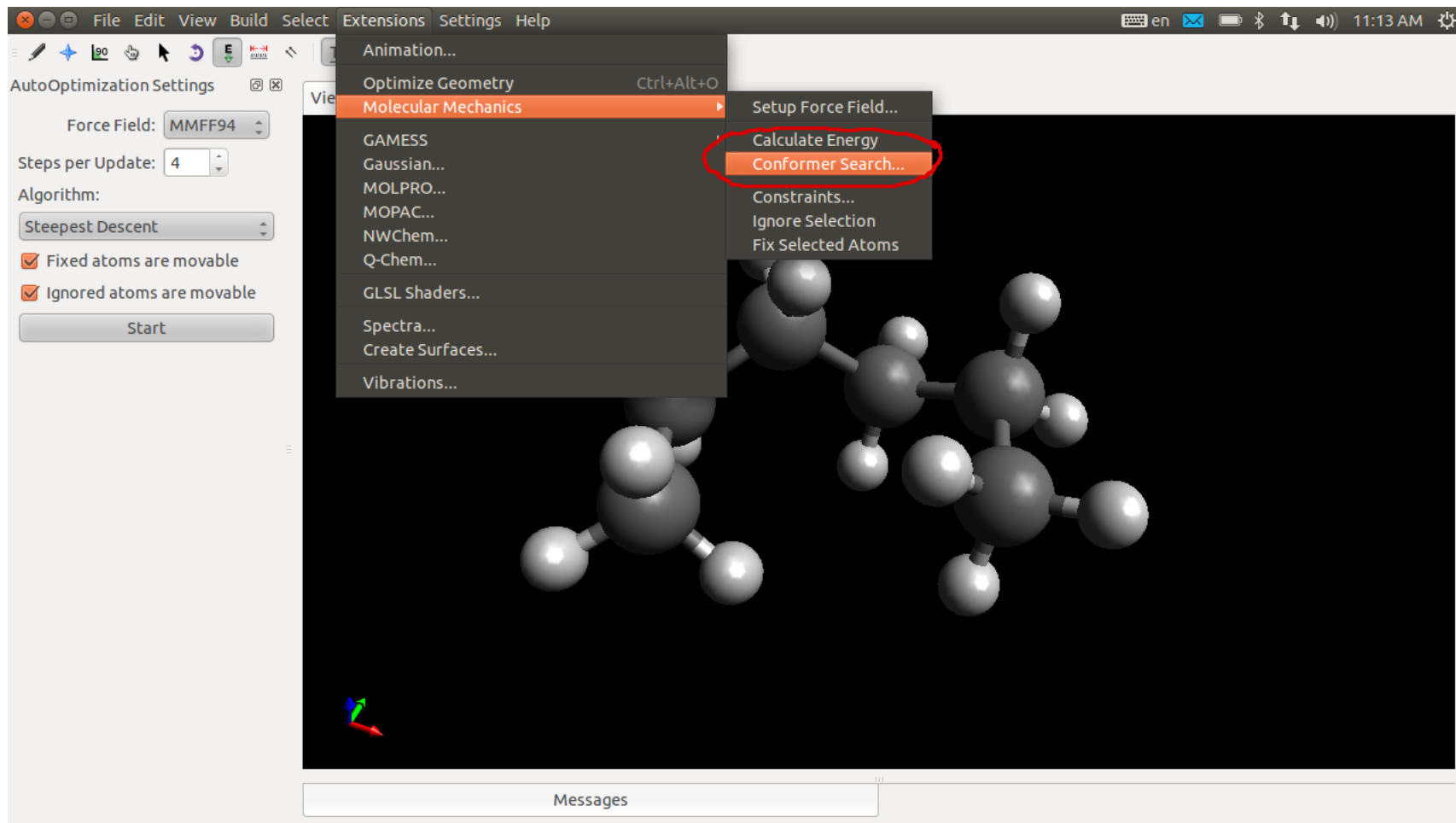
Default optimized geometry of the hexane has energy 2.5 kJ/mol (MMFF94). It is a local minimum on the potential energy surface, which is not the lowest.





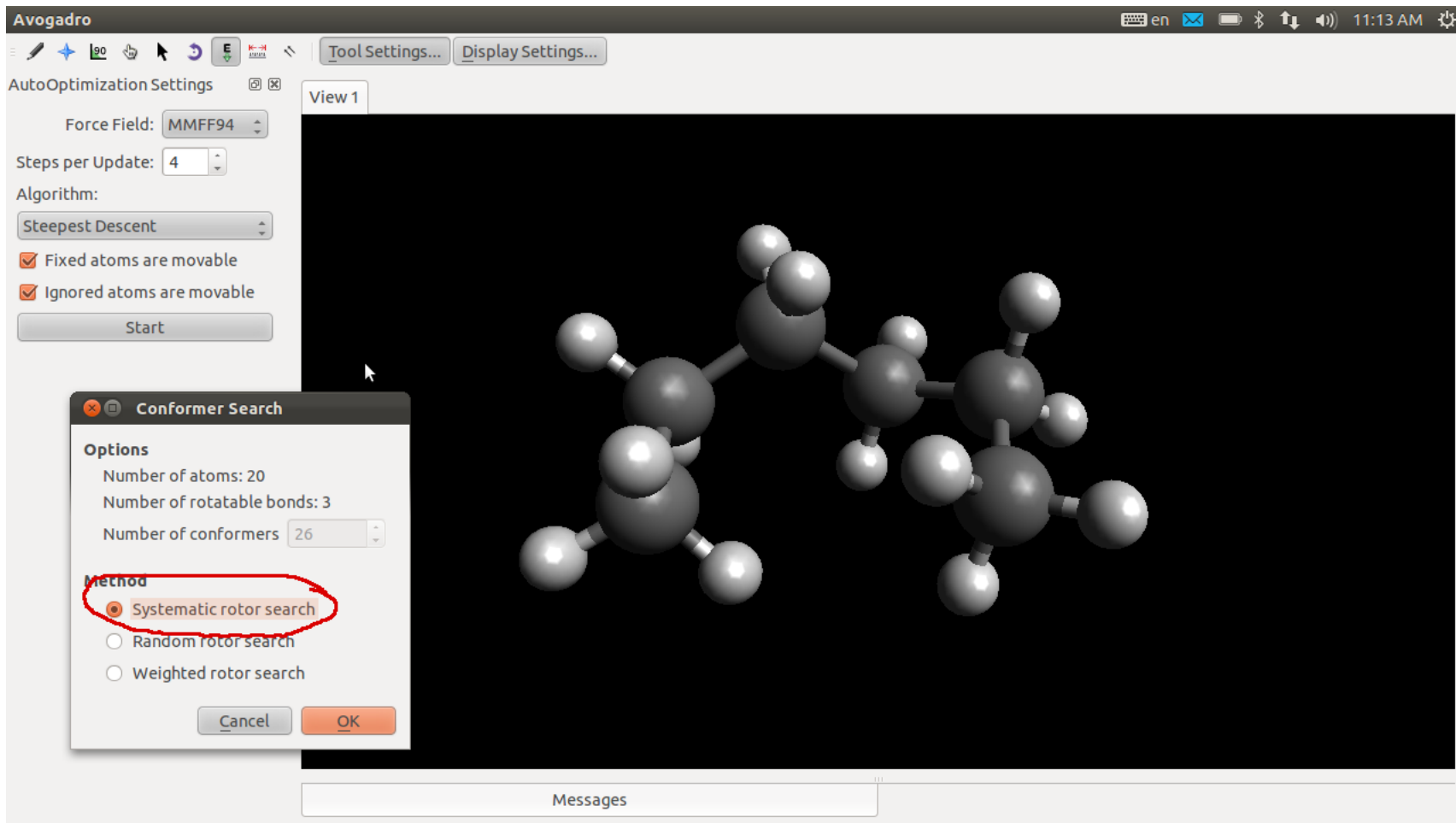
# Finding the most stable geometry, II

Avogadro contains methods for finding the most stable conformer (structures).



# Finding the most stable geometry, III

To find the most stable conformer we will use the systematic search method.



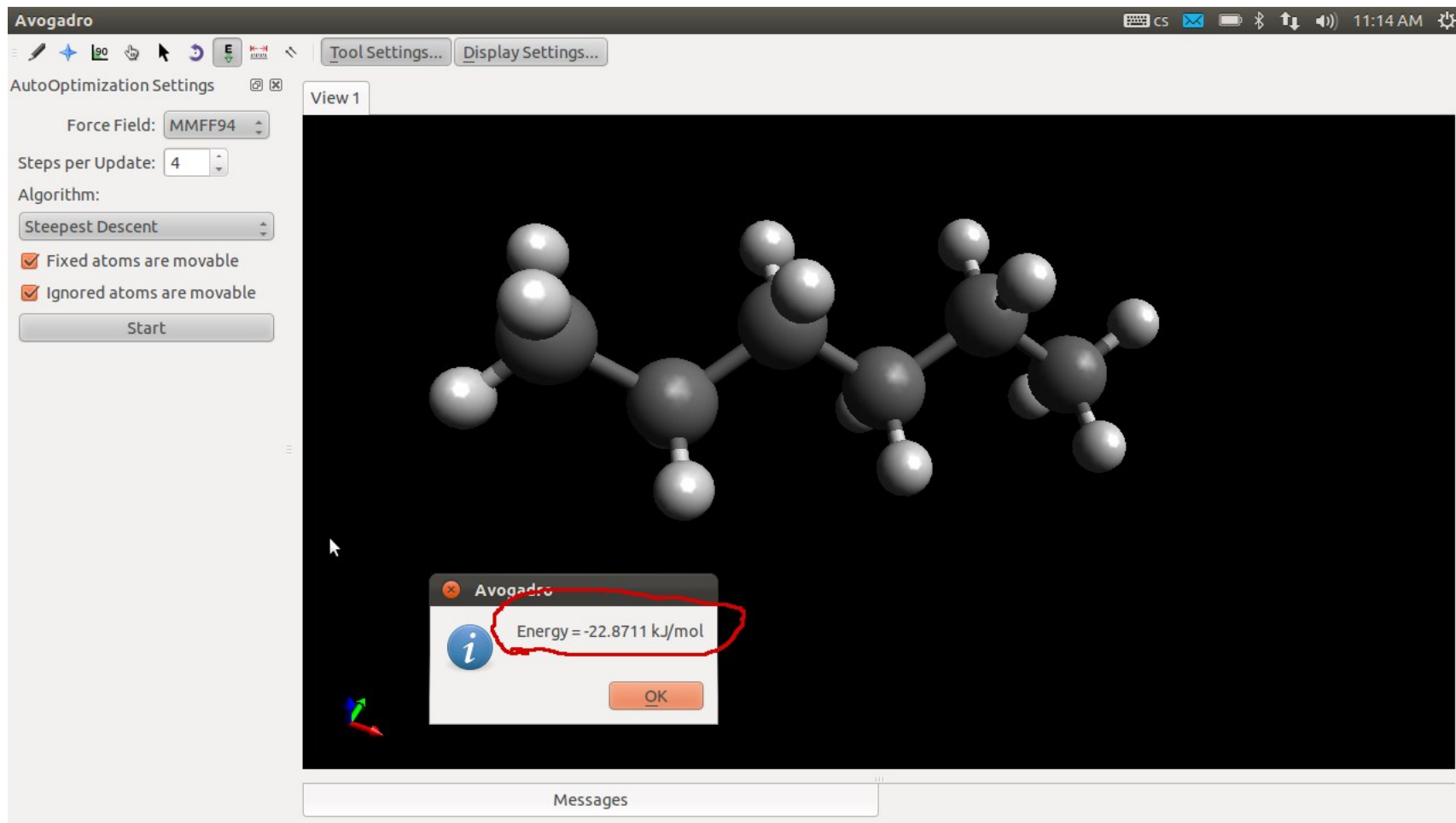
The screenshot displays the Avogadro software interface. The main window shows a 3D ball-and-stick model of a molecule. On the left, the 'AutoOptimization Settings' panel is visible, with 'Force Field' set to 'MMFF94', 'Steps per Update' set to 4, and 'Algorithm' set to 'Steepest Descent'. A 'Conformer Search' dialog box is open in the foreground, showing the following options:

- Options
  - Number of atoms: 20
  - Number of rotatable bonds: 3
  - Number of conformers: 26
- Method
  - Systematic rotor search
  - Random rotor search
  - Weighted rotor search

The 'Systematic rotor search' option is highlighted with a red circle. The dialog box also includes 'Cancel' and 'OK' buttons. The background shows the Avogadro interface with a toolbar and a 'Messages' panel at the bottom.

# Finding the most stable geometry, IV

The most stable hexane conformer has energy -22.9 kJ/mol (MMFF94). The geometry of the found structure should be optimized again.



# Vibration visualization

# Vibration visualization

Load [soubor.log](#), containing results of vibration analysis, into Avogadro program. A summary of individual normal vibration frequencies can be found in the menu **Extensions->Vibrations**.

The screenshot shows the Avogadro interface with the 'Molecular Vibrations' dialog box open. The dialog box contains a table with two columns: 'Frequency (cm<sup>-1</sup>)' and 'Intensity (km/mol)'. The table lists 8 vibrational modes. A blue arrow points from the 'Start Animation' button to the 'vibration visualization' label. Another blue arrow points from the '1,119.9' frequency value in the table to the 'vibration frequency' label. The background shows a 3D ball-and-stick model of a molecule.

	Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
1	223.7	0.0
2	877.8	1.5
3	878.0	1.5
4	1,119.8	0.0
5	1,119.9	0.0
6	1,138.0	0.0
7	1,359.2	0.3
8	1,408.1	0.3

Options:

- Scale: [Slider]
- Display force vectors
- Animation speed set by frequency

Buttons: Start Animation, Export..., Close

Labels: vibration visualization, vibration frequency