Explore Chemistry with Avogadro

About Avogadro…

- Free and Open Source software
- Construct, edit and view molecules in 3D
- 3D Molecular Editor and Visualization tool
- Designed for use on Mac, Windows, and Linux OS
- Downloaded from http://avogadro.cc

MSN India | Breaking News, Ente | Avogadro - Free cross-platform

Not secure | avogadro.cc

Paused

Avogadro

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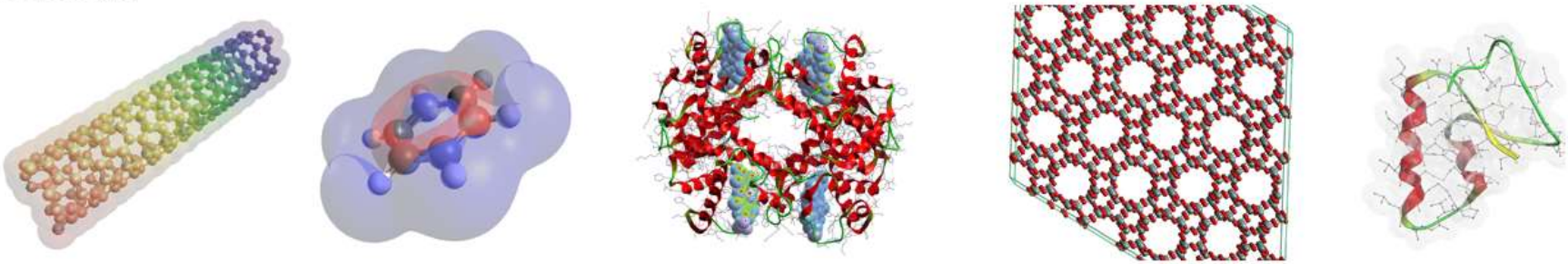
Avogadro is an advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high quality rendering and a powerful plugin architecture.



- **Cross-Platform:** Molecular builder/editor for Windows, Linux, and Mac OS X.
- **Free, Open Source**: Easy to install and all source code and documentation is available to modify or extend.
- **International**: Translations into Chinese, French, German, Italian, Russian, Spanish, and others, with more languages to come.
- **Intuitive**: Built to work easily for students and advanced researchers both

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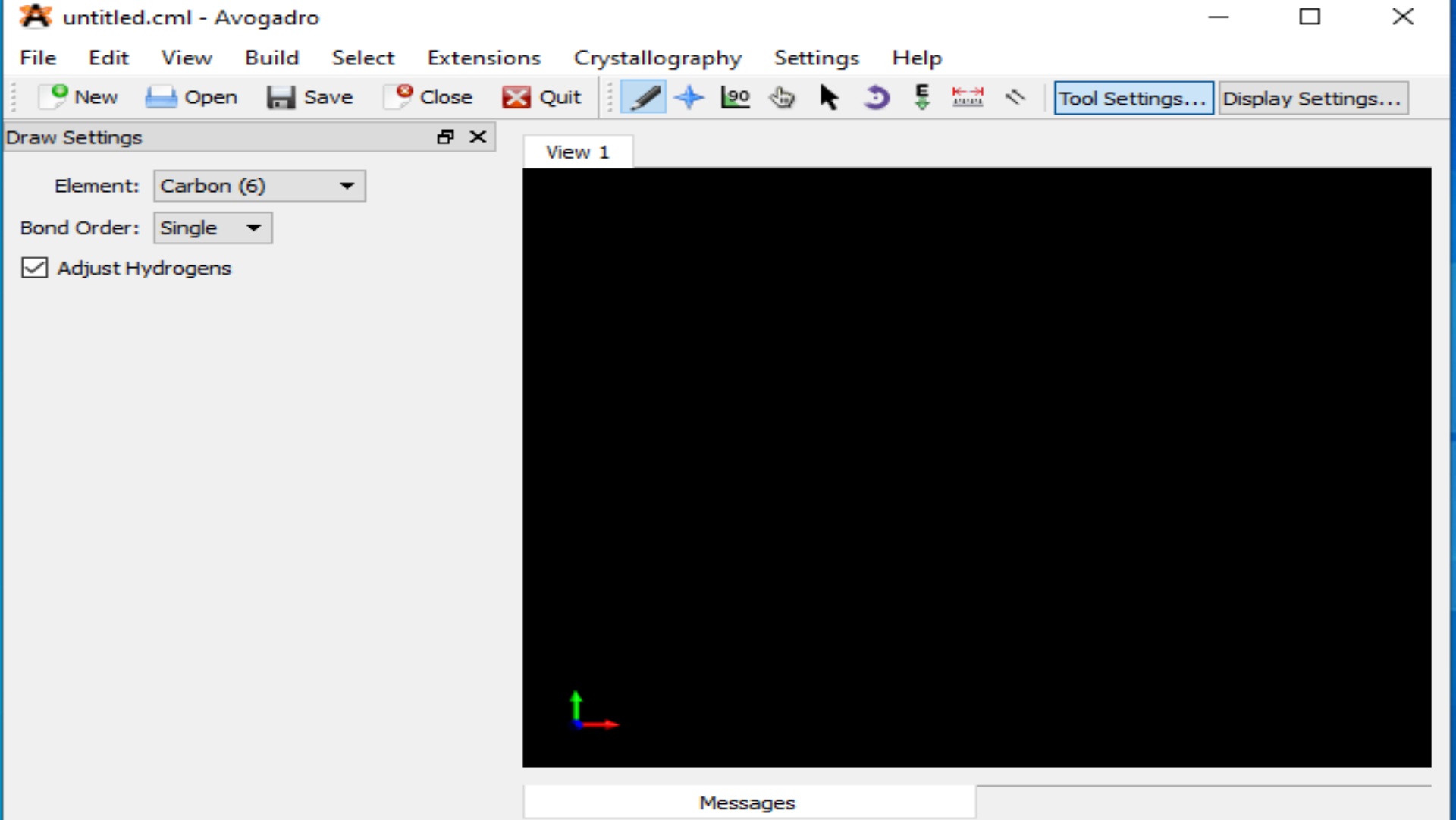
untitled.cml - Avogadro
File
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View
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Select
Extensions
Crystallography
Settings
Help
New
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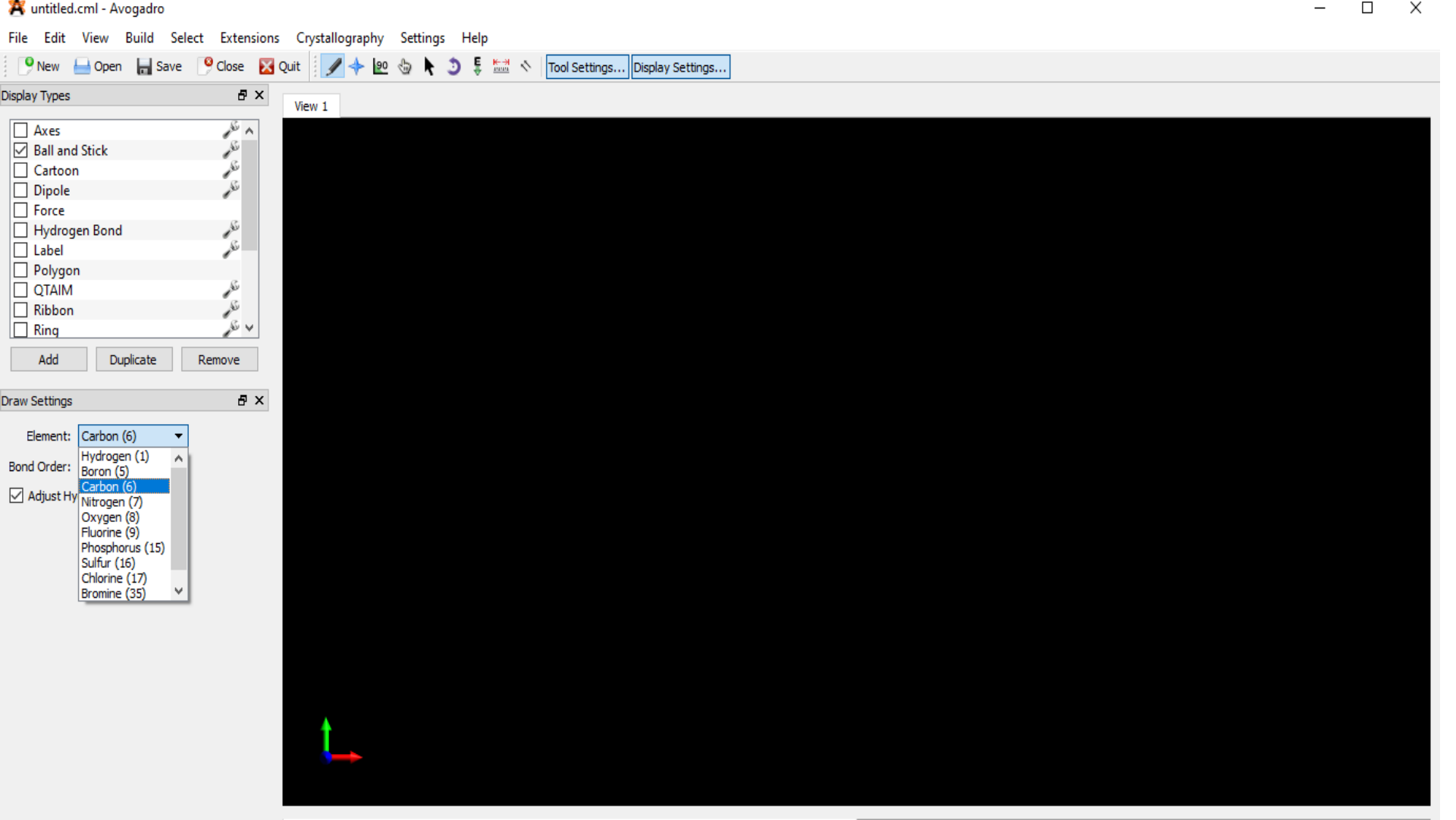
Save
Close
Quit
Tool Settings...
Display Settings...
Draw Settings
Element:
Carbon (6)
Bond Order:
Single
Adjust Hydrogens
View 1
Messages

Let us

Build molecule…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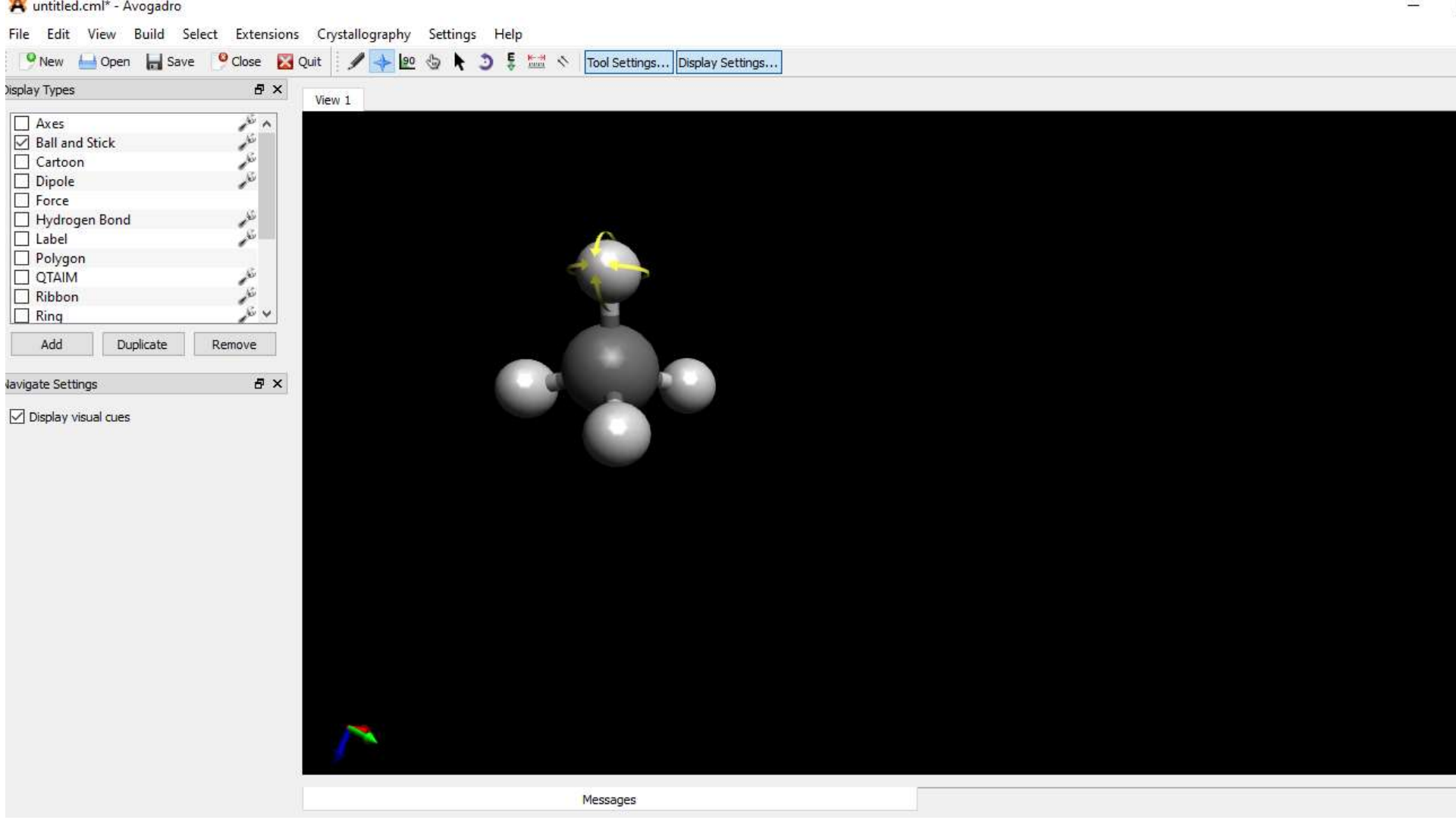
Display Settings...
Display Types
Axes
Ball and Stick
Cartoon
Dipole
Force
Hydrogen Bond
Label
Polygon
QTAIM
Ribbon
Ring
Add
Duplicate
Remove
Draw Settings
Element:
Carbon (6)
Bond Order:
Adjust Hy
Hydrogen (1)
Boron (5)
Carbon (6)
Nitrogen (7)
Oxygen (8)
Fluorine (9)
Phosphorus (15)
Sulfur (16)
Chlorine (17)
Bromine (35)
View 1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Display Settings...
Display Types
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Ball and Stick
Cartoon
Dipole
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Hydrogen Bond
Label
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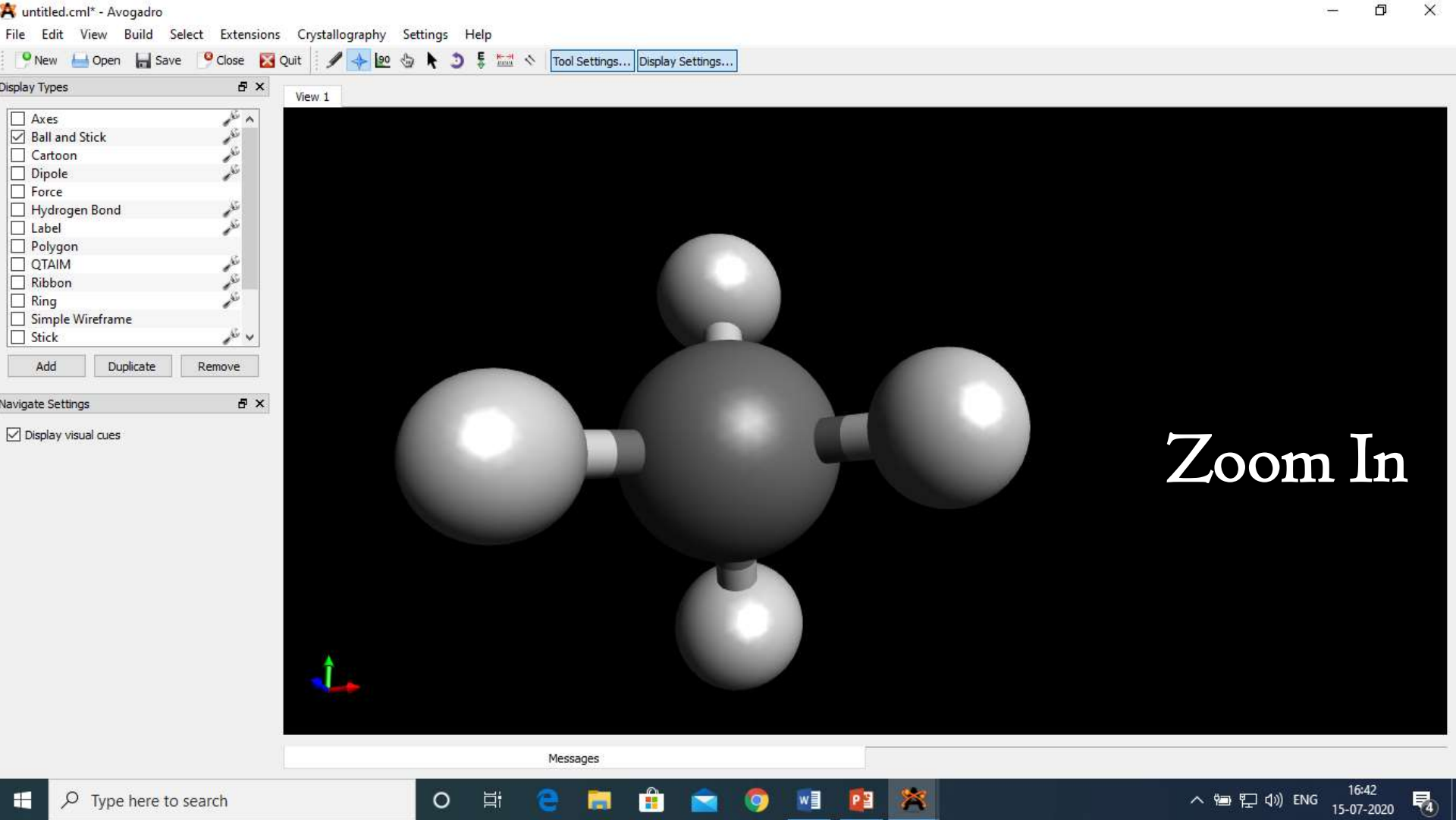
QTAIM
Ribbon
Ring
Add
Duplicate
Remove
Navigate Settings
Display visual cues
View 1
Messages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Hydrogen Bond
Label
Polygon
QTAIM
Ribbon
Ring
Simple Wireframe
Stick
Add Duplicate Remove
Navigate Settings
Display visual cues
View 1
Zoom In
Messages
Type here to search
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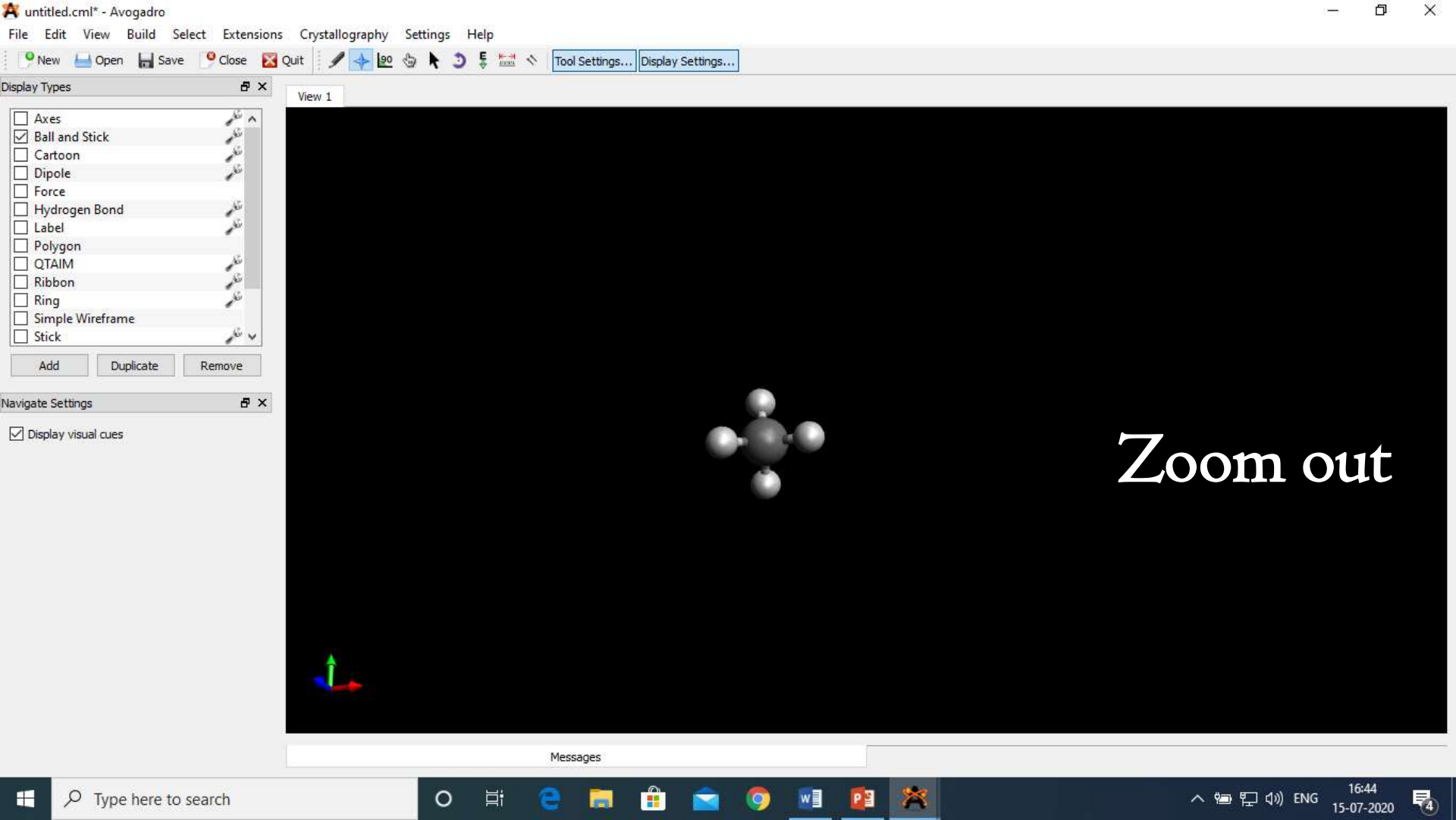
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Hydrogen Bond
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Polygon
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Ribbon
Ring
Simple Wireframe
Stick
Add Duplicate Remove
Navigate Settings
Display visual cues
View 1
Zoom out
Messages
Type here to search
ENG
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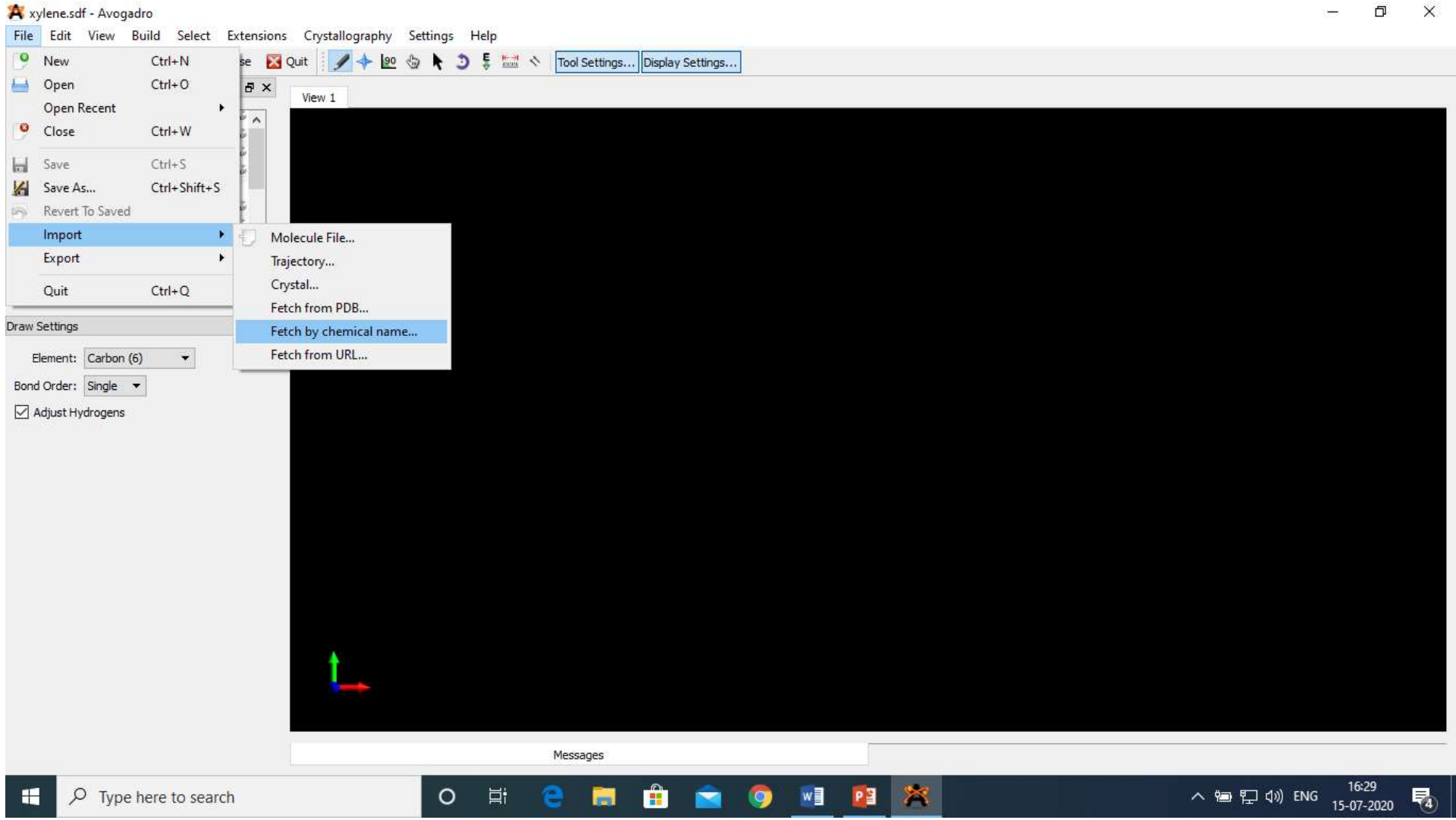
15-07-2020

Explore to Import molecule from Avogadro data base


xylene.sdf - Avogadro
File
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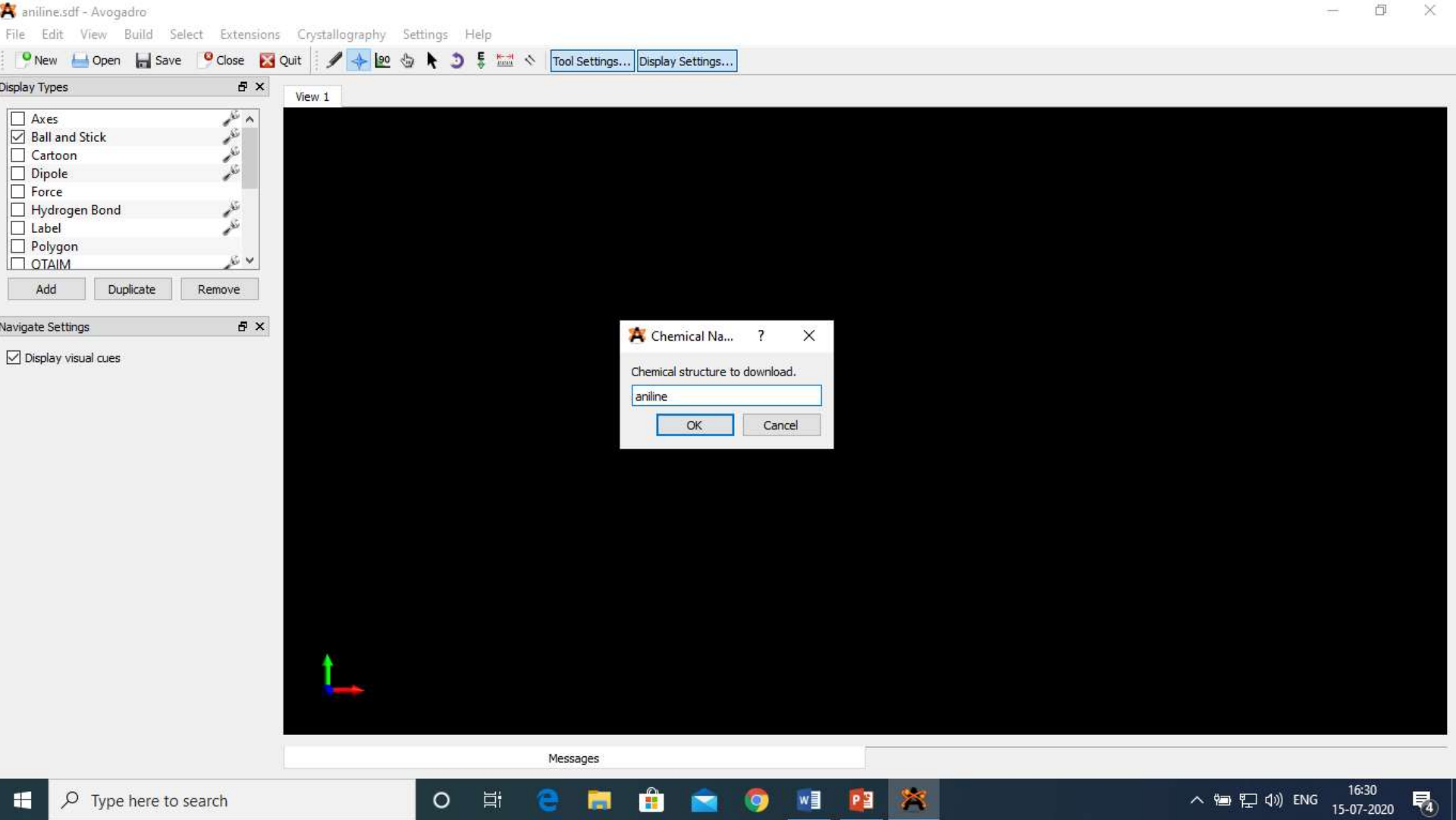
View
Build
Select
Extensions
Crystallography
Settings
Help
New Ctrl+N
Open Ctrl+O
Open Recent
Close Ctrl+W
Save Ctrl+S
Save As... Ctrl+Shift+S
Revert To Saved
Import
Export
Quit Ctrl+Q
Molecule File...
Trajectory...
Crystal...
Fetch from PDB...
Fetch by chemical name...
Fetch from URL...
Quit
Tool Settings...
Display Settings...
View 1
Draw Settings
Element: Carbon (6)
Bond Order: Single
Adjust Hydrogens
Messages
Type here to search
ENG
16:29
15-07-2020


aniline.sdf - Avogadro
File Edit View Build Select Extensions Crystallography Settings Help
New Open Save Close Quit
Tool Settings... Display Settings...
Display Types
Axes
Ball and Stick
Cartoon
Dipole
Force
Hydrogen Bond
Label
Polygon
QTAIM
Add Duplicate Remove
Navigate Settings
Display visual cues
View 1
Chemical Na...
Chemical structure to download.
aniline
OK Cancel
Messages
Type here to search
ENG
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15-07-2020

Aniline.cml - Avogadro

File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

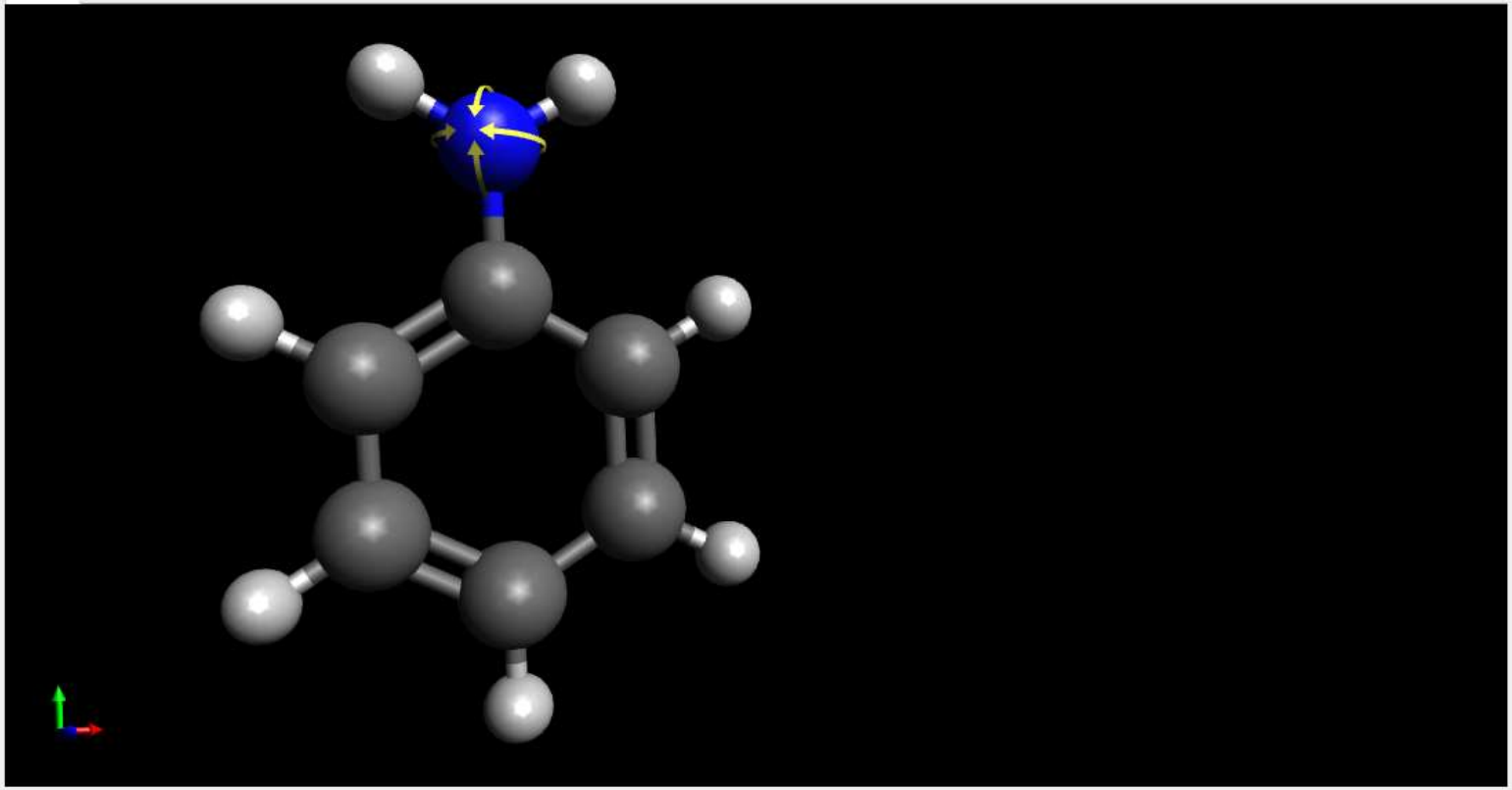
- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [ ] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick
- [ ] Surfaces
- [ ] Van der Waals Spheres
- [ ] Wireframe

Add Duplicate Remove

Navigate Settings

- [x] Display visual cues

View 1



Messages

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Draw and Edit a molecule

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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [ ] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick
- [ ] Surfaces
- [ ] Van der Waals Spheres
- [ ] Wireframe

Add Duplicate Remove

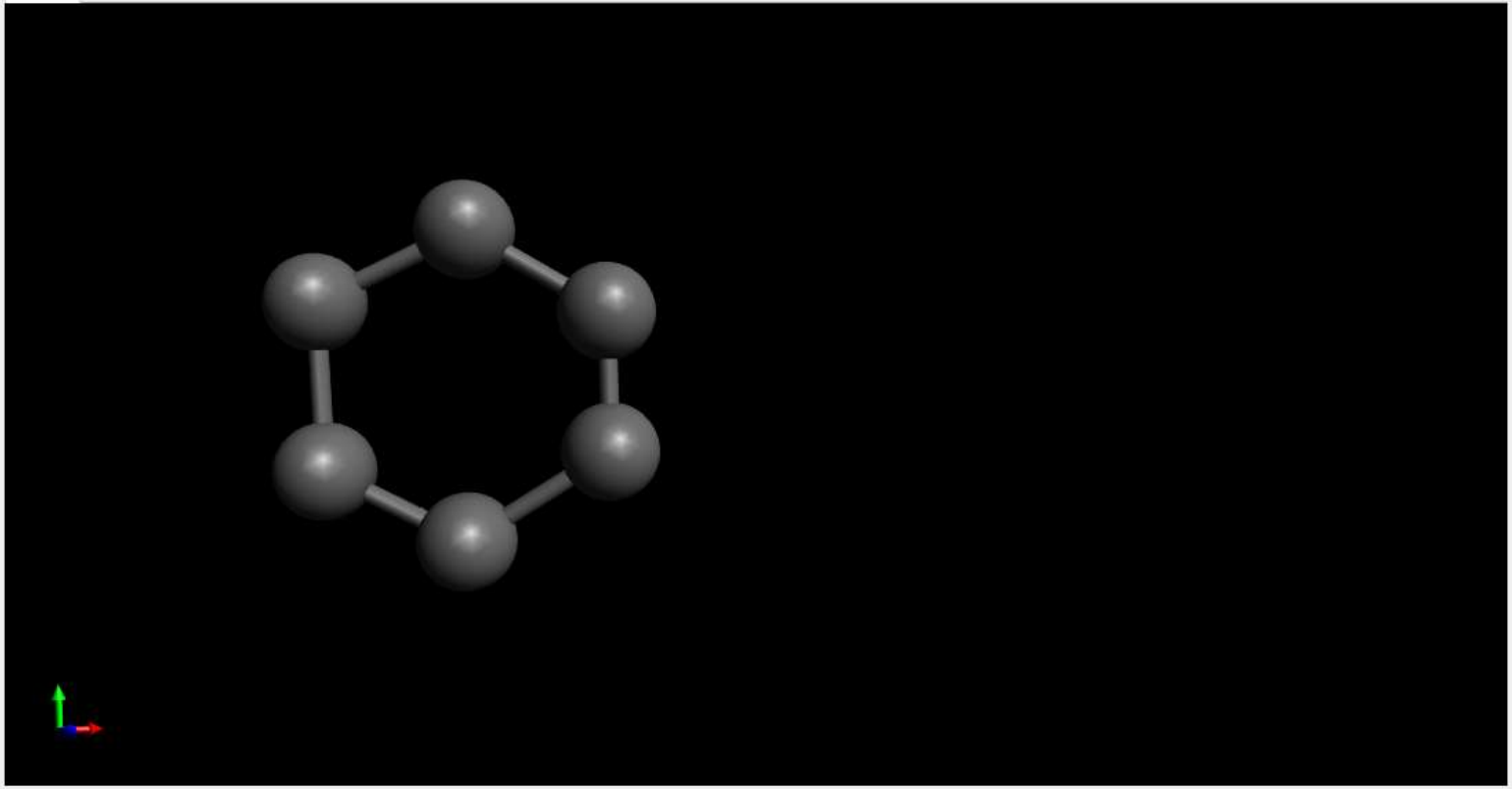
Draw Settings

Element: Carbon (6)

Bond Order: Single

- [ ] Adjust Hydrogens

View 1



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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [ ] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick

Add Duplicate Remove

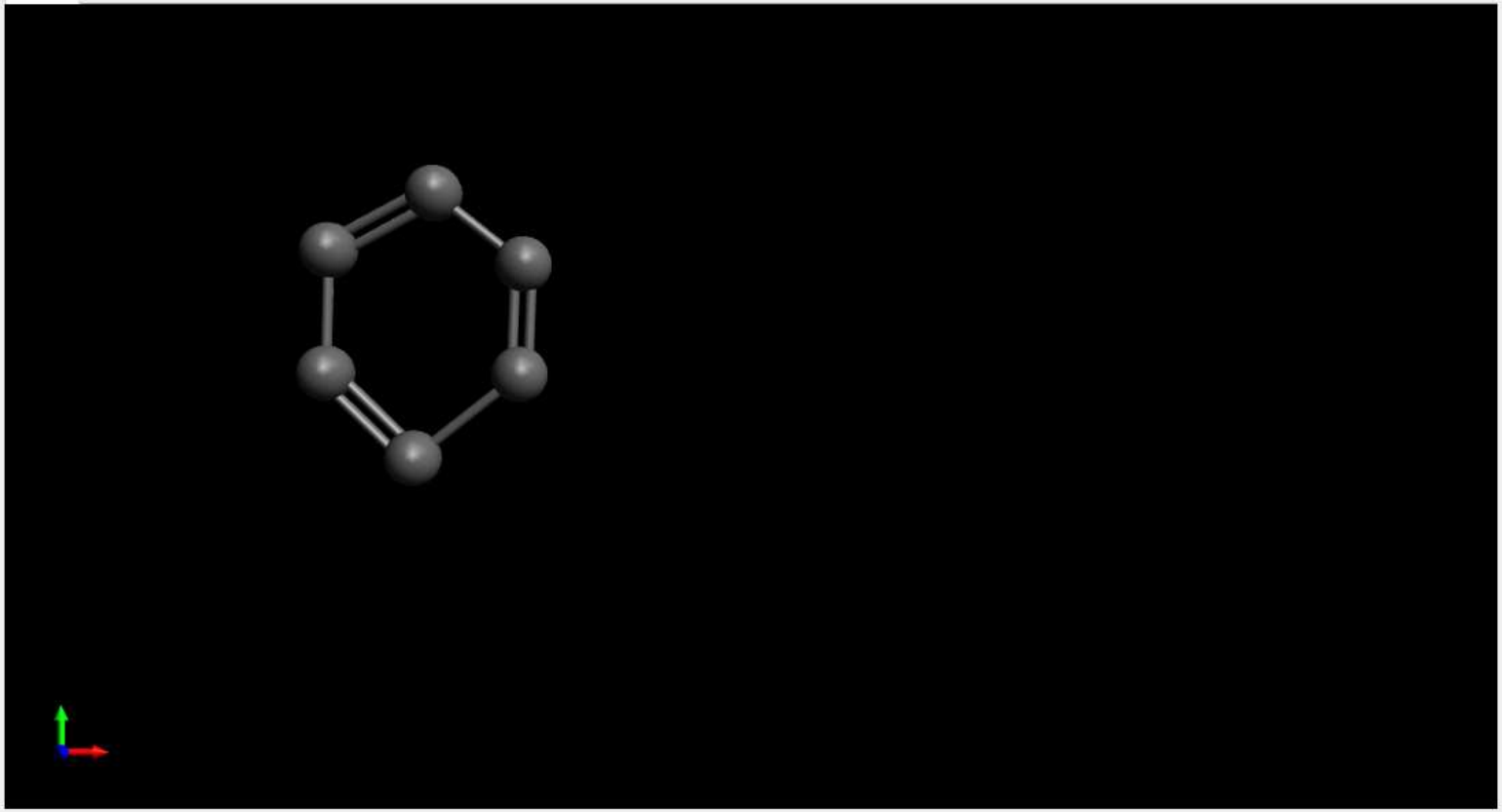
Draw Settings

Element: Nitrogen (7)

Bond Order: Single

- [ ] Adjust Hydrogens

View 1



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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [ ] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick

Add Duplicate Remove

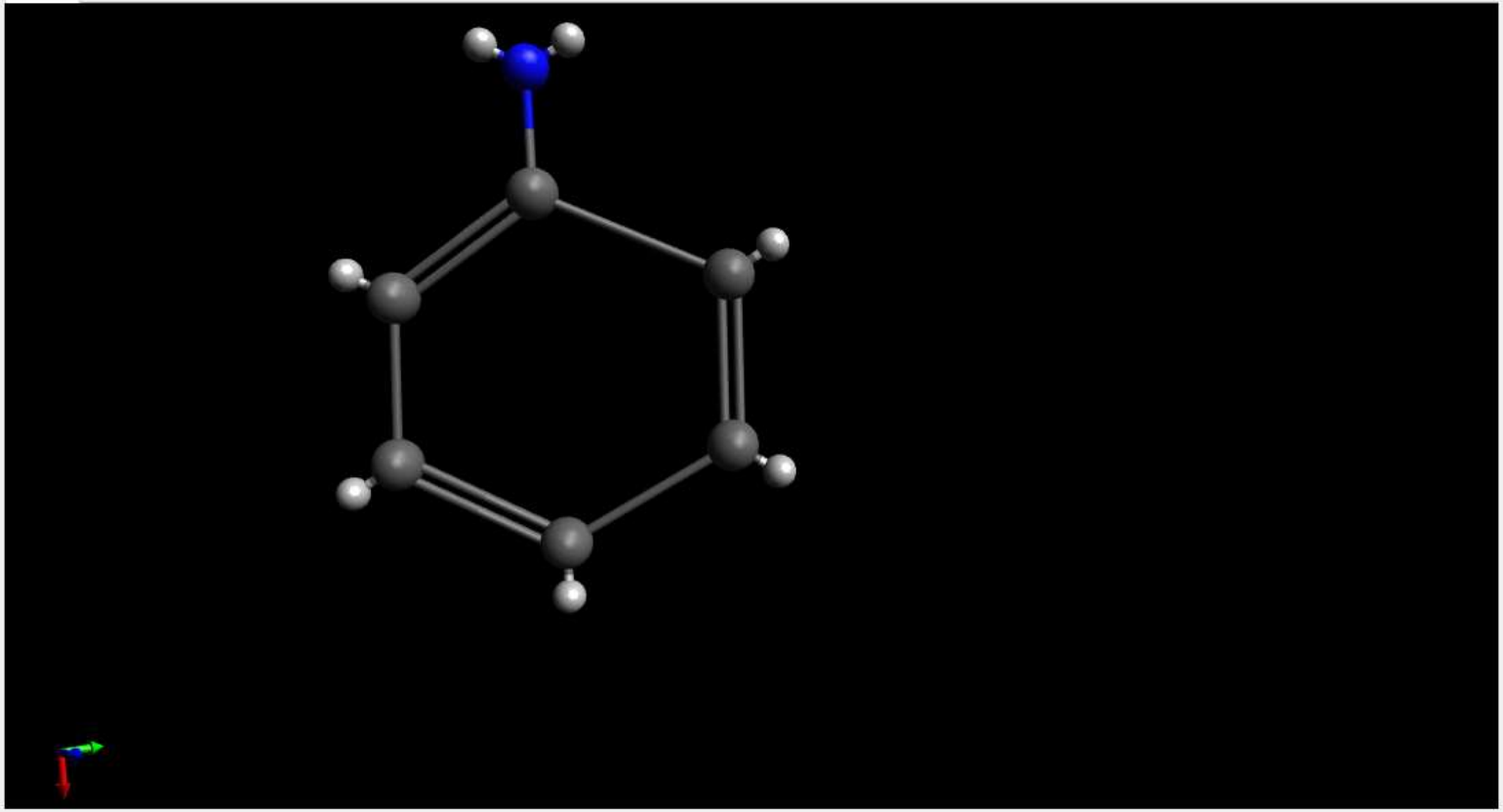
Draw Settings

Element: Nitrogen (7)

Bond Order: Single

- [ ] Adjust Hydrogens

View 1



Messages

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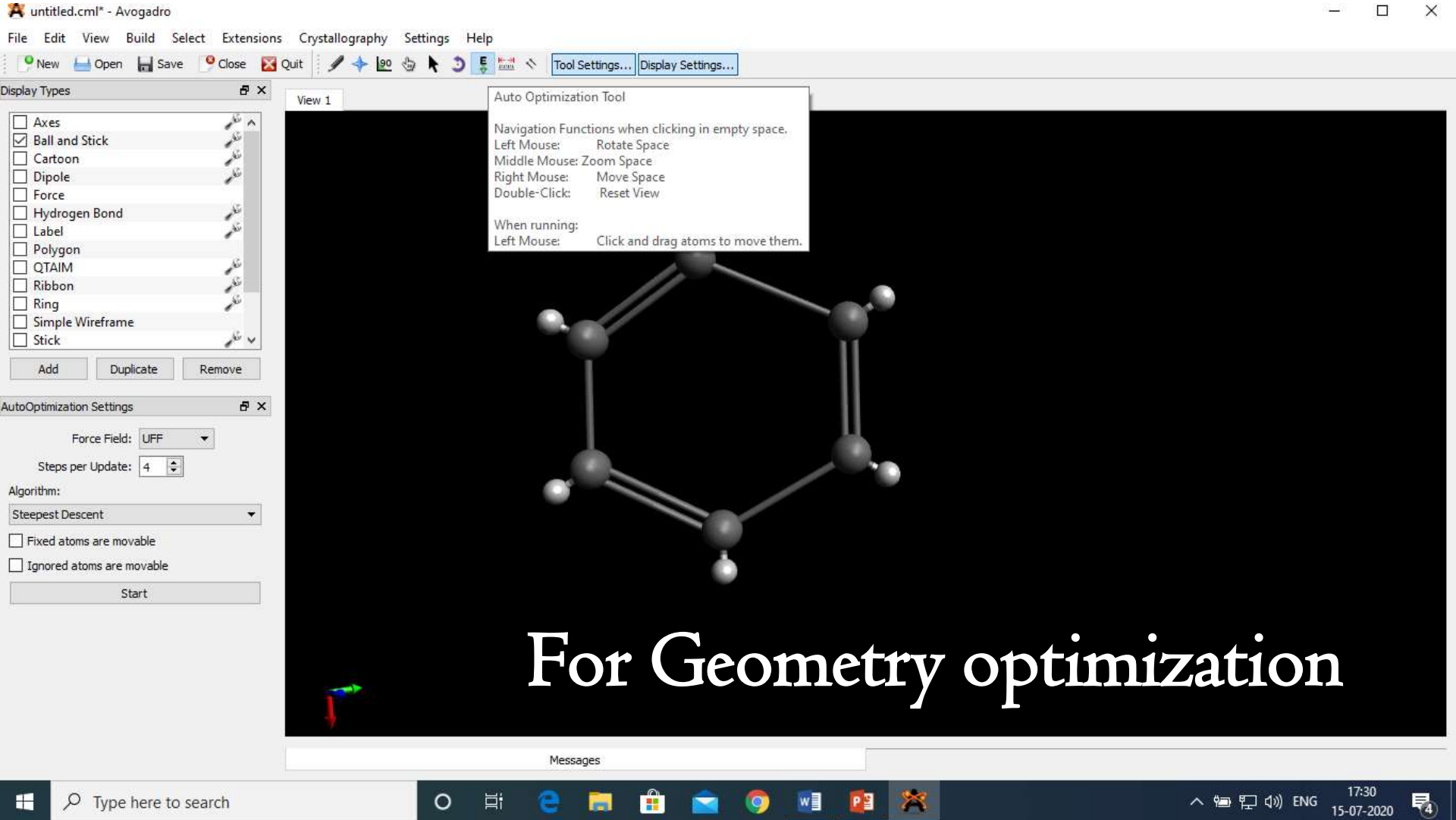
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Display Types
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Ball and Stick
Cartoon
Dipole
Force
Hydrogen Bond
Label
Polygon
QTAIM
Ribbon
Ring
Simple Wireframe
Stick
Add Duplicate Remove
AutoOptimization Settings
Force Field: UFF
Steps per Update: 4
Algorithm:
Steepest Descent
Fixed atoms are movable
Ignored atoms are movable
Start
View 1
Auto Optimization Tool
Navigation Functions when clicking in empty space.
Left Mouse: Rotate Space
Middle Mouse: Zoom Space
Right Mouse: Move Space
Double-Click: Reset View
When running:
Left Mouse: Click and drag atoms to move them.
For Geometry optimization
Messages
Type here to search
ENG
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15-07-2020

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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [ ] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick

Add Duplicate Remove

AutoOptimization Settings

Force Field: UFF

Steps per Update: 4

Algorithm:

Steepest Descent

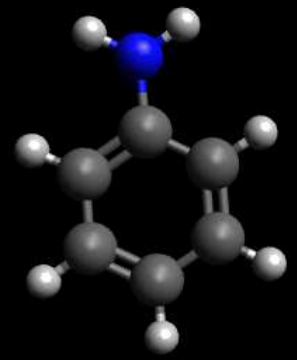
- [ ] Fixed atoms are movable
- [ ] Ignored atoms are movable

Stop

View 1

AutoOpt: E = 49.4359 kJ/mol (dE = 0)

Num Constraints: 0



Messages

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Bond Length, Bond angle and Dihedral angle in a Molecule

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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

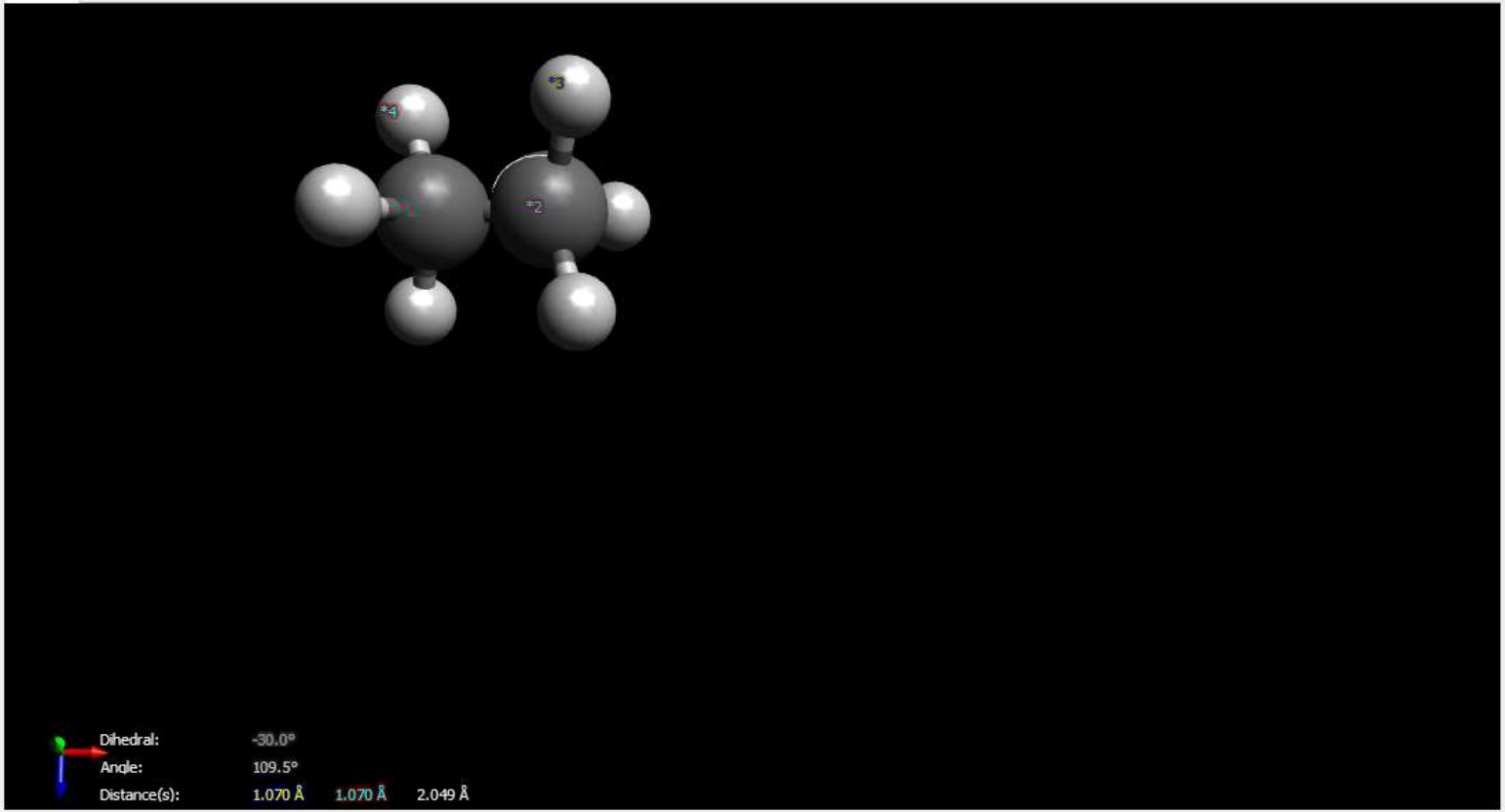
Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [ ] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM

Add Duplicate Remove

Measure Settings

View 1



Messages

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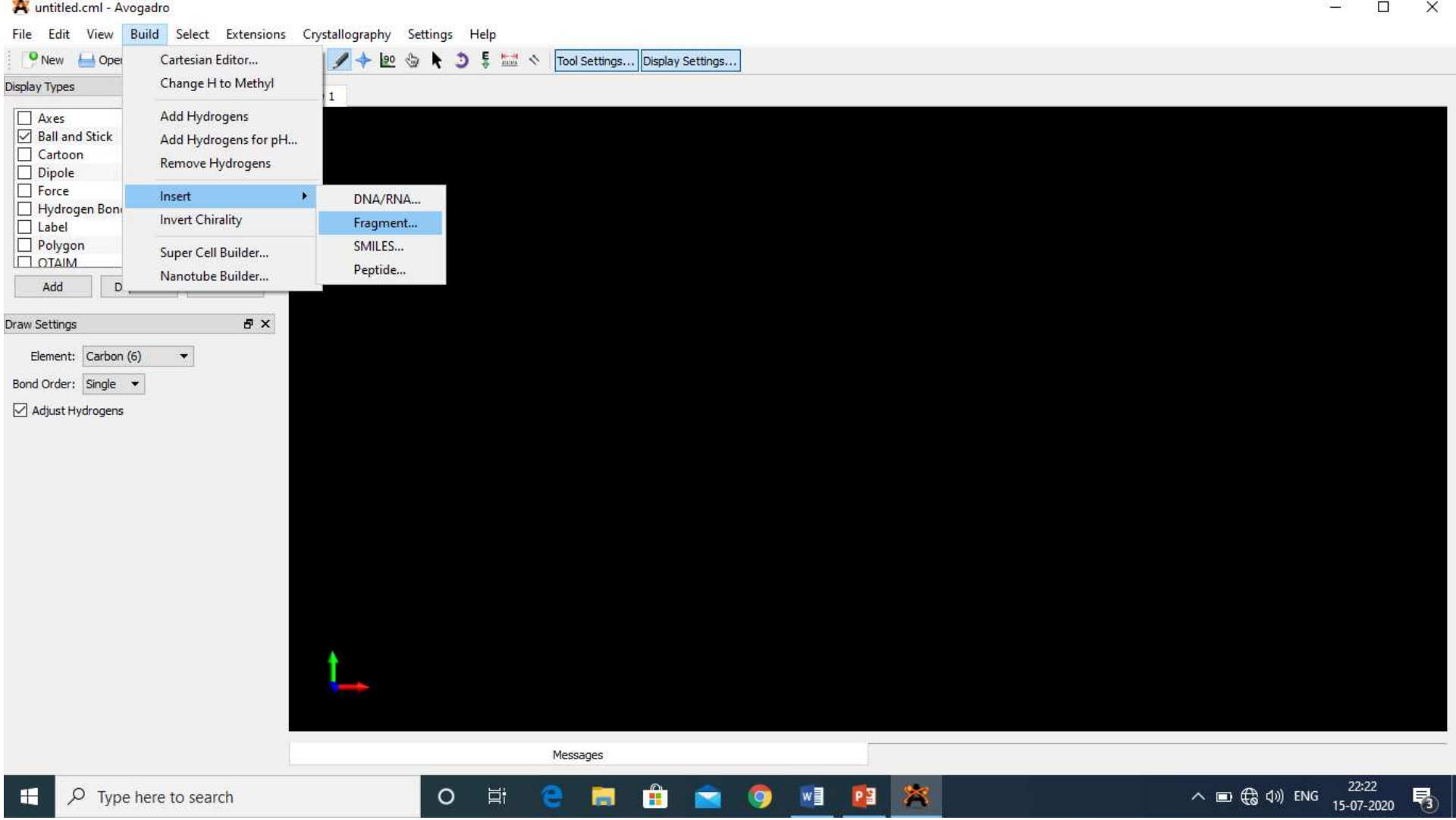
Export molecules from fragment library


untitled.cml - Avogadro
File
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View
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Select
Extensions
Crystallography
Settings
Help
New
Cartesian Editor...
Change H to Methyl
Add Hydrogens
Add Hydrogens for pH...
Remove Hydrogens
Insert
Invert Chirality
Super Cell Builder...
Nanotube Builder...
DNA/RNA...
Fragment...
SMILES...
Peptide...
Tool Settings...
Display Settings...
Display Types
Axes
Ball and Stick
Cartoon
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Force
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Polygon
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Draw Settings
Element:
Carbon (6)
Bond Order:
Single
Adjust Hydrogens
Messages
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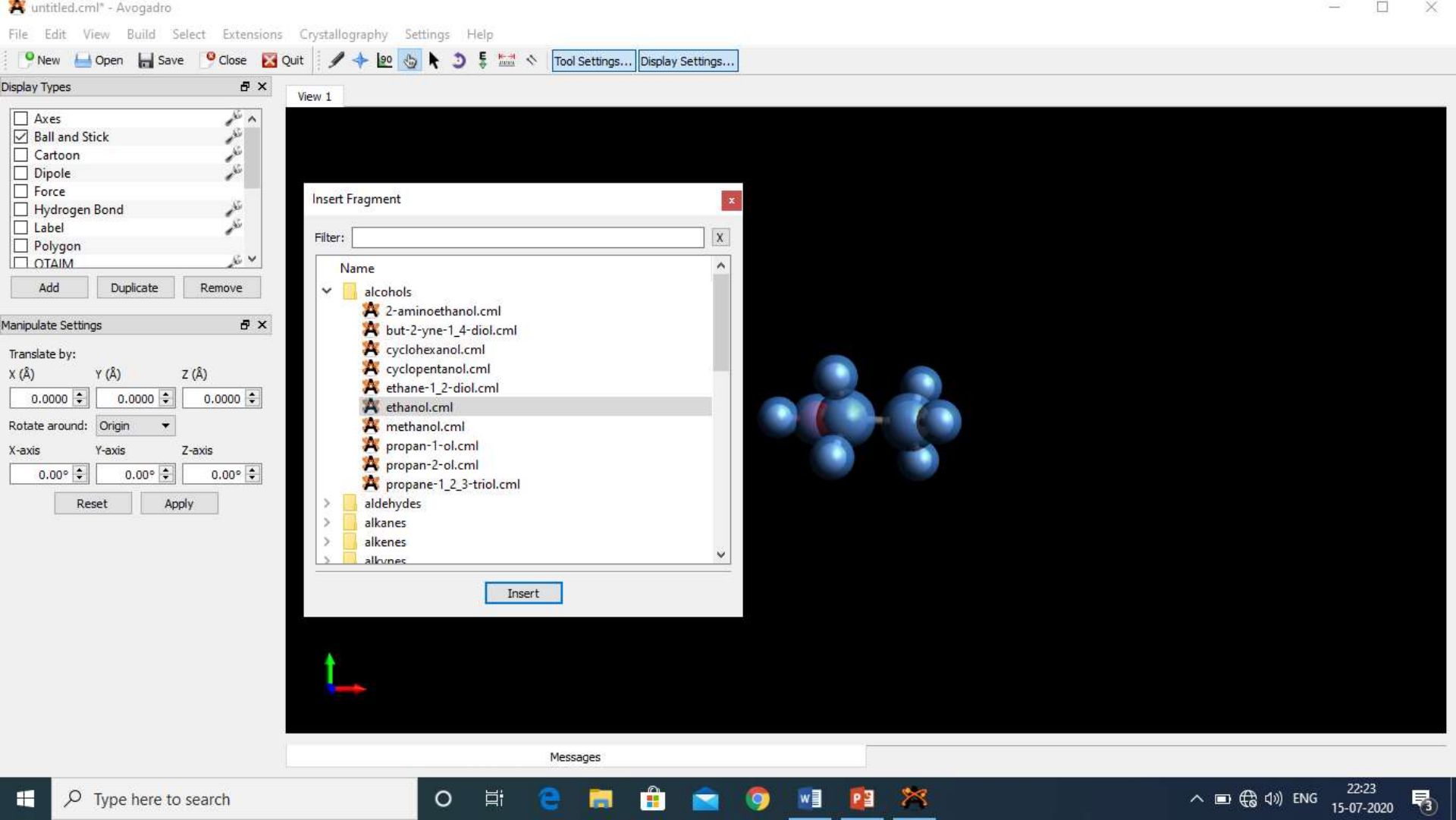
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Add Duplicate Remove
Manipulate Settings
Translate by:
X (Å) Y (Å) Z (Å)
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Rotate around: Origin
X-axis Y-axis Z-axis
0.00° 0.00° 0.00°
Reset Apply
View 1
Insert Fragment
Filter:
Name
alcohols
2-aminoethanol.cml
but-2-yne-1_4-diol.cml
cyclohexanol.cml
cyclopentanol.cml
ethane-1_2-diol.cml
ethanol.cml
methanol.cml
propan-1-ol.cml
propan-2-ol.cml
propane-1_2_3-triol.cml
aldehydes
alkanes
alkenes
alkynes
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Messages
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Exploring Hydrogen Bonding..

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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [x] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick

Add Duplicate Remove

AutoOptimization Settings

Force Field: MMFF94

Steps per Update: 4

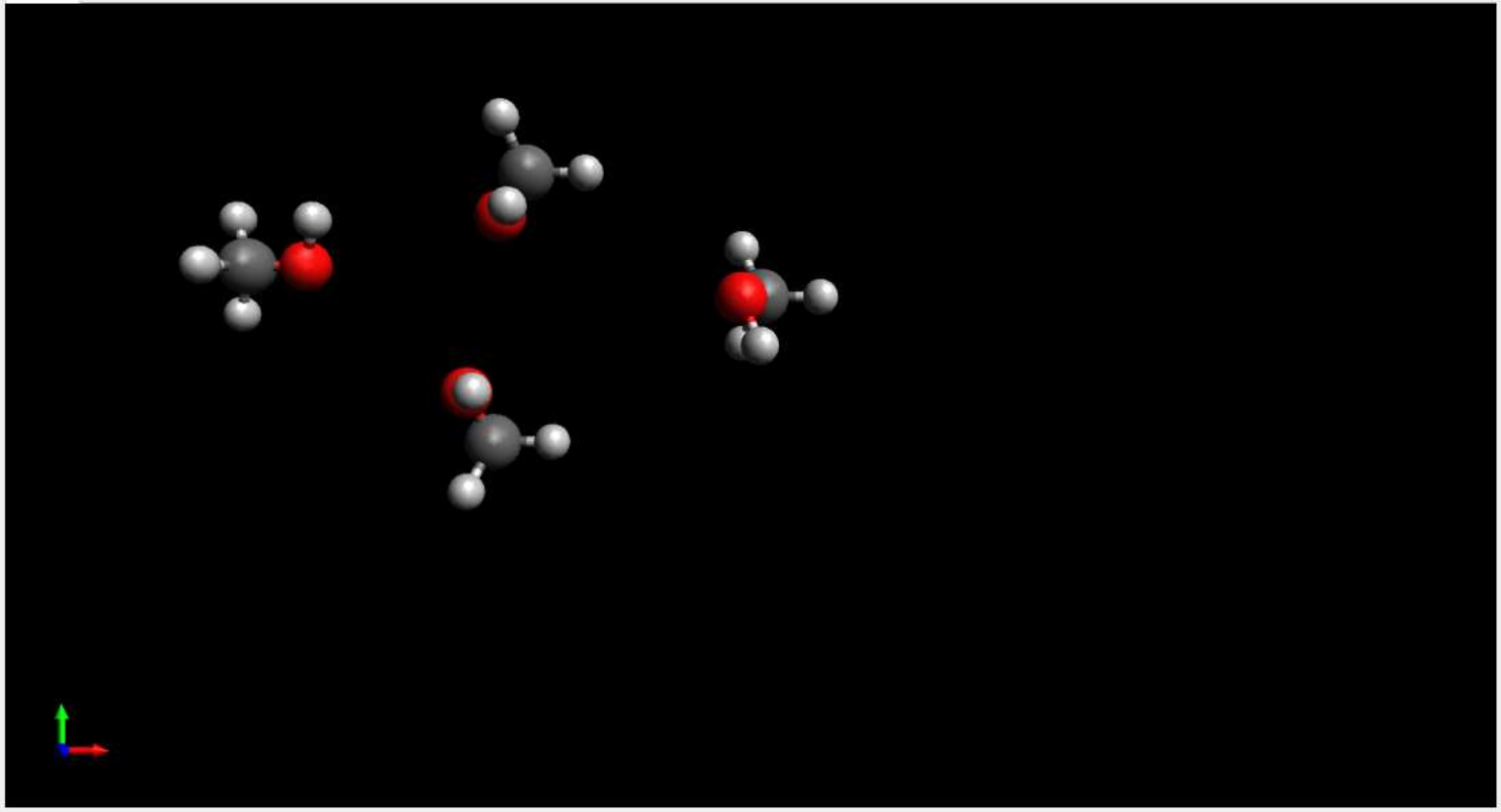
Algorithm:

Steepest Descent

- [ ] Fixed atoms are movable
- [ ] Ignored atoms are movable

Start

View 1



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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [x] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick

Add Duplicate Remove

AutoOptimization Settings

Force Field: MMFF94

Steps per Update: 4

Algorithm:

Steepest Descent

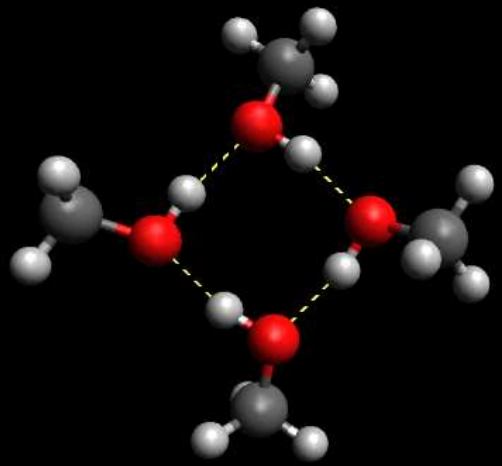
- [ ] Fixed atoms are movable
- [ ] Ignored atoms are movable

Stop

View 1

AutoOpt: E = -100.693 kJ/mol (dE = 7.44777e-06)

Num Constraints: 0



Messages

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Exploring Stereoisomerism...

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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

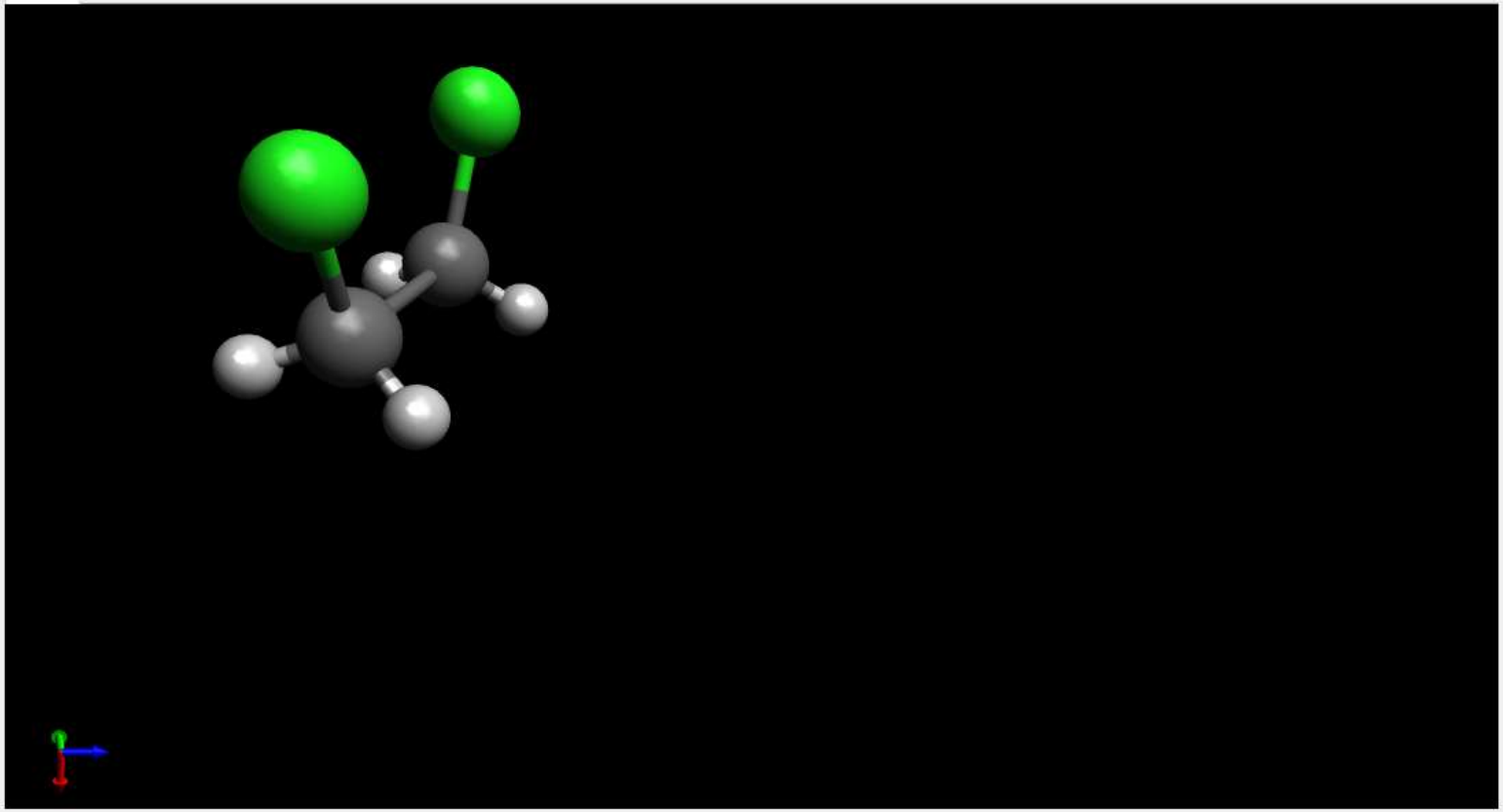
- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [x] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick

Add Duplicate Remove

Navigate Settings

- [x] Display visual cues

View 1



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File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [x] Hydrogen Bond
- [ ] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring
- [ ] Simple Wireframe
- [ ] Stick

Add Duplicate Remove

AutoOptimization Settings

Force Field: MMFF94

Steps per Update: 4

Algorithm:

Steepest Descent

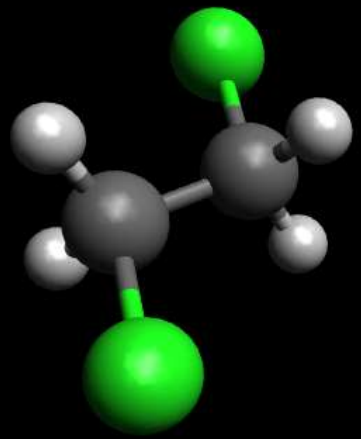
- [ ] Fixed atoms are movable
- [ ] Ignored atoms are movable

Stop

View 1

AutoOpt: E = 20.9933 kJ/mol (dE = 1.33761e-05)

Num Constraints: 0



Messages

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untitled.cml* - Avogadro

File Edit View Build Select Extensions Crystallography Settings Help

New Open Save Close Quit Tool Settings... Display Settings...

Display Types

- [ ] Axes
- [x] Ball and Stick
- [ ] Cartoon
- [ ] Dipole
- [ ] Force
- [ ] Hydrogen Bond
- [x] Label
- [ ] Polygon
- [ ] QTAIM
- [ ] Ribbon
- [ ] Ring

Add Duplicate Remove

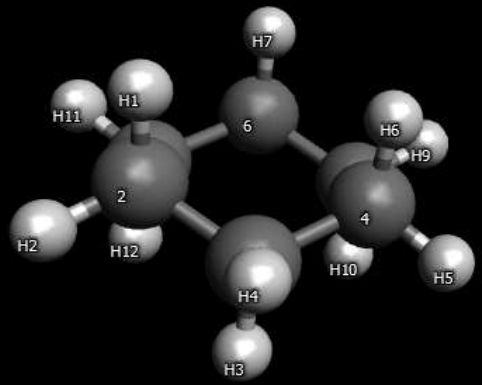
Navigate Settings

- [x] Display visual cues

View 1

AutoOpt: E = -14.909 kJ/mol (dE = 0)

Num Constraints: 0



Messages

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Benefits of Avogadro…

- It offers flexible, high quality rendering.
- Molecule may be Constructed, edited and visualized in 3D
- Energy minimization to obtain stable conformations
- Huge fragment library to load inbuilt structures
- Files can be exported to desired formats such as png, jpg, bmp file

Thanks for your attention

for any queries…

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NCERT, New Delhi
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9461068296