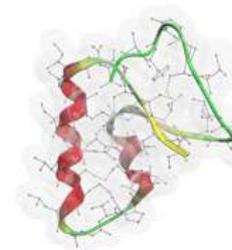
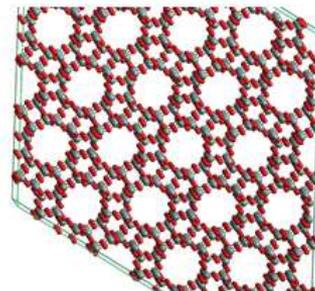
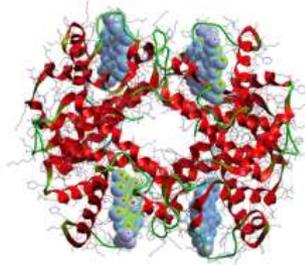
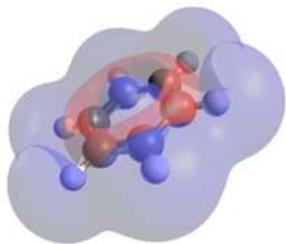


Explore Chemistry
with
Avogadro (Hindi)

Avogadro ...

- फ्री और ओपन सोर्स सॉफ्टवेयर
 - अणुओं का 3D (त्रिविमीय) में निर्माण, संपादन और दृश्य
 - 3D (त्रिविमीय) आणविक संपादक और दृश्यावलोकन उपकरण
 - Mac, Windows, और Linux OS पर उपयोग के लिए डिज़ाइन किया गया
 - डाउनलोड हेतु <http://avogadro.cc>
- <http://avogadro.cc>

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

Draw Settings

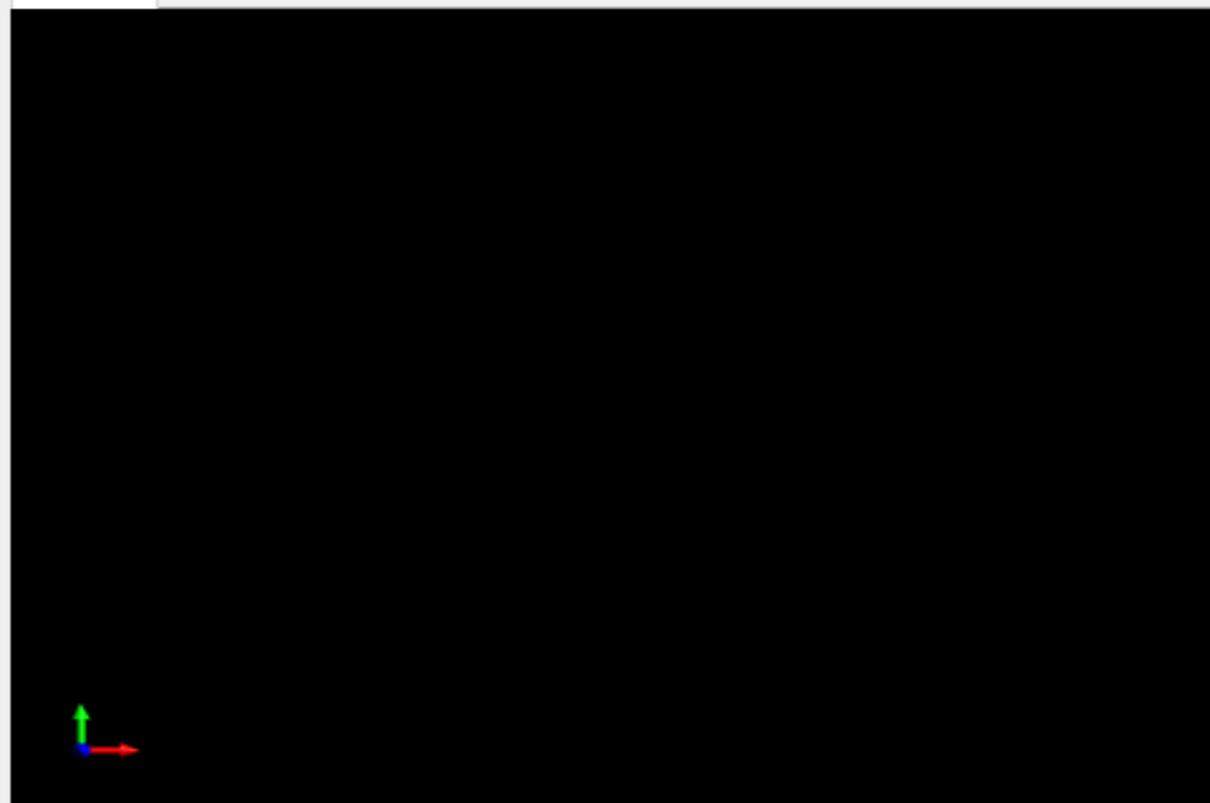


Element: Carbon (6) ▾

Bond Order: Single ▾

 Adjust Hydrogens

View 1



Messages

चलिए...

अणु का निर्माण करे...

Display Types

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

Add

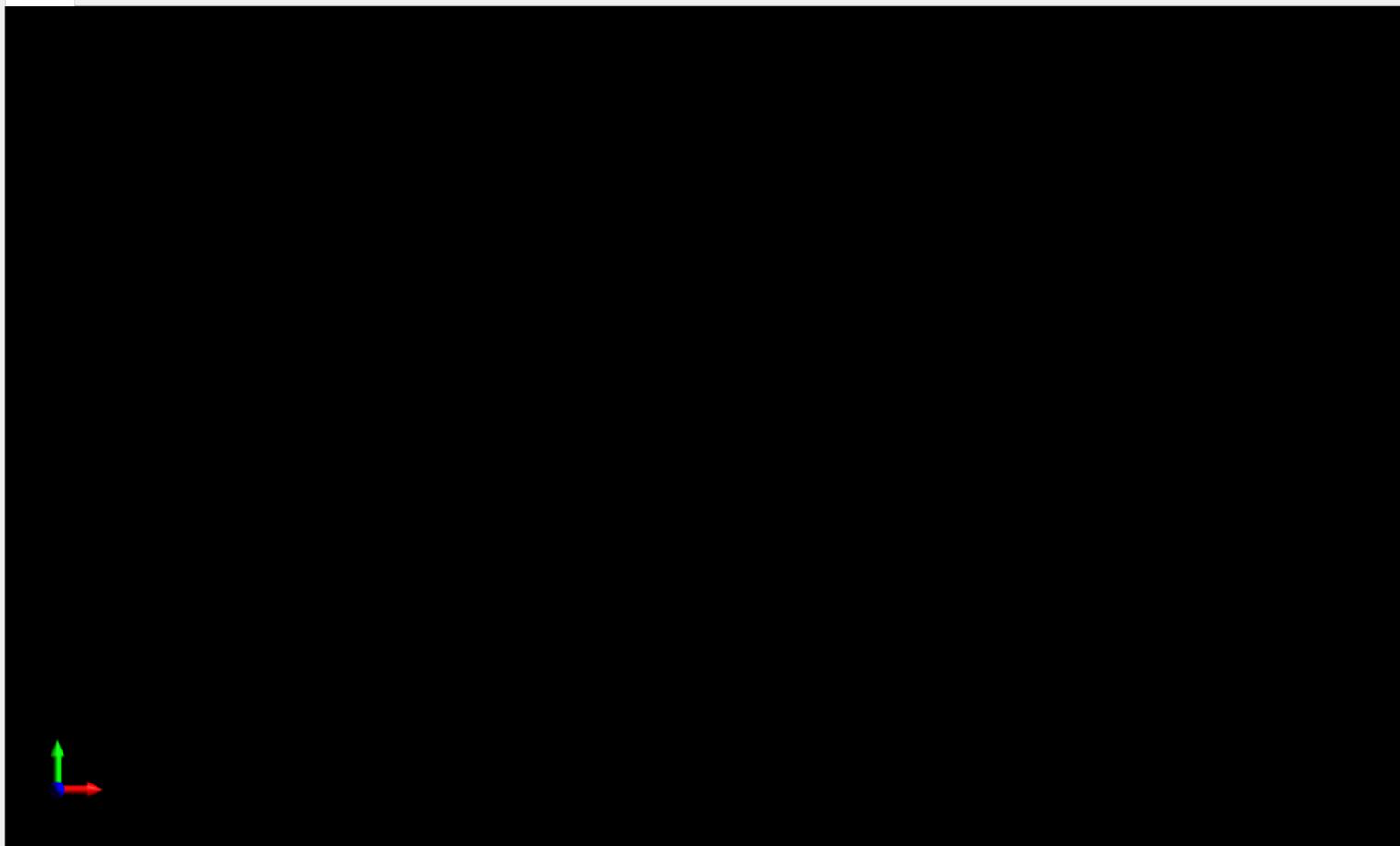
Duplicate

Remove

Draw Settings

- Element: Carbon (6)
- Bond Order: Boron (5)
- Adjust H's
- Carbon (6)
 - Nitrogen (7)
 - Oxygen (8)
 - Fluorine (9)
 - Phosphorus (15)
 - Sulfur (16)
 - Chlorine (17)
 - Bromine (35)

View 1



Display Types

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

Add

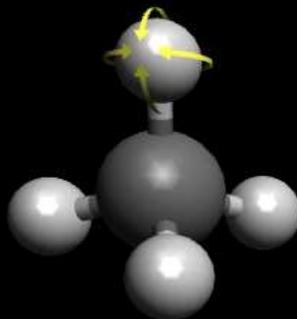
Duplicate

Remove

Navigate Settings

- Display visual cues

View 1



Display Types

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

Add

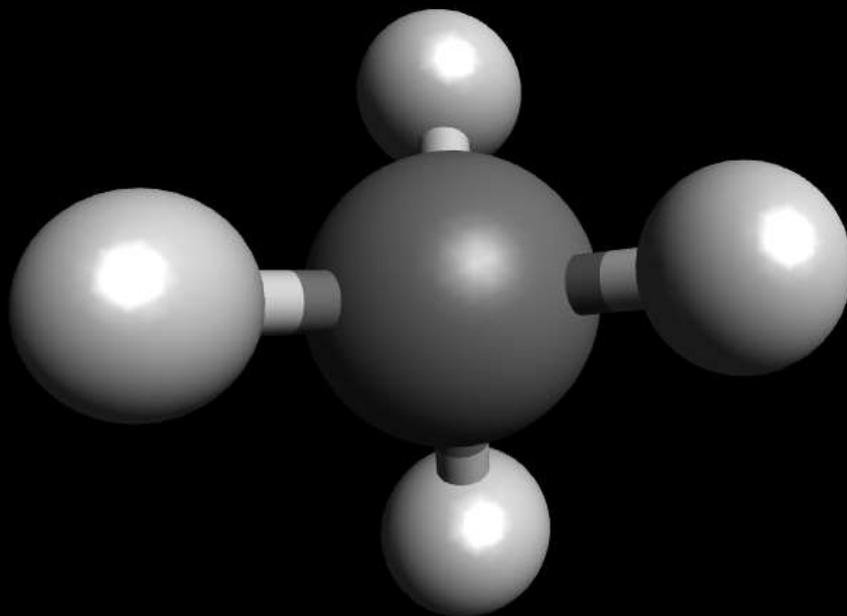
Duplicate

Remove

Navigate Settings

- Display visual cues

View 1



Zoom In

Messages

Display Types

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

Add

Duplicate

Remove

Navigate Settings

- Display visual cues

View 1



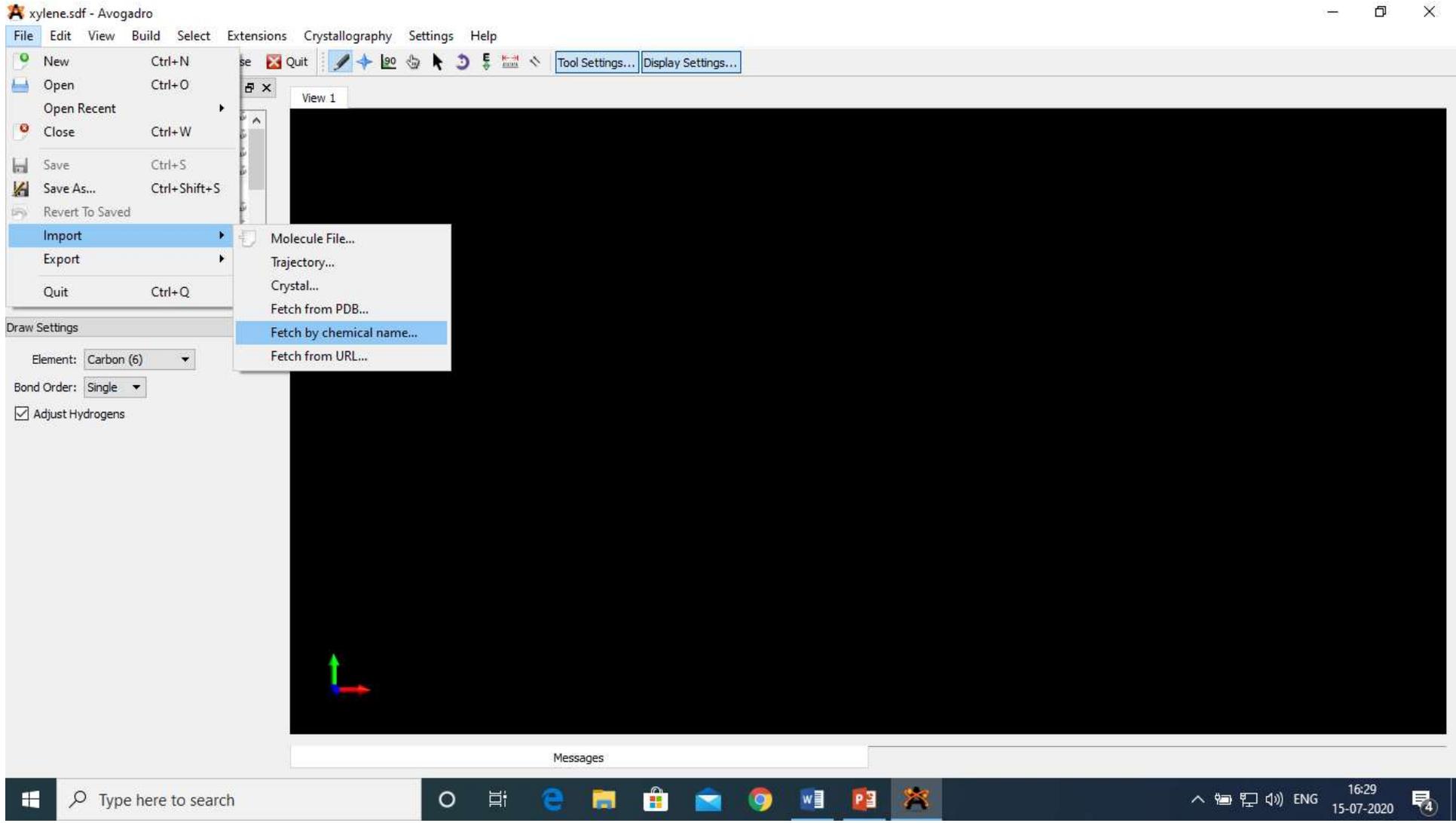
Zoom out



Messages

चलिए...

Avogadro डेटा बेस से अणु को
आयातित करें



- 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

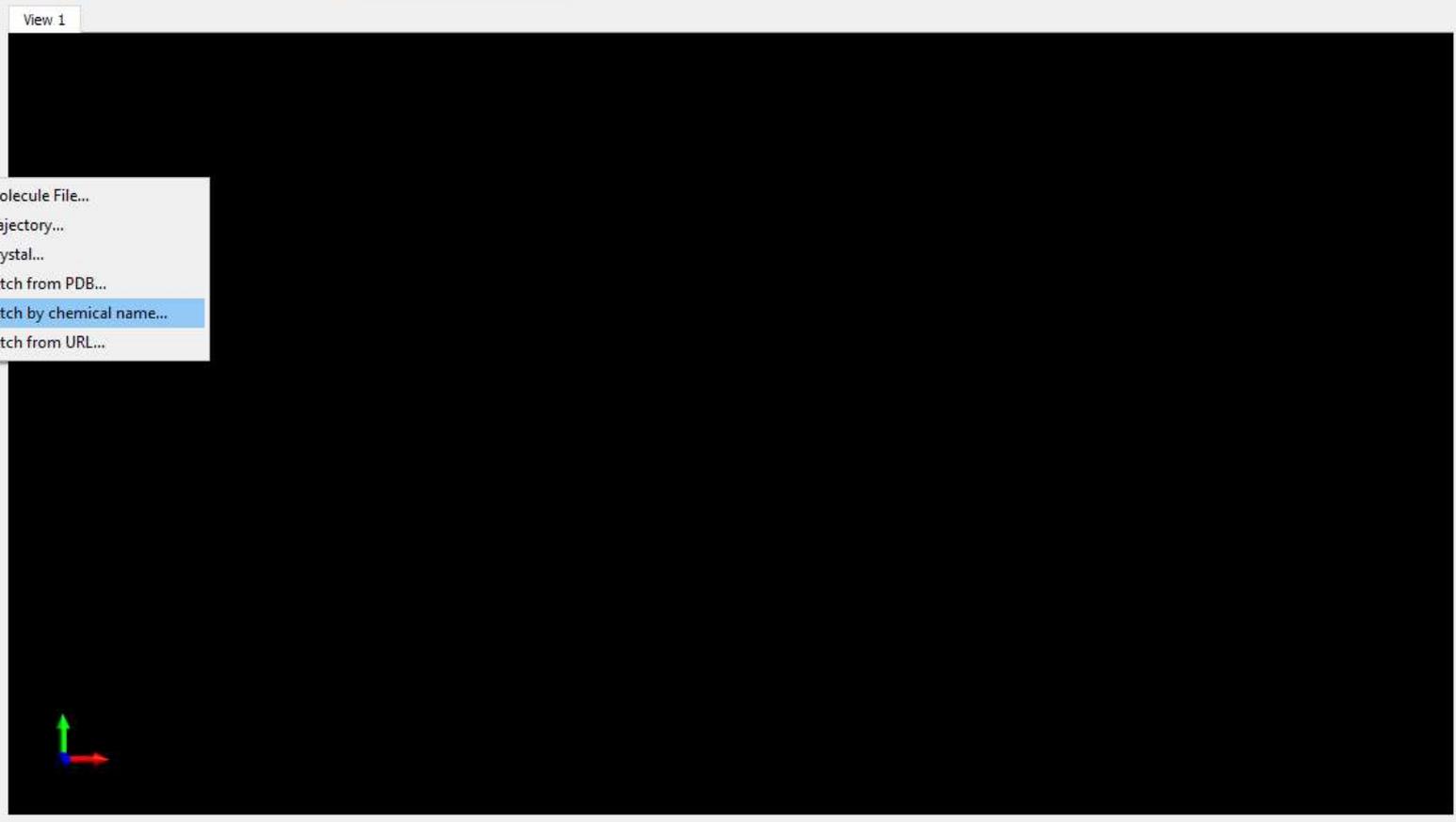
- Molecule File...
- Trajectory...
- Crystal...
- Fetch from PDB...
- Fetch by chemical name...**
- Fetch from URL...

Draw Settings

Element: Carbon (6)

Bond Order: Single

Adjust Hydrogens



Messages

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... ? X

Chemical structure to download.

aniline

OK Cancel

Messages

Type here to search

16:30 15-07-2020

Display Types

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

Add

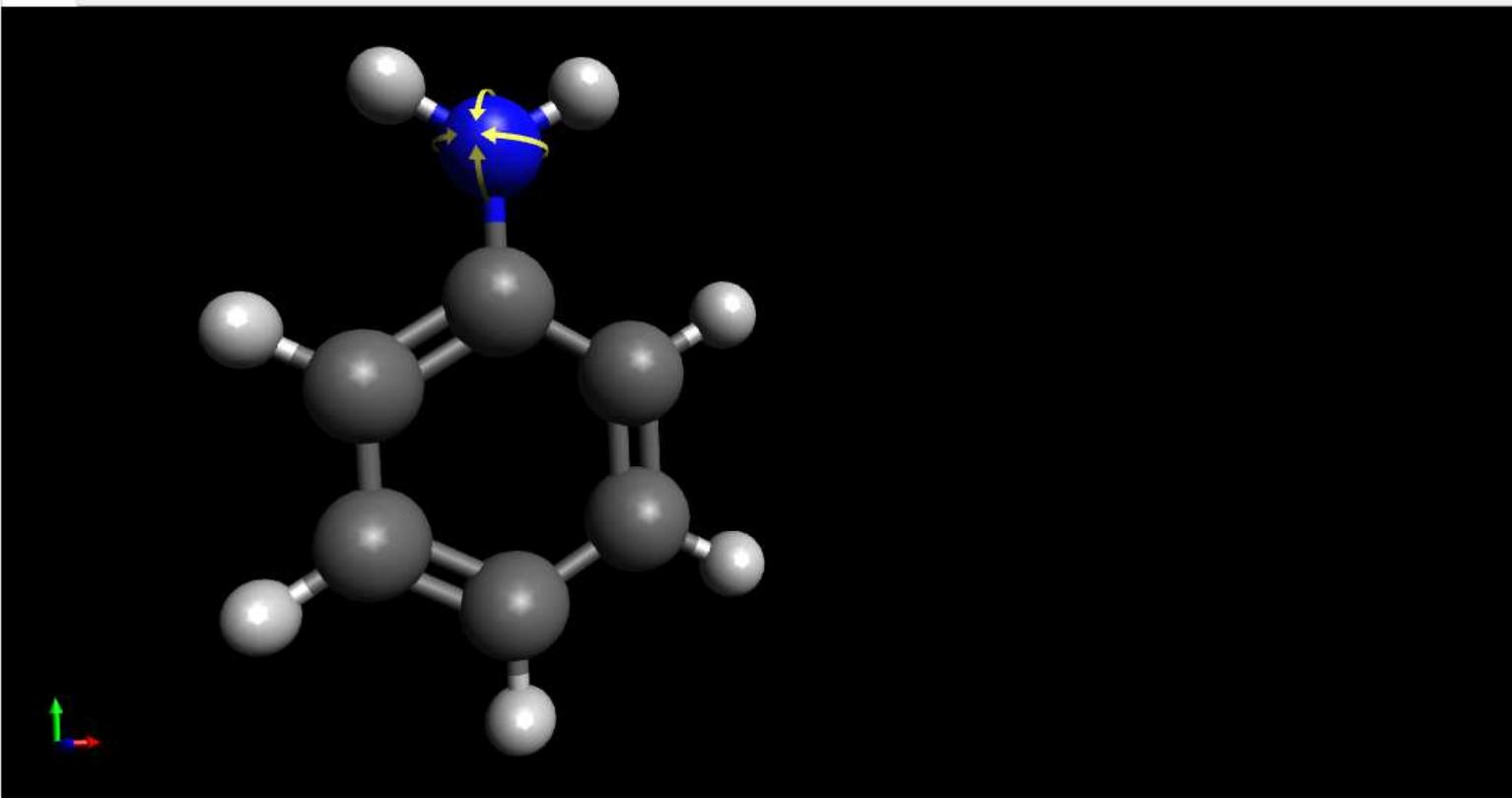
Duplicate

Remove

Navigate Settings

- Display visual cues

View 1



Messages

चलिए....

अणुओं को आरेखित और संपादित करते हैं..

Display Types

- Axes
- 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

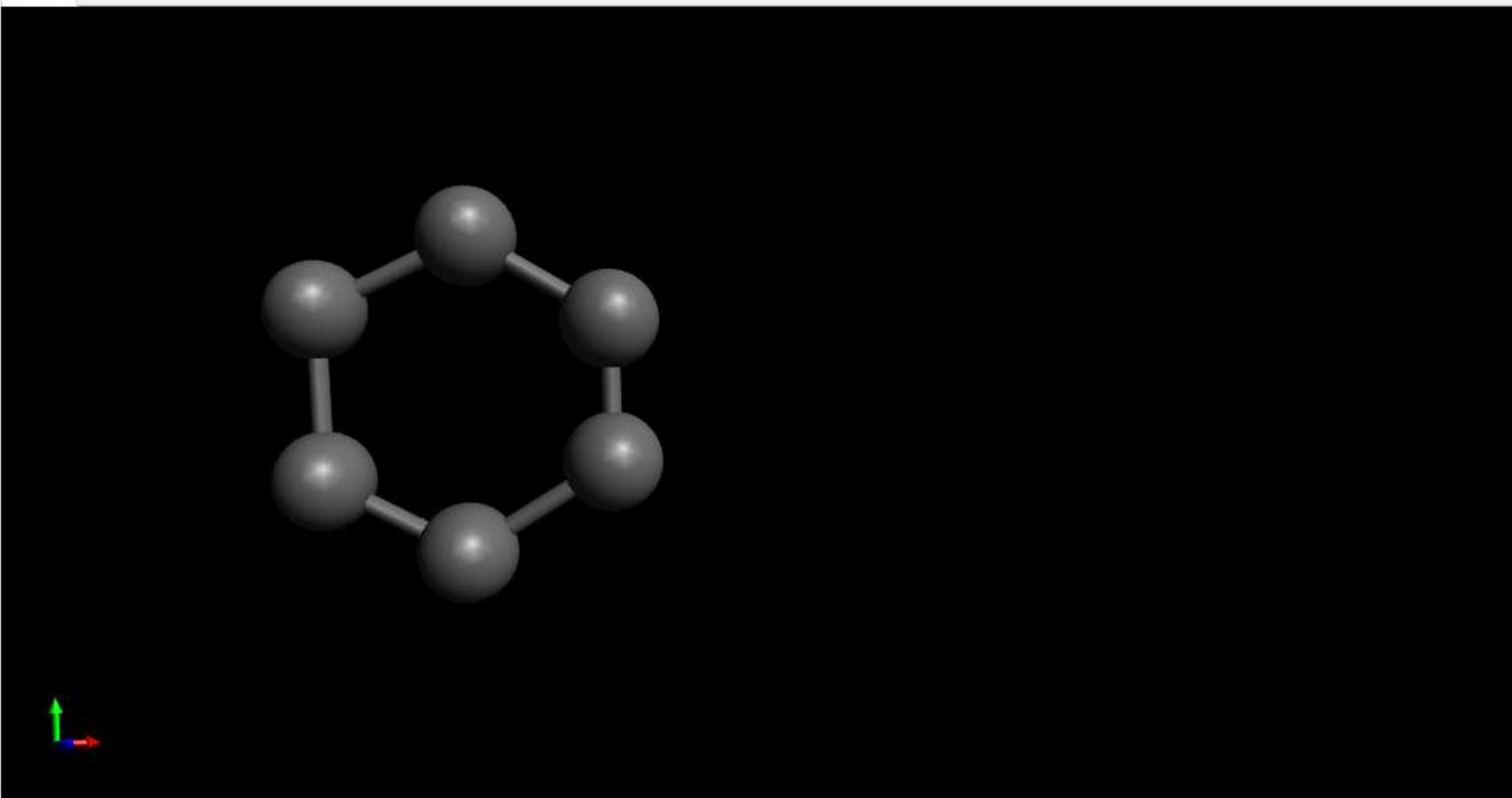
Draw Settings

Element: Carbon (6)

Bond Order: Single

 Adjust Hydrogens

View 1



Messages

Display Types

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

Add

Duplicate

Remove

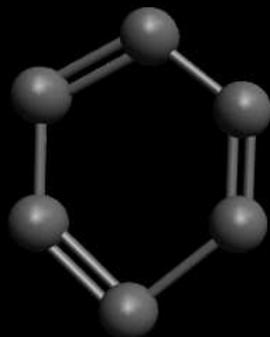
Draw Settings

Element: Nitrogen (7)

Bond Order: Single

 Adjust Hydrogens

View 1



Messages

Display Types

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

Add

Duplicate

Remove

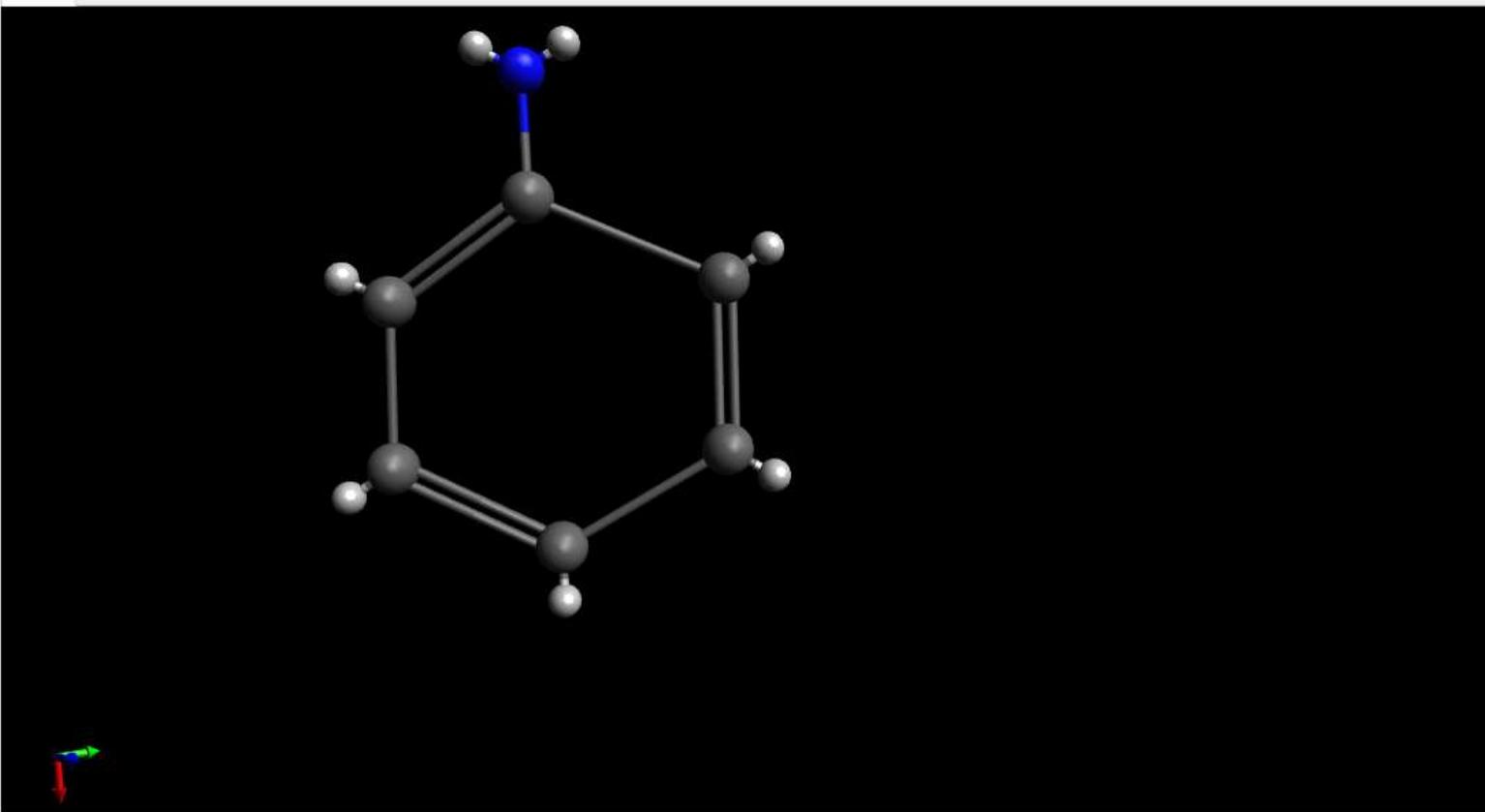
Draw Settings

Element: Nitrogen (7)

Bond Order: Single

 Adjust Hydrogens

View 1



Messages

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

Add Duplicate Remove

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

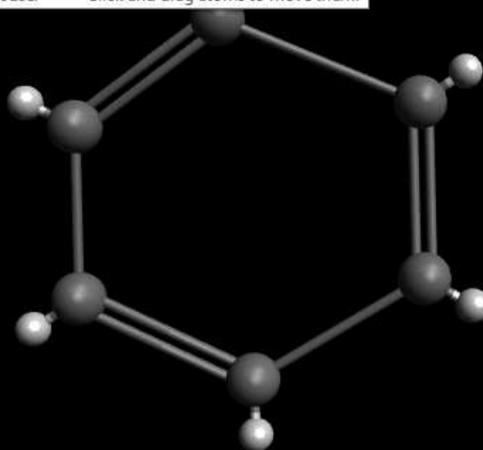
Middle Mouse: Zoom Space

Right Mouse: Move Space

Double-Click: Reset View

When running:

Left Mouse: Click and drag atoms to move them.



For Geometry optimization

Messages

Display Types

- Axes
- 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

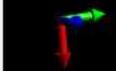
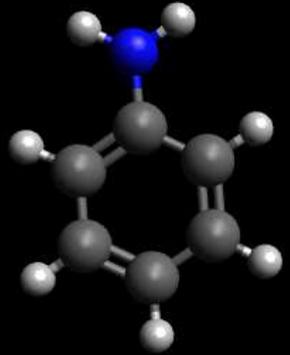
Ignored atoms are movable

Stop

View 1

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

Num Constraints: 0



Messages

अणु की बंध लंबाई, बंध कोण और
द्वितल कोण

Display Types

- Axes
- Ball and Stick
- Cartoon
- Dipole
- Force
- Hydrogen Bond
- Label
- Polygon
- OTAIM

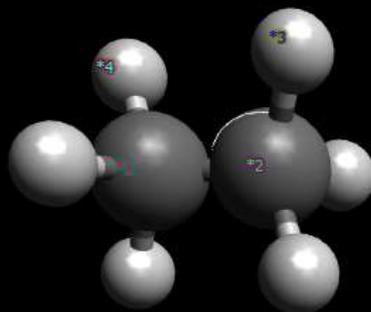
Add

Duplicate

Remove

Measure Settings

View 1



 Dihedral: -30.0°
 Angle: 109.5°
 Distance(s): 1.070 Å 1.070 Å 2.049 Å

Messages

Fragment library से अणुओं को निर्यात
करना

- Axes
 - Ball and Stick
 - Cartoon
 - Dipole
 - Force
 - Hydrogen Bond
 - Label
 - Polygon
 - OTAIM
- Add D

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...

Element: Carbon (6)

Bond Order: Single

 Adjust Hydrogens

Display Types

- Axes
- Ball and Stick
- Cartoon
- Dipole
- Force
- Hydrogen Bond
- Label
- Polygon
- OTAIM

Add Duplicate Remove

Manipulate Settings

Translate by:

X (Å) Y (Å) Z (Å)
0.0000 0.0000 0.0000

Rotate around: Origin

X-axis Y-axis Z-axis
0.00° 0.00° 0.00°

Reset Apply

View 1

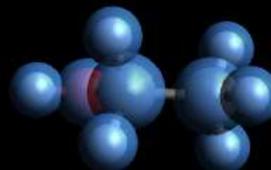
Insert Fragment

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

Insert



Messages

Exploring Hydrogen Bonding...
हाइड्रोजन बंध का अन्वेषण ...

Display Types

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

Add Duplicate Remove

AutoOptimization Settings

Force Field: MMFF94

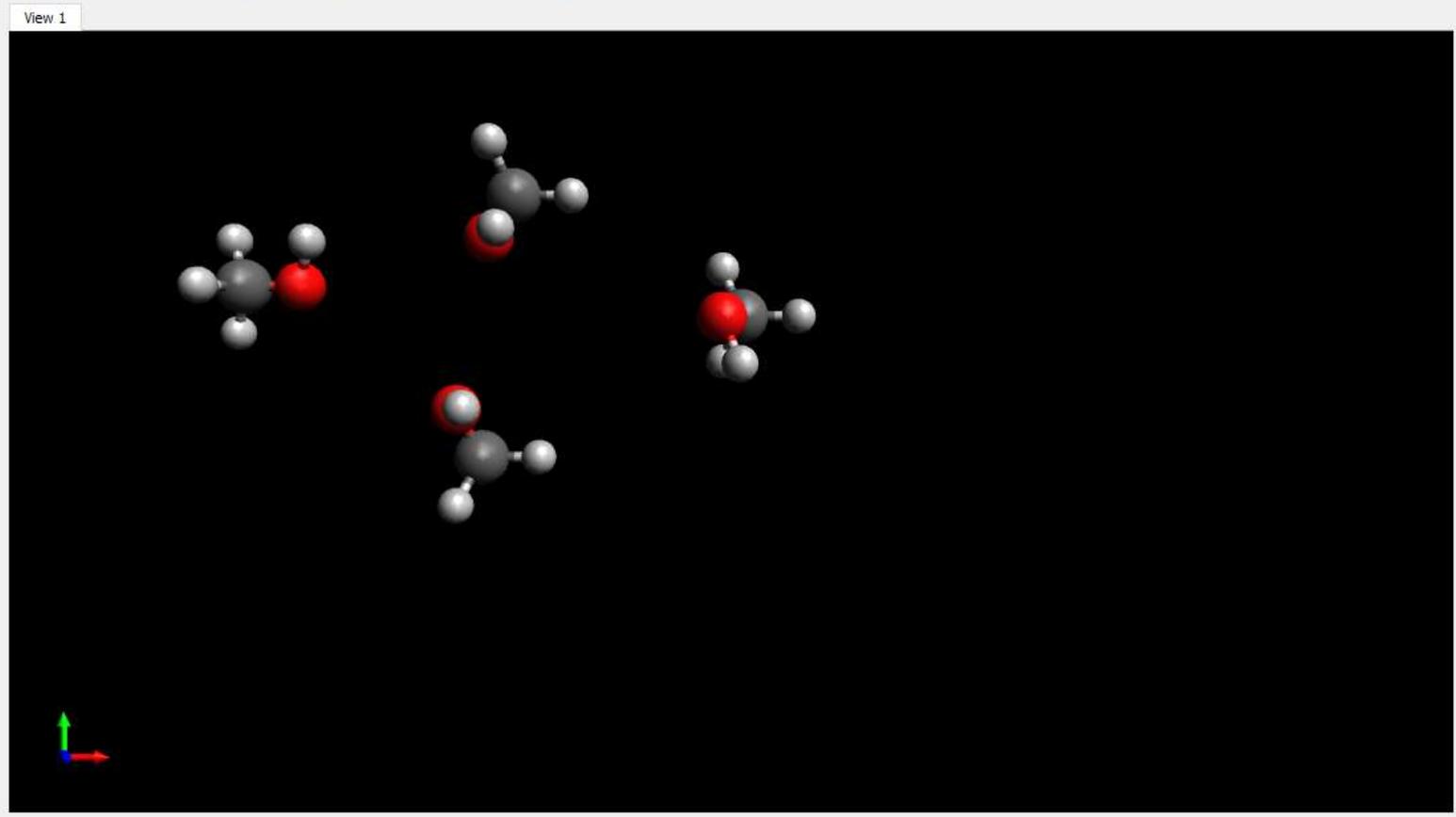
Steps per Update: 4

Algorithm: Steepest Descent

Fixed atoms are movable

Ignored atoms are movable

Start



Messages

Display Types

- Axes
- Ball and Stick
- Cartoon
- Dipole
- Force
- 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

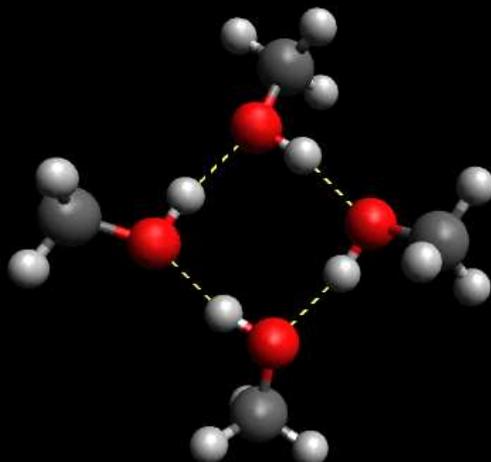
 Fixed atoms are movable Ignored atoms are movable

Stop

View 1

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

Num Constraints: 0



Messages

Exploring Stereoisomerism...

त्रिविम समावयवी का अन्वेषण ...

Display Types

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

Add

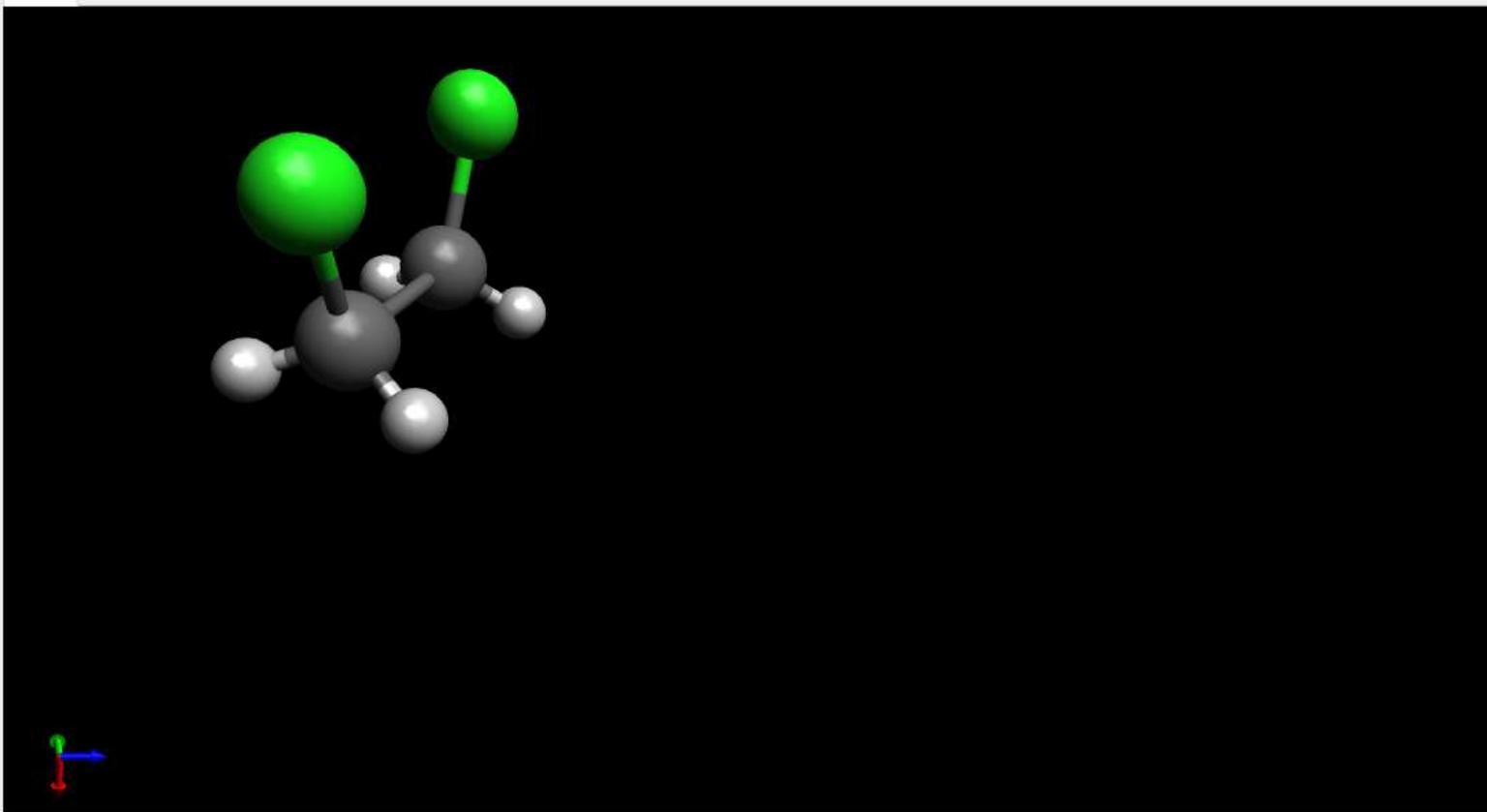
Duplicate

Remove

Navigate Settings

- Display visual cues

View 1



Messages

Display Types

- Axes
- Ball and Stick
- Cartoon
- Dipole
- Force
- 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

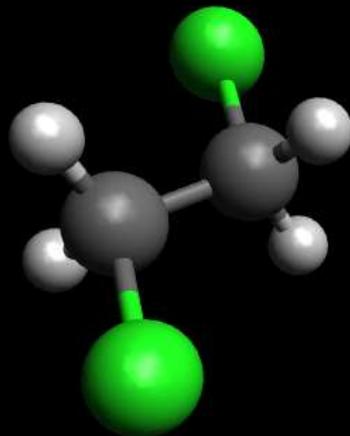
 Fixed atoms are movable Ignored atoms are movable

Stop

View 1

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

Num Constraints: 0



Messages

Display Types

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

Add

Duplicate

Remove

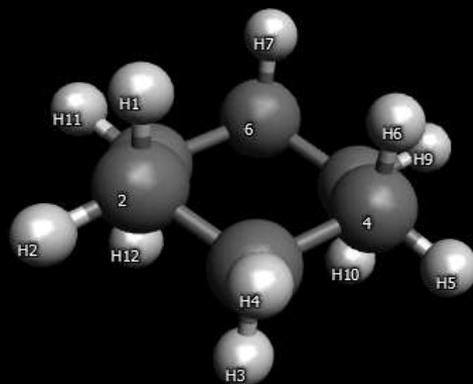
Navigate Settings

- Display visual cues

View 1

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

Num Constraints: 0



Messages

Benefits of Avogadro...

Avogadro के लाभ...

- अणु का निर्माण, संपादन और त्रिविमीय दृश्यावलोकन किया जा सकता है।
- Energy minimization to obtain stable conformations.
स्थिर अनुरूपता (stable conformations) प्राप्त करने के लिए ऊर्जा का कम से कम उपयोग।
- अंतर्निहित संरचनाओं को लोड करने के लिए विशाल खंड पुस्तकालय (Huge fragment library)।
- Files can be exported to desired formats such as png, jpg, bmp file
फ़ाइलों को वांछित स्वरूपों में निर्यात किया जा सकता है जैसे कि png, jpg, bmp फ़ाइल

Thanks for your attention

for any queries...

Dr. Anand Kumar Arya

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NCERT, New Delhi

anandarya2001@yahoo.com

9461068296