

Comparative Structural Analysis of Diamond and Graphite using Jmol : A Molecular Perspective

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1. Introduction

Though Diamond and Graphite are made of purely carbon atoms, they differ significantly in their physical properties, which is due to their diverse atomic arrangements. Being aware of how fundamental configurations at atomic level and nature of bonding are in diamond or graphite form can enable discovery of their special characteristics being utilized within different technological domains such as nanotechnology, electronics among many others.

Details of symmetry	Diamond	Graphite
Lattice type	cubic crystal	Hexagonal
Lattice Parameters	$a = b = c = 3.56 \text{ \AA}$	$a = b = 2.461 \text{ \AA}; c = 6.707 \text{ \AA}$
Angles	$\alpha = \beta = \gamma = 90^\circ$	$\alpha = \beta = 90^\circ; \gamma = 120^\circ$

1.1 Structural Properties of Diamond

1.1.1 Atomic Structure:

- Diamond consists of carbon atoms arranged in a three-dimensional network
- Each carbon atom is bonded to four other carbon atoms in a tetrahedral arrangement through sp^3 hybridization
- This configuration results in a very strong and rigid structure

1.1.2 Physical Characteristics:

- **Hardness:** Diamond is the hardest known natural material, making it highly valuable for cutting and grinding applications.
- **Density:** Due to its closely packed structure, diamond has a high density.
- **Transparency:** The strong covalent bonds in diamond result in a transparent material, often used in gemstones.
- **Electrical Conductivity:** Diamond is an electrical insulator because there are no free electrons to carry an electric current.

1.1.3 Chemical Characteristics:

- **Reactivity:** Diamond is highly resistant to chemical reactions, making it stable in various environments.
- **Combustibility:** Diamond is non-combustible and can only burn at very high temperatures under specific conditions.

1.1.4 Applications:

- Widely used in cutting, grinding, and drilling tools
- Valued in the jewelry industry for its brilliance and transparency
- Potential uses in advanced electronics and high-performance components due to its thermal conductivity and insulating properties.

1.2 Structural Analysis of Graphite

1.2.1 Atomic Structure:

- Graphite is composed of carbon atoms arranged in layers of hexagonal rings
- Each carbon atom is bonded to three other carbon atoms within the same plane through sp^2 hybridization, forming strong covalent bonds
- The layers are held together by weak van der Waals forces, allowing them to slide over each other easily

1.2.2 Physical Characteristics:

- **Hardness:** Graphite is soft and slippery due to the weak forces between layers, making it an excellent lubricant.
- **Density:** Graphite has a lower density compared to diamond due to the greater distance between layers.
- **Opacity:** Graphite is opaque and usually black or gray in appearance.
- **Electrical Conductivity:** Graphite is an excellent conductor of electricity because of the presence of delocalized electrons within its layers

1.2.3 Chemical Characteristics:

- **Reactivity:** Graphite is generally inert but can react with strong oxidizers.
- **Combustibility:** Graphite is combustible and burns at high temperatures, forming carbon dioxide.

1.2.4 Applications:

- Used as a lubricant in various mechanical applications.
- Employed in the production of electrodes and batteries due to its electrical conductivity
- Utilized in high-temperature crucibles and as a moderator in nuclear reactors due to its thermal stability and conductivity

2. Importing 3D structure of molecules in Jmol

2.1 Downloading COD (Crystallography Open Database) database

2.1.1 Downloading unit cell of Diamond

- Go to the COD database in your search engine and open it
- On your left side you will notice Accessing COD data, click on **search**
- It appears like Search by COD ID, in that enter COD id for Diamond (already obtained from internet) (i.e 9012243)
- Now click on cif for download, as show in below.
- Then automatically our required cif file is downloaded

The screenshot shows the Crystallography Open Database (COD) search results page. The browser address bar shows crystallography.net/cod/result.php. The page title is "Crystallography Open Database". On the left sidebar, under "Accessing COD Data", the "Search" link is highlighted. The main content area shows "Search results" for COD ID 9012243. It indicates "Result: there are 1 entries in the selection". Below this, there are links to "Switch to the old layout of the page", "Download all results as: list of COD numbers", "list of CIF URLs", "data in CSV format", and "archive of CIF files (ZIP)". The search criteria are "Searching COD ID like 9012243 including duplicate structures including structures with errors including theoretical structures". The results table shows one entry with COD ID 9012243, formula C, space group Fd-3m:1, cell parameters 3.567; 3.567; 3.567, and cell volume 45.385. The bibliography lists "Fayos, J. Possible 3D carbon structures as progressive intermediates in graphite to diamond phase transition Note: mathematical model, phase: diamond(cub) Journal of Solid State Chemistry, 1999, 148, 278-285".

Crystallography Open Database

Search results

Result: there are 1 entries in the selection

[Switch to the old layout of the page](#)

Download all results as: [list of COD numbers](#) | [list of CIF URLs](#) | [data in CSV format](#) | [archive of CIF files \(ZIP\)](#)

Searching COD ID like 9012243 including duplicate structures including structures with errors including theoretical structures

◀◀ First | ◀ Previous 5 | Page 1 of 1 | Next 5 ▶ | Last ▶▶ | Display 5 20 50 100 200 300 500 1000 entries per page

COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
9012243	CIF	C	Fd-3m:1	3.567; 3.567; 3.567 90; 90; 90	45.385	Fayos, J. Possible 3D carbon structures as progressive intermediates in graphite to diamond phase transition Note: mathematical model, phase: diamond(cub) Journal of Solid State Chemistry, 1999, 148, 278-285

◀◀ First | ◀ Previous 5 | Page 1 of 1 | Next 5 ▶ | Last ▶▶ | Display 5 20 50 100 200 300 500 1000 entries per page

[Back to the search form](#)

[Your own data is not in the COD? Deposit it, thanks!](#)

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All data in the COD and the database itself are dedicated to the public domain and licensed under the [CCO License](#). Users of the data should acknowledge the original authors of the structural data.

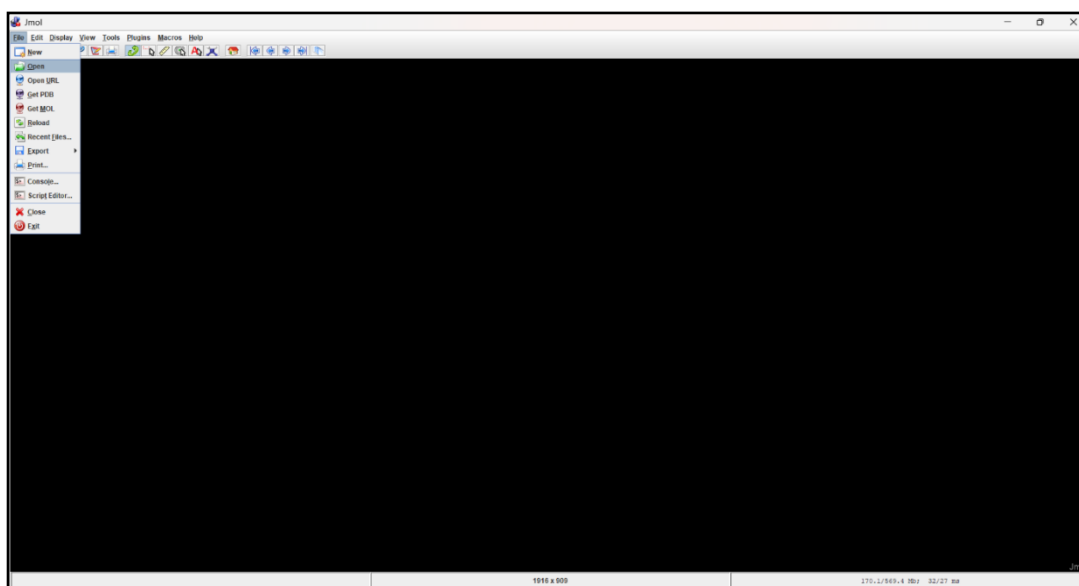
2.1.2 Download unit cell of Graphite

- Proceed with the same procedure as before for graphite too
- The COD id for graphite structure is 9912230

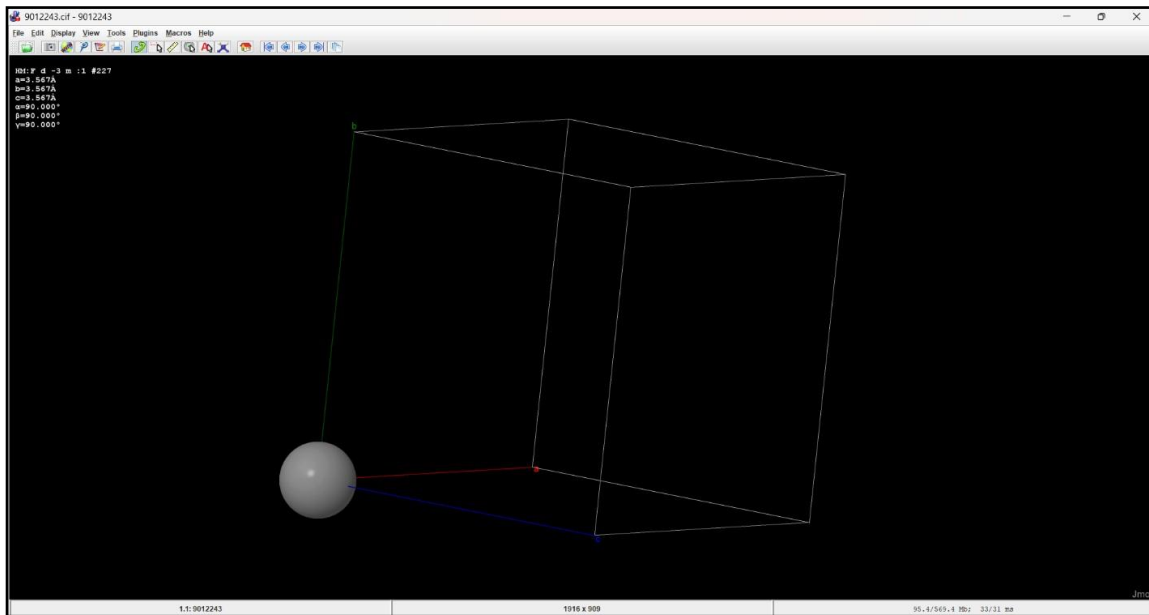
The screenshot shows the Crystallography Open Database (COD) search results page. The browser address bar shows crystallography.net/cod/result.php. The page title is "Crystallography Open Database". On the left, there are navigation links under "COD Home", "Accessing COD Data", "Add Your Data", and "Documentation". The main content area is titled "Search results" and shows "Result: there are 1 entries in the selection". Below this, there are links to download results in various formats: "list of COD numbers", "list of CIF URLs", "data in CSV format", and "archive of CIF files (ZIP)". The search criteria are "Searching COD ID like 9912230 including duplicate structures including structures with errors including theoretical structures". The results are displayed in a table with columns: COD ID, Links, Formula, Space group, Cell parameters, Cell volume, and Bibliography. The first entry is for COD ID 9912230, with formula C, space group P63/mc, cell parameters 2.461; 2.461; 6.708, and cell volume 35.184. The bibliography entry is by Fayos, J., titled "Possible 3D carbon structures as progressive intermediates in graphite to diamond phase transition Note: mathematical model", published in *Journal of Solid State Chemistry*, 1999, 148, 278-285. At the bottom, there is a footer with a "Top of the page" link and a disclaimer: "All data in the COD and the database itself are dedicated to the public domain and licensed under the CC0 License. Users of the data should acknowledge the original authors of the structural data."

2.2 Open CIF files in Jmol

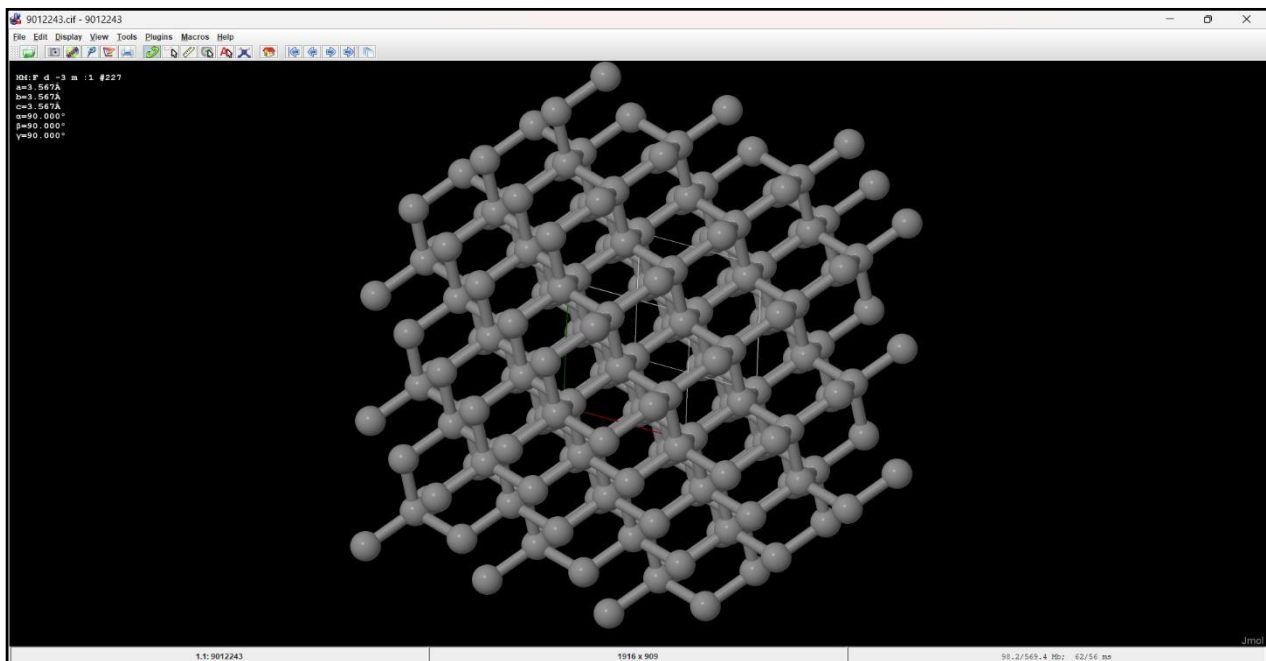
- Open Jmol interface
- Click the file menu in the tool bar
- Select open in that pop up menu as shown in below



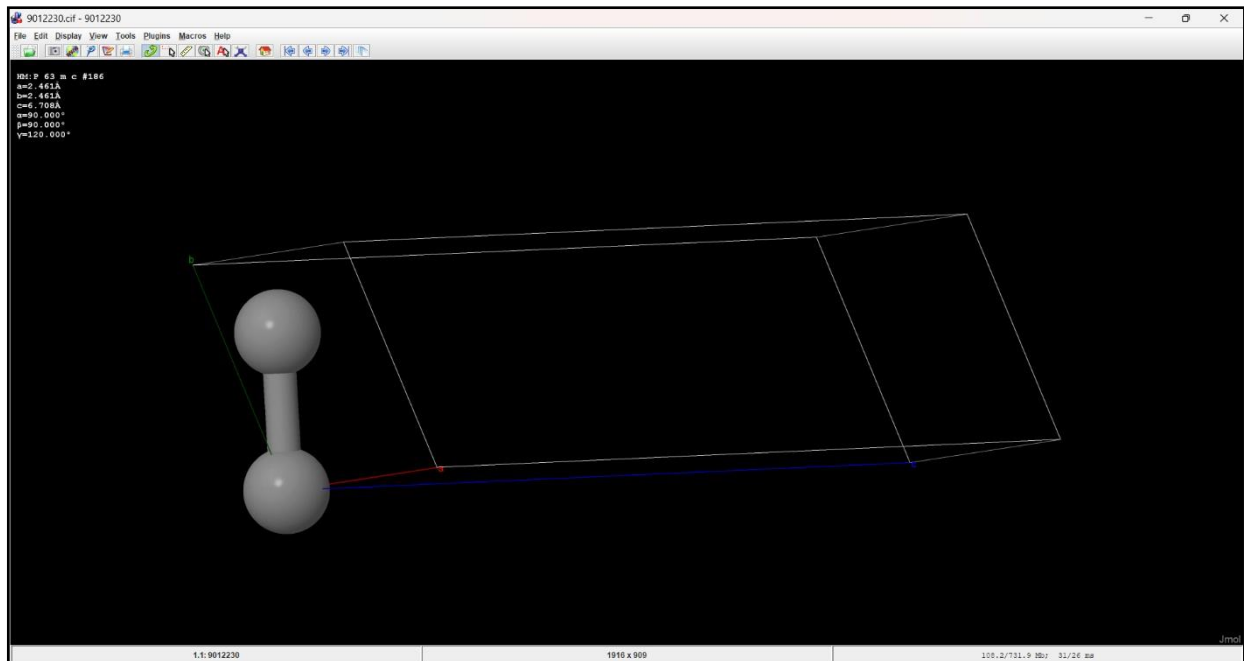
2.2.1 Now open the downloaded cif file of Diamond (Initial view of unit cell)



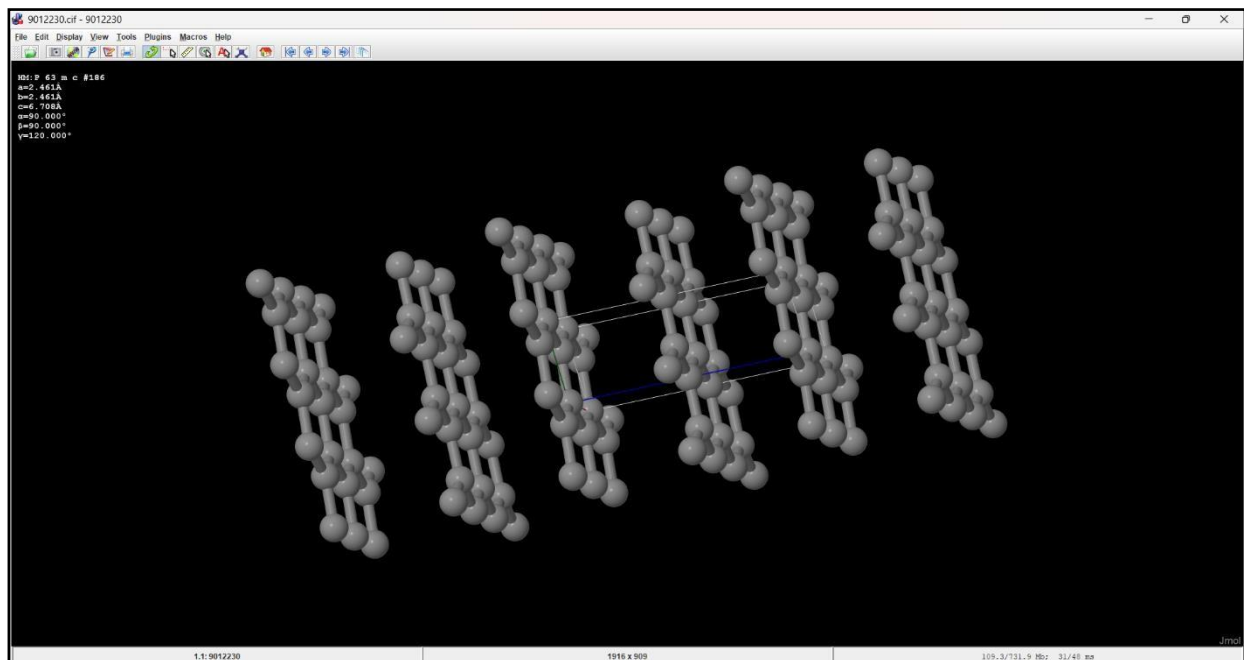
- Perform right click on the mouse, select *symmetry*, now reload {444 666 1} for multi chain of carbon arrangements in diamond
- Our final outcome of Diamond structure is follows



2.2.2 Open the downloaded cif file of graphite (Initial view of unit cell)

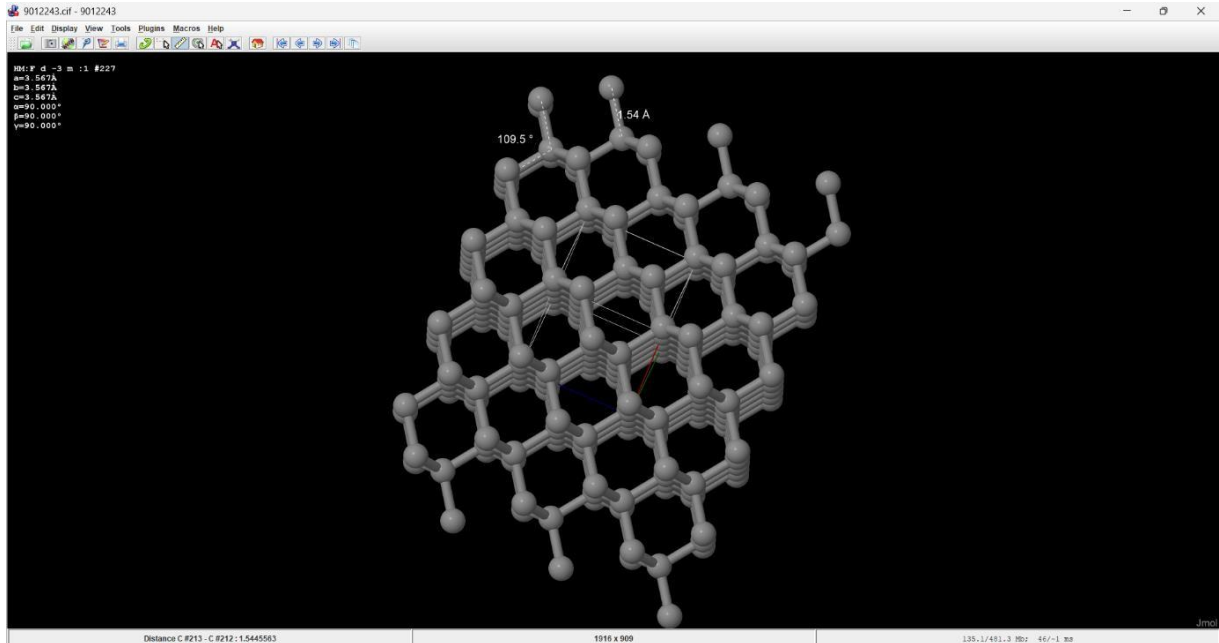


- Perform right click on the mouse, select *symmetry*, now reload {444 666 1} for multi chain of carbon arrangements in graphite
- Our final outcome of graphite structure is follows



3. Additional features in Diamond and Graphite

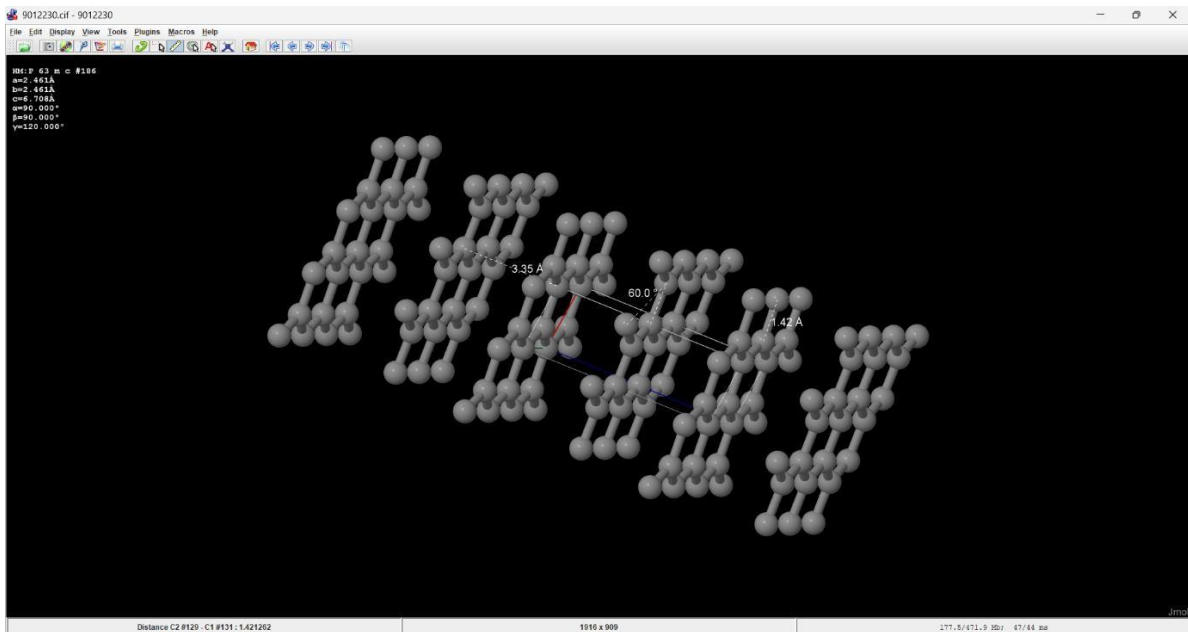
3.1 bond angle and bond length between two carbon atoms in Diamond



conclusion for Diamond structure

- **Structure:** Diamond has a cubic crystal structure, specifically a face-centered cubic (FCC) lattice.
- **Lattice Parameters:**
 - Lattice constant (a,b,c): The lattice parameter for diamond is approximately 3.567 Å.
- **Lattice Angles:**
 - All angles between the lattice vectors in diamond are 90°, consistent with its cubic symmetry.
- **Bond Length:** The C-C bond length is approximately 1.54 Å.
- **Bond Angle:** The bond angle between adjacent carbon atoms is approximately 109.5°, characteristic of sp^3 hybridization.

3.2 bond angle and bond length between two carbon atoms in Graphite and also layers in Graphite



conclusion for Graphite structure

- **Structure:** Graphite has a hexagonal crystal structure.
- **Lattice Parameters:**
 - Lattice constants (a,b and c):
 - The in-plane lattice constant (a,b) is approximately 2.46 Å.
 - The interlayer spacing (c) is approximately 6.70 Å .
- **Lattice Angles:**
 - The angles between the in-plane lattice vectors are 120°, while the angle between the planes is 90°.
- **Bond Length:** The in-plane C-C bond length is approximately 1.42 Å.
The distance between layers (interlayer distance) in graphite is approximately 3.35 Å.
- **Bond Angle:** The bond angle between adjacent carbon atoms in the plane is approximately 120°, characteristic of sp² hybridization.

Conclusion

Due this structural difference only we noticed different physical and chemical properties of Diamond and Graphite even with same chemical formulae

Acknowledgement

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