

Visualisation and Comparative Study of the Allotropes of Carbon Using Jmol Application

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1. Introduction

Carbon is one of the most versatile elements in the periodic table. Due to its ability to bond in multiple ways, carbon can form a wide range of allotropes. This project focuses on three key allotropes of carbon: diamond, graphite, and buckminsterfullerene (C₆₀). Each form has unique structures and properties despite being made of the same element. Using Jmol, an open-source molecular visualisation tool, their structures are explored and compared to better understand their characteristics and applications.

1.1 Structural Analysis of Diamond

1.1.1 Atomic Structure:

A diamond consists of carbon atoms arranged in a three-dimensional tetrahedral lattice. Each carbon atom forms four strong covalent bonds with neighbouring carbon atoms through sp³ hybridisation, resulting in a rigid, repeating framework.

1.1.2 Bonding and Hybridisation

- **Hybridisation:** sp³
- **Bond Angle:** 109.5° (ideal tetrahedral angle)
- **Bond Type:** Covalent, sigma bonds
- **Bond Length:** ~1.54 Å

1.1.3 Crystal Structure

- **Crystal System:** Cubic (Face-Centred Cubic, FCC)
- **Space Group:** Fd $\bar{3}$ m

- **Unit Cell:** Contains 8 carbon atoms in a diamond cubic arrangement

1.1.4 Physical Implications

- Very high hardness due to strong 3d covalent bonding
- High thermal conductivity
- Electrically insulating
- Optically transparent

1. 2 Structural Analysis of Graphite

1.2.1 Atomic Structure

Graphite is composed of **layers of carbon atoms** arranged in **hexagonal rings**. Each carbon atom forms **three sigma bonds** with adjacent carbon atoms using **sp² hybridisation**, and the fourth valence electron occupies a **π-orbital** that contributes to delocalised electron clouds above and below the layers.

1.2.2 Bonding and Hybridisation

- **Hybridisation:** sp²
- **Bond Angle:** 120°
- **In-plane Bond Length:** ~1.42 Å
- **Interlayer Spacing:** ~3.35 Å
- **Bond Type:** Covalent within layers, weak van der Waals between layers

1.2.3 Crystal Structure

- **Crystal System:** Hexagonal
- **Space Group:** P6₃/mmc
- **Structure:** ABAB stacking of 2D hexagonal layers

1.2.4 Physical Implications

- High electrical conductivity in-plane (due to delocalized π -electrons)
- Soft and slippery due to weak interlayer forces
- Opaque and black in appearance
- Good lubricant and electrode material

1.3 Buckminsterfullerene (C_{60})

1.3.1 Atomic Structure

C_{60} is a molecule composed of **60 carbon atoms** arranged in a **spherical cage-like structure** resembling a soccer ball. It consists of **12 pentagons and 20 hexagons**, forming a truncated icosahedron.

1.3.2 Bonding and Hybridisation

- **Hybridisation:** sp^2
- **Bond Angles:** $\sim 108^\circ - 120^\circ$
- **Bond Lengths:** Two types —
 - $\sim 1.40 \text{ \AA}$ (between hexagons)
 - $\sim 1.45 \text{ \AA}$ (between hexagon and pentagon)
- **Bond Type:** Covalent with partial double-bond character due to resonance

1.3.3 Crystal Structure

- **Crystal Form:** Molecular solid in crystalline form
Packing: Often forms face-centred cubic (FCC) lattices at room temperature
- **Space Group:** Varies (commonly $Fm\bar{3}m$ in solid state)

1.3.4 Physical Implications

- Electrically semiconducting or insulating
- Can accept and donate electrons (used in organic photovoltaics and superconductors)
- High symmetry and stability
- Used in drug delivery, materials science, and nanotech applications

2. Importing 3d structure of molecules in Jmol

2.1 Downloading the COD (Crystallography Open Database) database.

- Access the COD database using the hyperlink: <https://www.crystallography.net/cod/>
- Find the Search by COD ID option on the left side of the screen
- Enter the COD ID of the required molecular structures.
- Diamond COD ID - 9012243
- Buckminsterfullerene COD ID-9012244
- Export the structures as CIF

2.1.1 Downloading structures from The Material Projects.

- Access the Material Project website using the hyperlink: <https://next-gen.materialsproject.org/>
- Find the “Start exploring materials” option.
- Enter the material project ID of the required structure
- Graphite - mp-48
- Follow the hyperlink and export the structure as CIF.

crystallography.net/cod/result.php

Crystallography Open Database

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9012244	CIF	Ga H4 N O8 P2 Zn	P 1 21/a 1	9.406; 9.881; 8.612 90; 90.58; 90	800.364	Logar, N. Z.; Mrak, M.; Kaucic, V. Syntheses and structures of two ammonium zinc gallophosphates: analcime and paracelsian analogs Sample: Paracelsian analog <i>Journal of Solid State Chemistry</i> , 2001 , <i>156</i> , 480-486

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doi 10.17188/1208406

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Energy Above Hull 0.003 eV/atom

Space Group P6₃/mmc

Band Gap 0.00 eV

Predicted Formation Energy 0.003 eV/atom

Magnetic Ordering Non-magnetic

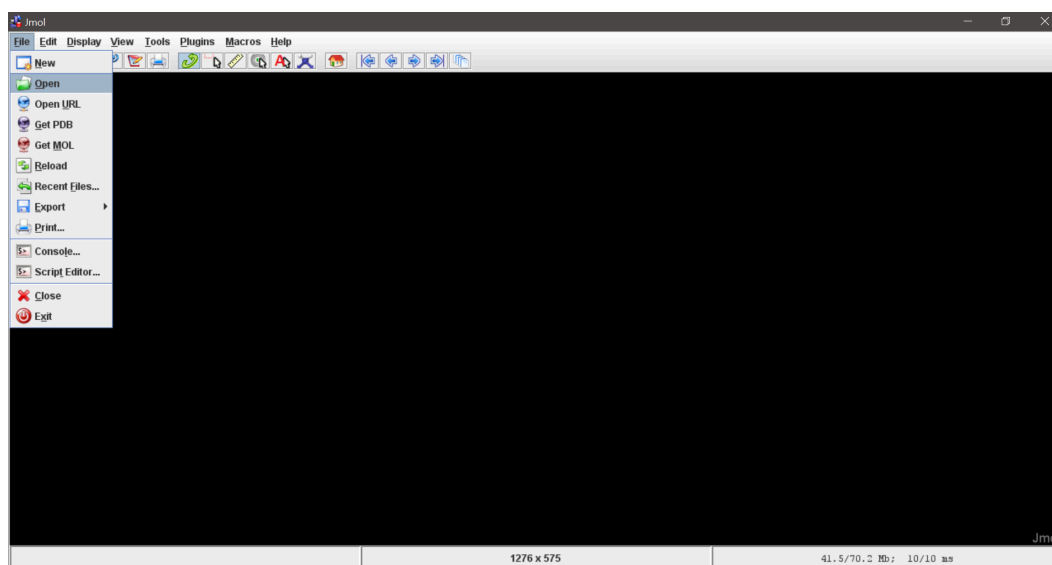
Total Magnetization 0.00 μB/f.u.

Experimentally Observed Yes

Description (Auto-generated)
C is graphite structured and crystallizes in the hexagonal P6₃/mmc space group. The structure is two-dimensional and consists of two C sheets oriented in the (0, 0, 1) direction. C is bonded in a trigonal planar geometry to three equivalent C atoms. All C-C bond lengths are 1.42 Å.

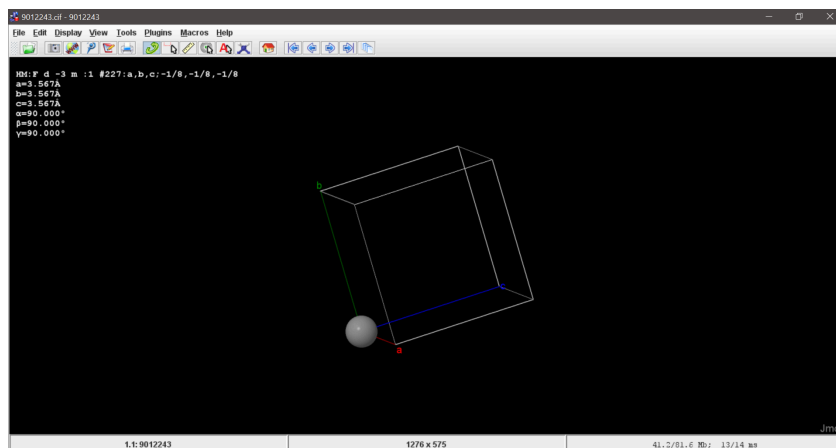
2.2 Loading CIF Files in Jmol

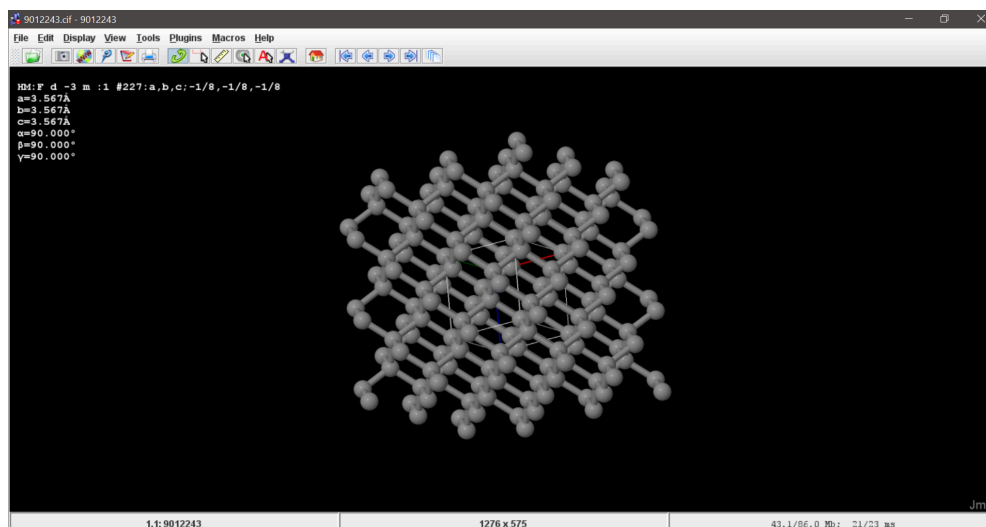
- Launch the Jmol application.
- Click on the file menu located in the toolbar.
- In the resulting dropdown menu, choose 'open' as illustrated below.



2.2.1 Open the structure of the diamond downloaded earlier

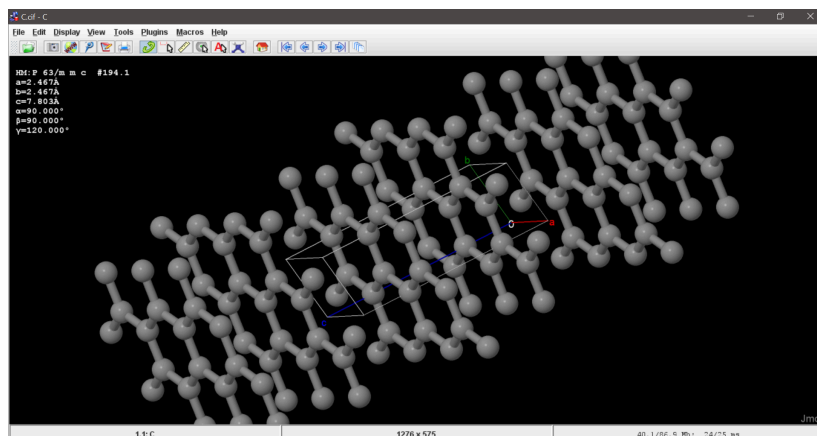
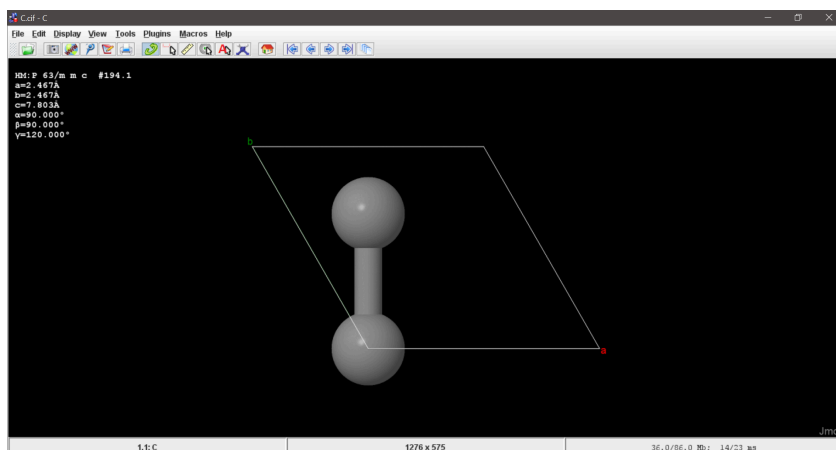
- Right-click the mouse and choose the symmetry option, then reload {444 666 1} to create multiple carbon chain arrangements in diamond.
- Refer to the attached picture for the resulting structure of the diamond.





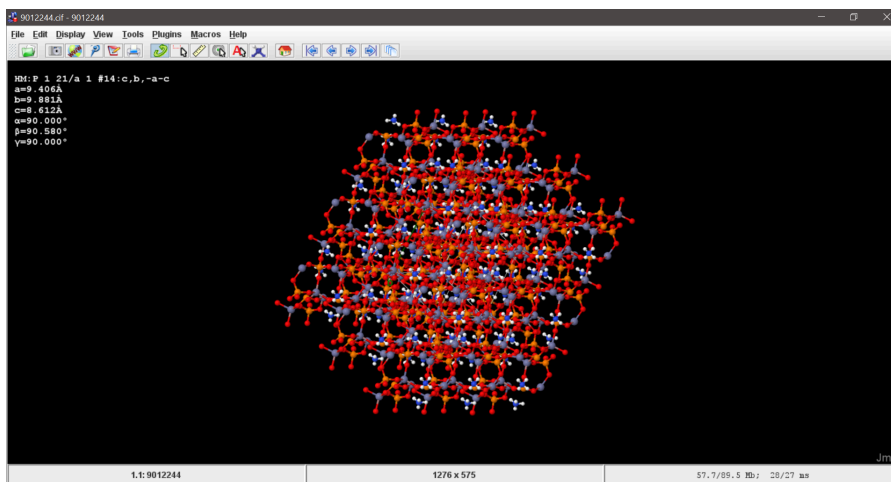
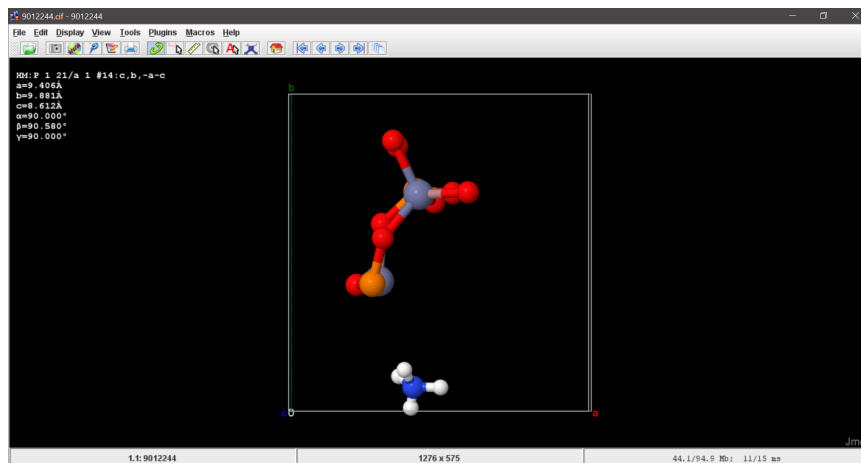
2.2.2 Open the structure of the graphite downloaded earlier

- Right-click on the mouse, choose symmetry, and then reload $\{444\ 666\ 1\}$ for the multiple carbon chains in graphite.
- Refer to the attached picture for the resulting structure of graphite.



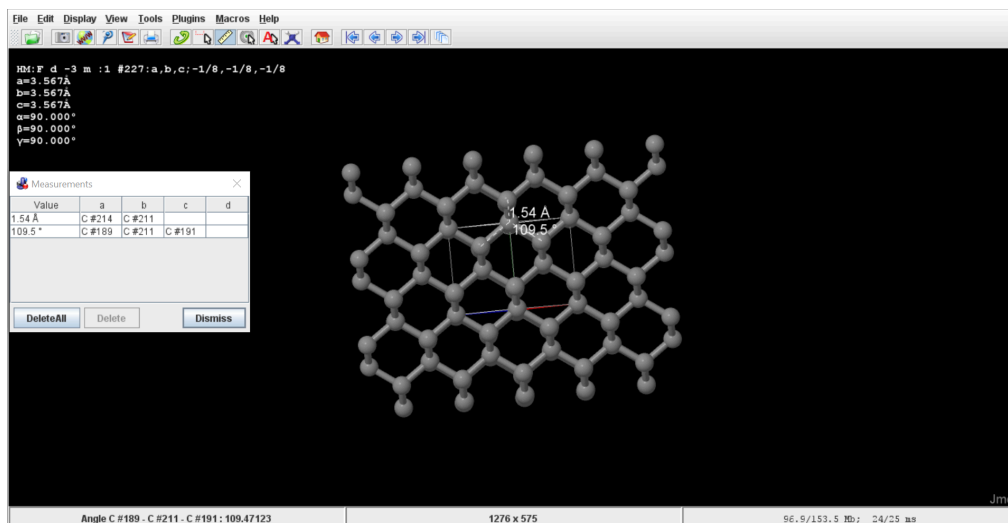
2.2.3 Open the structure of Buckminsterfullerene (C₆₀) downloaded earlier

- Right-click on the mouse, choose symmetry, and then reload {444 666 1} for the multiple carbon chains in Buckminsterfullerene.
- Refer to the attached picture for the resulting structure of Buckminsterfullerene.

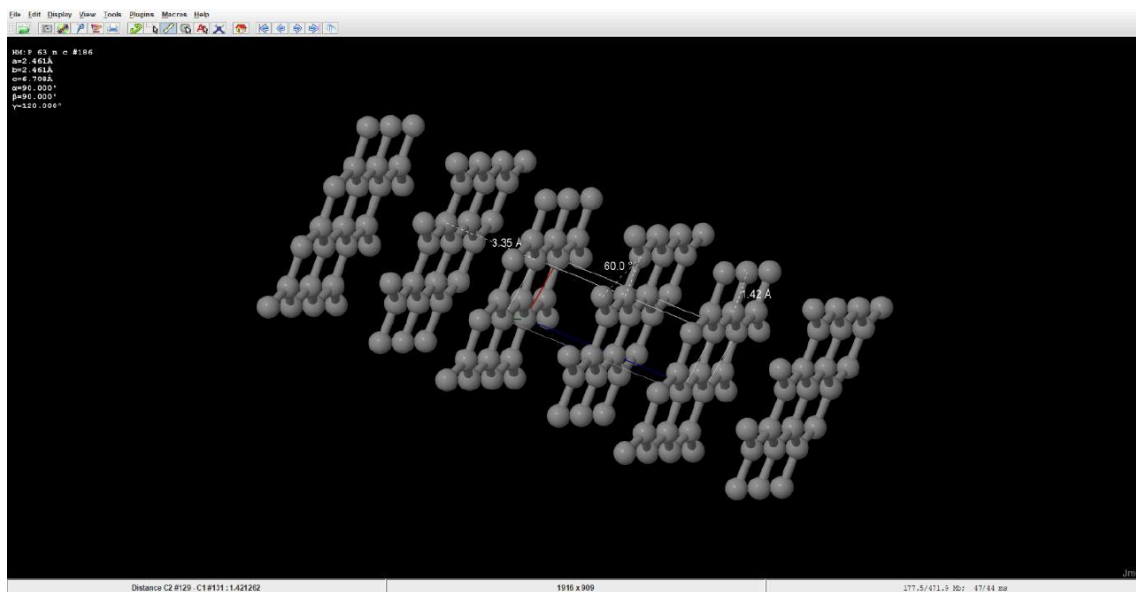


3. Visualisation of bond angles and bond lengths of diamond and graphite

- 3.1 Bond Length And Bond Angle Between A Pair Of Carbon Atoms In Diamond



- 3.2 The Bond Angle And Bond Length Between A Pair Of Carbon Atoms In Graphite And The Layers Present In Graphite.



Comparative Analysis of Carbon Allotropes: Diamond, Graphite, and Buckminsterfullerene (C₆₀)

Aspect	Diamond	Graphite	Buckminsterfullerene (C ₆₀)
Hybridization	sp ³ (tetrahedral)	sp ² (planar)	sp ² (curved)
Bond Length (Å)	1.54 (C–C)	1.42 (in-plane)	1.40 (6:6), 1.45 (6:5)
Bond Angle (°)	109.5 (tetrahedral)	120 (hexagonal)	108 (pentagon), 120 (hexagon)
Crystal System	Cubic (FCC)	Hexagonal	Cubic (*Pa-3*)
Lattice Parameters (Å)	*a* = *b* = *c* = 3.567	*a* = *b* = 2.461, *c* = 6.707	*a* = *b* = *c* = 14.17
Electrical Conductivity	Insulator (no free electrons)	Conductor (delocalized π -electrons)	Semiconductor (limited delocalisation)
Hardness	Hardest natural material (10 Mohs)	Soft (1–2 Mohs)	Brittle (molecular crystal)
Key Applications	Cutting tools, jewelry, electronics	Lubricants, batteries, electrodes	Drug delivery, nanotechnology
Jmol Confirmation	✓ Bond angles/lengths verified	✓ Bond angles/lengths verified	✓ Layered structure visualized

Conclusion:

This project conducted a comparative structural analysis of three carbon allotropes—diamond, graphite, and Buckminsterfullerene (C_{60})—using Jmol for visualization and measurement. The study confirmed that atomic hybridization (sp^3 vs. sp^2) and lattice geometry dictate their mechanical, electrical, and chemical properties.

Acknowledgement:

I would like to convey our gratitude to the management of Kalasalingam Academy of Research and Education for the fabrication resources they provided. Additionally, we sincerely thank Dr. M. Kalpana, Dean of Freshman Engineering, and Dr. D. Geetha, my project guide, for her encouragement and support.