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

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Abstract

Diamond and graphite are made up of carbon atoms. They are two unique allotropes of carbon in nature with dramatically different properties. In this study, we will examine the atomic-level structural properties of graphite and diamond using Jmol, a molecular visualization tool. Our focus will be on elucidating the unique atomic arrangements of carbon atoms in each allotrope, emphasizing variations in bonding, symmetry, and crystalline structure, using molecular modeling and visualization. In particular, we study the sp^2 hybridization in graphite, which is responsible for its layered structure and conductivity. Whereas in diamond the sp^3 hybridization of carbon atoms results in its hardness and transparency. Our investigation sheds light on the fundamental disparities between these two allotropes and their wide range of applications in materials science, electronics, and nanotechnology.

Keywords: Jmol, Diamond, Graphite, Carbon allotropes, Molecular visualization, Atomic structure, sp^3 hybridization, sp^2 hybridization, Materials science.