What Are its Crystal Structure and Chemistry?

*Crystal Structure*

Diamond is comprised entirely of carbon and its chemical formula is simply C. Diamond belongs to theisometric or cubic crystal system meaning that each of the crystallographic axes is the same length and at 90 degrees to one another (i.e., the unit cell building blocks are simple cubes). This particular arrangement has very strong covalently bonded carbon atoms in a highly symmetrical three dimensional network, which makes for an impressively hard, durable and dense material. This differentiates diamond from many other minerals in this respect, as ionic bonding is more common than covalent bonding in minerals.

But diamond does have its weakness. Diamond has a set of *imaginary* flat planes within its atomic structure that display perfect cleavage. We describe these planes as being at [111], or a plane intersecting each of the three orthogonal axes at an equal unit of 1 away from the origin. The shape of the intersecting planes is that of an octahedron (an eight-sided polyhedron), hence the descriptor "octahedral" for its cleavage.

Diamond cutters require a good understanding of the mineral's crystallography and where its inherent weaknesses lie in order to expertly cut stones and grind the flat parts (facets) on a polished stone. Before the advent of analytical techniques using x-ray diffraction, information on the weakness of diamond were derived from observations that often came from gemstone cutters.

The images below show 3 views of the crystal structure of diamond, looking down a crystallographic axis, perpendicular to a perfect cleavage plane, and at an oblique angle to the cleavage plane to show the inherent weakness in the crystal. The red balls symbolize carbon atoms, and the grey bars illustrate the covalent bonds that link them together.

Diamond's crystal structure looking along a crystallographic axis (left image); along [111], perpendicular to the plane that characterizes (111) (middle image); and looking at an oblique angle to emphasize where the C–C bonds are the furthest apart and weakest (right image). This last view allows a cleavage plane (in light red) to be described in 3D space. The black 3D cube is the unit cell or building block for diamond.

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| Click here for 3D animation of [diamond's octahedral form](http://webmineral.com/java/Diamond.shtml) (opens an external window from webmineral.com) | Click here for interactive 3D animation of [diamond's crystal structure](http://webmineral.com/jpowd/JPX/jpowd.php?target_file=Diamond.jpx) (opens an external window from webmineral.com) |

Interestingly, graphite, like diamond, is also a material composed entirely of carbon. However, it has a significantly different crystal structure and therefore significantly different physical properties. This phenomenon of a material being of the same composition but having a different crystal structure is known as polymorphism and both diamond and graphite are 'polymorphs' with the composition "C".

Carbon atoms within graphite are partially covalently bonded, but strong bonds only exist in 2-dimensional sheets.  Bonding between these sheets (ie, perpendicular to these planes) is of the Van der Waals type and are very weak. Graphite therefore cleaves parallel to these sheets along the (001) plane. Comparing the crystal structures of diamond and graphite using the linked 3D models below, you'll notice that in diamond the C atoms are strongly bonded to each other in 3-dimensions.  Each carbon atom is bonded to 4 other carbon atoms forming a tetrahedron. When you rotate the crystal structure of graphite, you'll notice that the C atoms are only strongly bonded to each other in 2-dimensions forming infinitely linked hexagons.  Each carbon atom is bonded to 3 other carbon atoms. It is between these planes that the Van der Waals bonding occurs.

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| Click here for 3D animation of [graphite's crystal structure](http://webmineral.com/jpowd/JPX/jpowd.php?target_file=Graphite.jpx) (opens an external window from webmineral.com) | Click here for interactive 3D animation of[diamond's crystal structure](http://webmineral.com/jpowd/JPX/jpowd.php?target_file=Diamond.jpx) (opens an external window from webmineral.com) |

*Crystal Chemistry and Type Classification of Diamond*

Although gemologists and jewellers typically group diamonds based on the 4Cs, scientists classify diamonds based on crystal chemistry variations. The first subdivision in the scientist's classification scheme is based on the amount of nitrogen (N) that has substituted into the crystal structure.

Classification of diamonds based on its crystal chemistry. From [Breeding and Shigley 2009](https://connect.ubc.ca/bbcswebdav/pid-2559739-dt-content-rid-10494221_1/courses/SIS.UBC.EOSC.118.99C.2014WC.44220/Course_Files/moduleB/lesson09/download/DiamondTypesBreeding2009.pdf)

Type I diamonds have N concentrations greater than 10 ppm (and up to ~3000 ppm) and Type II diamonds have N less than 10 ppm (i.e., considered to be nitrogen-free). Type I diamonds are further grouped into two: Type Ia where N atoms occur in aggregates within the diamond and Type Ib where N in the diamond structure is dispersed. In the next level, Type Ia diamonds with clustered N are subdivided into Types IaA with paired N atoms and IaB where 4 N atoms (quads) are clustered often with a vacancy (void/absence of atoms) at their center. Type II diamonds with little to no N in their crystal structure can be subdivided into Type IIa, those that are boron (B)-free and Type IIb, those that contain minute amounts of B, up to about 10 ppm.

Most diamonds (~98%) belong to the Type Ia group, those containing appreciable amounts of N that are clustered in the crystal structure. Type Ia diamonds exhibit absorption of blue light and therefore show an overall yellow hue. Type IIa is the next most common type of diamond (<2%). These diamonds have no appreciable N or B substituting for carbon in the crystal structure. Due to a lack of impurities, these diamonds tend to show the whitest colour with little to no absorption of light across the visible spectrum. Physical deformation and resulting crystal defects in Type IIa crystals give rise to most pink, purple, and brown diamonds.

Type IIb diamonds are very rare and contain minute amounts of B in the crystal structure but no appreciable N. Optically, the incorporation of boron causes most light except blue to be absorbed, imparting a blue to grey hue. These diamonds are very rare and include specimens like the Hope Diamond. Finally, Type Ib diamonds are also very rare and are characterized by appreciable N, but scattered about the crystal lattice. Diamonds of this type occur in a range in colours including yellow, brown, orange, and green or can be colourless.