Ionic, Simple Molecular and Giant Molecular Crystals

A crystal is a solid substance, which has an ordered arrangement of atoms, molecules or ions. Such solids may be classified as either an ionic crystal, a simple molecular crystal or a giant molecular crystal, depending on the type of bonding (ionic or covalent), as well as the arrangement of the atoms or molecules in the compound. Solids that do not have a crystalline structure are called amorphous.

Structure and Properties of Ionic Compounds

Ionic Crystals (E.g. Sodium Chloride)

A feature of ionic compounds is that they form structures that have a well-defined lattice. This is facilitated by the oppositely charged ions, which arrange themselves in an ordered and regular way. Sodium chloride (NaCl) is a common example of an ionic compound. The ions are arranged in such a way that each Na⁺ is surrounded by six Cl⁻, and each Cl⁻ is surrounded by six Na⁺.

Properties of Ionic Compounds

- They are hard, brittle crystalline solids
- They have high melting points and heats of fusion
- They conduct electricity well when molten or in aqueous solution
- They do not conduct electricity in the solid state
- (Most) dissolve readily in water
- They react readily with each other in solution

Structure of Ionic Compounds

Ionic solids are formed by ionic bonding. The solids are crystals because of their structure. In a crystal, the regular structure tells that the ions are arranged in an orderly manner to form a crystal lattice.

The sodium chloride structure is a regular, repeating arrangement of ions. Each sodium ion is surrounded by six chloride ions as its nearest neighbours. This arrangement results in a closely packed three-dimensional structure. Two models of sodium chloride crystal structures are shown below:



Ionic compounds are said to consist of a "giant structure of ions".

Properties of Ionic	Comment
Compounds	
Crystalline solid	Due to regular arrangement of ions, resulting from strong attractions
	between opposite charges
Conduct electricity	On melting, ions are set free: these ions move to an oppositely charged
when molten	electrode when a voltage is applied
High melting points,	These high values indicate that the ions are held together strongly –
high boiling points,	therefore lots of energy is needed to separate the ions
high heats of fusion	
and vaporization	

Structure and Properties of Simple Covalent (Molecular) Substances

Properties of Simple Covalent Substances

Most substances that contain covalent bonds are also described as simple molecular substances, because they consist of separate molecules. The properties of covalent substances are shown below:

Properties of Molecular Substances	Comment
Some are liquids or gases at room temperature	They consist of small molecules with weak attractive forces between them
Low melting and boiling temperatures, low heats of fusion and vaporization	Due to weak intermolecular forces

Some are soluble in water, while some are soluble in non-polar organic solvents such as methylbenzene	The non-polar molecular substances dissolve in non-polar solvents; polar substances dissolve in both types of solvent
Do not conduct electricity when molten	This is due to the absence of ions (N.B. A few may react with water to produce ions and the resulting solution conducts electricity)

Covalent substances tend to be liquids or gases at room temperature because the forces between the molecules (intermolecular forces) are weak.

Simple Molecular Crystals

In simple molecular compounds, the number and arrangement of each different type of atom is fixed in the molecule. The bond between any two atoms is a covalent one. So, for instance, in CO_2 , for every molecule present, there is one atom of carbon separately and covalently bonded to two atoms of oxygen. In molecular iodine, I_2 , there are two atoms of iodine covalently bonded to each other.

In a crystal of iodine, the I_2 molecules pack together in layers, described as a herring-bone pattern. In this pattern, the iodine molecules are further away from the molecules above and below them, than they are from molecules in their own layer.

Intermolecular Forces

Intermolecular forces are the weak forces between individual molecules. Two types of intermolecular forces are Van der Waals forces and Hydrogen bonds. These forces are neither ionic nor covalent.

Van der Waals Forces

The uneven movement of all the electrons within molecules results in an uneven distribution of electronic charge leads to positive and negative charges within molecules. These are called dipoles. All covalent molecules (polar or non-polar), develop temporary or instantaneous dipoles. Van der Waals forces are the weak attractions between oppositely charged ends of molecules with temporary dipoles.

Hydrogen Bonds

The hydrogen bond is the weak attraction between the slightly positive hydrogen atom in one polar molecule and the slightly electronegative atom in another polar molecule of the same type or of a different type.



Structure of Simple Covalent Solids

Solids containing discrete covalent molecules generally have lower melting and boiling points than giant ionic solids, because of the weak intermolecular forces present in the covalent molecules.

Examples of simple molecular solids are the elements sulphur (S_8) , phosphorus (P_4) and iodine (I_2) , solid carbon dioxide (dry ice) and water (ice).

Sometimes the particles of the same element can be arranged in different ways, giving rise to different forms. For example, the elements sulphur and phosphorus have more than one crystalline form. When an element can exist in different forms in the same physical state, it is said to exhibit allotropy. The different forms of the element are known as allotropes. (The two allotropes of sulphur are rhombic sulphur or alpha sulphur, and monoclinic sulphur or beta sulphur)



- Giant Covalent Solids

A few covalent solids (such as diamond, graphite and silica) have high melting and boiling points as well as high heats of fusion and vaporization. Like simple covalent solids, these solids are also formed by covalent bonding, but they do not form individual molecules. Instead, they exist as macromolecules in which very strong covalent bonds exist in three dimensions. These compounds are usually insoluble in polar and non-polar solvents.

Giant Molecular Crystals

Just as with simple molecular compounds, compounds with a giant molecular structure have covalent bonds that join the atoms together. However, unlike simple molecular structures, the number of atoms joined to each other in giant molecular structures is not definite, with the size of the molecule theoretically continuing indefinitely for the size of the sample. Even though the size of the molecule is undefined, the arrangement of atoms follows a clearly defined and ordered structure, called a repeat unit. This repeat unit represents what the expanded molecule looks like.

Some examples of giant molecular crystals include:

- Polymers
- Silicon dioxide (SiO₂) The major component of beach sand and glass is silicon dioxide.
- Diamond Diamond is composed of four covalently bonded carbon atoms. Each carbon atom is bonded to four other carbon atoms in a tetrahedral formation. This arrangement is repeated throughout the entire lattice in all directions.
- Graphite Graphite is made of covalently bonded carbon atoms (like diamond).
 However, the atoms are arranged differently in graphite, as the covalent bonds only exist in two dimensions. The structure of graphite comprises hexagonal layers of carbon atoms, and each carbon atom is bonded to only three other carbon atoms.



Structure of Diamond



