AS 91164 Bonding, structure, properties and energy changes

LEWIS DIAGRAMS, SHAPES OF MOLECULES, POLAR AND NON-POLAR MOLECULES

Lewis diagrams: use dots (or x) to represent electrons, show only outer electrons.

Multiple bonds: some atoms e.g. C, O and N can form double or triple bonds. (In drawing Lewis structures introduce = and ≡ only if there are unpaired electrons remaining and there are atoms which don't have a share in 8 electrons).

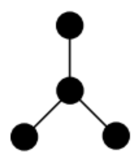
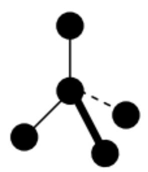
Bond polarity: when identical atoms are covalently bonded the electron pair is attracted equally by the 2 nuclei. The bond is non-polar. When the two atoms are different one nucleus will have a greater attraction for the electron pair in the bond than the other. The result is a polar covalent bond. One end is slightly negative with respect to the other. E.g. HCl. $^{\delta+}H-Cl^{\delta-}$.

Electronegativity: Is a measure of the attraction of an atom for the electron pair in a covalent bond. The most electronegative atom is fluorine. Electronegativity values increase across any period and decrease down a group. A polar bond results when there is a difference in electronegativity between the 2 atoms forming the bond. The more electronegative atom is the negative end of the bond. The bigger the difference in electronegativity between the 2 atoms forming the bond, the more polar the bond is.

Covalent or ionic? There is no distinct split between covalent and ionic bonding. (It may help to think of ionic bonds as the extreme of polar bonds where one atom takes over complete control of the electron pair).

Cl-Cl (non polar) ------------ $^{\delta+}H-Cl^{\delta-}$ (polar) ------------ Na^+ Cl^- (ionic)

Shapes of molecules: Covalent bonds are "directional". The rule is that regions of negative charge around the central atom repel each other as far as possible. The shape of a molecule or ion depends on the number of regions of negative charge around the central atom.
Double and triple bonds count as a region of negative charge for the purpose of determining shape. Don't draw the nonbonding (NB) pairs as part of the final shape of the molecule. Below they are shown as just to remind you they are there.

Regions of negative charge	2	3	3, one being non bonding	4	4, one being non bonding	4, two being non bonding
Shape	linear	Triangular planar	V-shaped or angular	tetrahedral	Trigonal pyramid	V-shaped or angular
Example	CO_2	H_2CO	SO_2	CH_4, NH_4^+	NH_3, PCl_3	H_2O, H_2S
						

Polarity of molecules: This depends on (1) whether the molecule has polar bonds (2) the symmetry of the molecule. Assuming the atoms bonded to the central atom are the same, symmetrical shapes are linear, trigonal planar and tetrahedral.

CO_2: has two regions of negative charge around the central atom. It has no unshared electron pairs and is therefore linear.

H_2CO: has three regions of negative charge around the central atom. It has no unshared electron pairs and is therefore trigonal planar. Having one very polar C=O bond and 2 virtually non-polar C-H bonds, it will be polar.

SO_2 has three regions of electron density (electron clouds) around the central atom (or S) and repulsions between them result in a bond angle of 120°. SO_2 is a polar molecule because the O atoms will attract bond pairs in the O – S bonds more closely. The two polar bonds are asymmetrically arranged, (therefore the dipoles will not cancel,) resulting in a polar molecule overall.

CH_4 has four regions of electron density around the central atom (C) and repulsions between them result in a bond angle of 109.5°.

NH_3: the molecule has four regions of negative charge around the central atom. These are arranged tetrahedrally. Three are bonding regions and there is one non-bonding region which results in the trigonal pyramid shape, bond angle approx. 109°. The lone pair of electrons on the N causes the asymmetry. The effect of the polar bonds is not cancelled out, making the molecule polar overall.

PCl_3: 3 polar bonds and unsymmetrical arrangement (trigonal pyramidal) of P–Cl bonds around central atom so polarities do not cancel out therefore polar.

H_2O has four regions of electron density around the central atom (O). 2 are bonding and 2 are non-bonding. Repulsions between them result in a bond angle of approx. 109°. H_2O is also a polar molecule for the same reasons as given above.

Polar molecules will dissolve in a polar solvent; therefore, SO_2 is soluble in water. There is attraction between positive end of one molecule and negative end of other in solution. PCl_3 and H_2S also dissolve in water. ('like' dissolves 'like'.) On the other hand non-polar CO_2 and CH_4 are virtually insoluble in water.

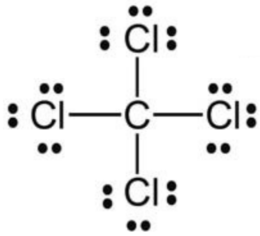
Practice explaining shape and polarity.

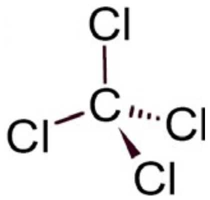
Remember:

Lewis diagram ⇒ shape of molecule (depends on electron repulsions around central atom) ⇒ consider polarity (if any) of bonds using idea of electronegativity (F O N/Cl S C H) ⇒ consider overall molecular shape ⇒ predict if molecule is polar or non-polar overall in terms of dipoles cancelling out or not.

Why is CCl_4 tetrahedral? Is it polar or non-polar?

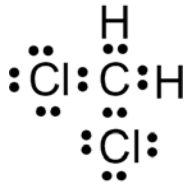
The molecule is tetrahedral, due to 4 regions of electron density around the central C atom.



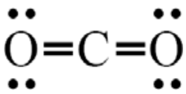


The C–Cl bond is polar (has a dipole), due to the difference in electronegativity of C and Cl. As these 4 identical dipoles are arranged symmetrically about the C atom in CCl_4, the dipoles cancel out, so the molecule is non-polar.

So why is CH_2Cl_2 the same shape but this molecule is polar?

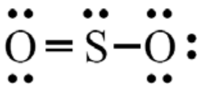


The molecule is tetrahedral due to 4 regions of electron density around the central C atom. The C–Cl bonds are polar due to the difference in electronegativity of C and Cl, while the C–H bonds are almost non–polar.
Although the bond arrangement around the C atom in CH_2Cl_2 is symmetrical, the differing dipoles of the C–H and C–Cl bonds means the effect of the polar bonds does not cancel out, so the molecule is polar overall.

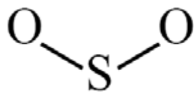
And CO_2? 

CO_2 has non-polar molecules. The C−O bonds of CO_2 are polar due to the different electronegativities of C and O.
As there are only 2 regions of electron density about the central C atom, the polar bonds are arranged symmetrically about the C atom giving the molecule a linear shape.

The effect of these polar bonds / bond dipoles cancel out so that the molecule is non polar.

So, what about SO_2 – is that the same? 

SO_2 has polar molecules. The S−O bonds of SO_2 are polar due to the differing electronegativities of S and O. There are 3 regions of electron density about the central S atom (which repel to a trigonal planar arrangement), however, the lone pair of electrons on the S atom causes the S−O bonds to occupy a bent or V shape around the central S atom. Therefore the effect of these polar bonds / bond dipoles is does not cancel out, so that overall the molecule is polar.



EXPLAINING SOME PROPERTIES IN TERMS OF STRUCTURE & BONDING

ELECTRICAL CONDUCTIVITY OF IONIC SUBSTANCES E.g. NaCl, $MgCl_2$

Explain - Solid sodium chloride does not conduct electricity. However, if it is melted, sodium chloride will conduct electricity.

In the solid state, sodium chloride consists of a 3–D lattice of Na^+ and Cl^- ions. Although charged particles are present, they are held in position by strong ionic bonds. As there is no charged particles able to move, the solid will not conduct electricity.

When the solid is melted (molten) the ions become free moving, and the free moving chargd particles means the liquid will conduct electricity. When molten, the charged ions are separated and free to move and conduct electricity.

THE HIGH MELTING POINT OF IONIC SUBSTANCES E.g. NaCl, KCl

Explain - NaCl has a high melting and boiling point

Sodium chloride consists of a 3–D lattice of Na^+ and Cl^- ions. The ions are held in position by strong ionic bonds. As a lot of energy is required to overcome these strong forces and separate the ions, the substances have high melting and boiling points.

THE SOLUBILITY OF (MANY) IONIC SUBSTANCES IN WATER E.g. KCl, NaCl

Explain - Potassium chloride will not dissolve in non-polar solvents, but will dissolve in water.

KCl is soluble in water as the polar water molecules are attracted towards the ions, and the attraction is sufficient to pull the ions from the lattice. The molecules of a non–polar solvent are not attracted towards the ions and so KCl is insoluble, for example, in cyclohexane.

METALS ARE EASILY SHAPED (MALLEABLE) OR CAN BE DRAWN INTO WIRES (DUCTILE) E.g. Cu, Ag, Zn

Explain - Copper is easily shaped to form wires.

Copper consists of Cu atoms held together in a 3D lattice by metallic bonding, in which valence electrons are attracted to the + nuclei of neighboring atoms. As this is a non-directional force, layers of atoms can slide over each other without breaking the metallic bond and disrupting the structure and breaking the metal.

METALS ARE GOOD CONDUCTORS OF ELECTRICITY

Explain - Copper (Cu) is a good conductor of electricity and is used for electrical wires.

Copper atoms are held together in a 3-D lattice by metallic bonding, in which delocalised valence electrons are attracted to the + nuclei of neighbouring atoms. Conduction of electricity requires free moving charges - the delocalised valence electrons.

COVALENT MOLECULAR SUBSTANCES HAVE LOW MELTING AND BOILING POINTS E.g. PCl_3, SCl_2

Explain - PCl_3 and SCl_2 both have low melting and boiling points.

These are molecular substances. They consist of molecules and the molecules are attracted to each other by weak intermolecular (or van der Waals) forces. As not much energy is required to overcome these weak forces and separate the molecules, the substances have low melting and boiling points.

SILICON DIOXIDE HAS A HIGH MELTING POINT & DOESN'T CONDUCT ELECTRICITY

Explain - Silicon dioxide has a high melting point

Silicon dioxide consists of silicon and oxygen atoms held together by covalent bonds in a tetrahedral arrangement, so that a 3D network exists. As the covalent bonds are strong, they are difficult to overcome and break, making it difficult to separate the atoms, so the structure has a high melting point.

Strong covalent bonds hold the Si and O atoms together in a 3D arrangement. As all valence electrons are involved in forming covalent bonds there are no free moving charges and so no electrical conduction.

EXPLAIN SOME PROPERTIES OF IODINE – SUBLIMATION & SOLUBILITY

Explain - Iodine sublimes when gently heated.

Iodine consists of I_2 *molecules and weak intermolecular forces / weak Van der Waals forces exist between the molecules. As these attractions are weak, the molecules are easily separated, and the melting point is low.*

Explain - It is soluble in cyclohexane.

Iodine molecules are non-polar, therefore iodine is soluble in a non-polar solvent such as cyclohexane. Since both molecules have similar weak intermolecular forces, then the same weak forces will exist between the two different molecules and this is why it will dissolve in cyclohexane.

EXPLAINING SOME PROPERTIES OF CARBON DIOXIDE

Explain - CO_2 sublimes at -78°C, is a poor conductor as a solid and is brittle as a solid.

CO_2 *exists as molecules. As the intermolecular forces between molecules are weak these are easily overcome hence little energy is required to separate the molecules (therefore has a low MP/sublimes at -78°C).*

As all valence electrons are involved in forming covalent bonds there are no free moving charges and so no electrical conduction.

Since the weak intermolecular forces allow the molecules to be easily separated this makes it brittle / (easy to break the solid).