4.3 Covalent structures

Nature of science:

Scientists use models as representations of the real world—the development of the model of molecular shape (VSEPR) to explain observable properties. (1.10)

Understandings:

- Lewis (electron dot) structures show all the valence electrons in a covalently bonded species.
- The “octet rule” refers to the tendency of atoms to gain a valence shell with a total of 8 electrons.
- Some atoms, like Be and B, might form stable compounds with incomplete octets of electrons.
- Resonance structures occur when there is more than one possible position for a double bond in a molecule.
- Shapes of species are determined by the repulsion of electron pairs according to VSEPR theory.
- Carbon and silicon form giant covalent/network covalent structures.

Applications and skills:

- Deduction of Lewis (electron dot) structure of molecules and ions showing all valence electrons for up to four electron pairs on each atom.
- The use of VSEPR theory to predict the electron domain geometry and the molecular geometry for species with two, three and four electron domains.
- Prediction of bond angles from molecular geometry and presence of non-bonding pairs of electrons.
- Prediction of molecular polarity from bond polarity and molecular geometry.
- Deduction of resonance structures, examples include but are not limited to C_6H_6, CO_3^{2-} and O_3.
- Explanation of the properties of giant covalent compounds in terms of their structures.

Guidance:

- The term “electron domain” should be used in place of “negative charge centre”.
- Electron pairs in a Lewis (electron dot) structure can be shown as dots, crosses, a dash or any combination.
- Allotropes of carbon (diamond, graphite, graphene, C_{60} buckminsterfullerene) and SiO_2 should be covered.
- Coordinate covalent bonds should be covered.

Theory of knowledge:

- Does the need for resonance structures decrease the value or validity of Lewis (electron dot) theory? What criteria do we use in assessing the validity of a scientific theory?

Utilization:

Syllabus and cross-curricular links:
Option A.7—biodegradability of plastics
Biology topic 2.3—3-D structure of molecules and relating structure to function

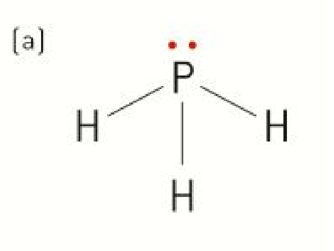
Aims:

- **Aim 7**: Computer simulations could be used to model VSEPR structures.

UNIT 4.3 – COVELENT STRUCTURES

LEWIS STRUCTURES

Lewis structures show bond between elements in a compound, as well as their lone pairs.

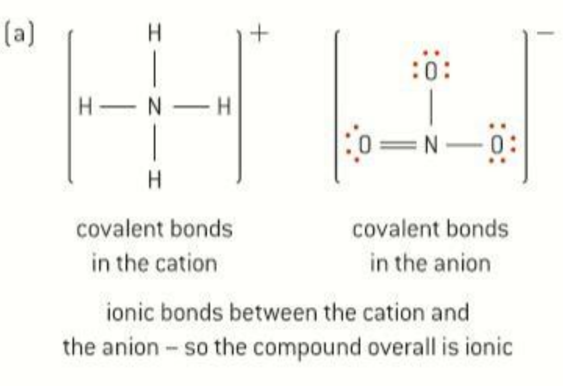


Important things to include

- **Bonding pairs of electrons** (showing the covalent bond as single, double, or triple bonds)
- **Non-bonding pairs of electrons,** often called **lone pairs**, which are pairs of electrons not involved in the bonding.

LEWIS STRUCTURES OF CATIONS AND ANIONS

When there is covalent bonding within an ion, it can still be shown as a Lewis structure.



When given a question to draw a Lewis structure of an ion, simple either add or subtract an election(s) where necessary.

VSEPR – VALENCE SHELL ELECTRON PAIR REPULSION THEORY

A model chemists use to predict the shape of individual molecules based upon the extent of electron-pair **electrostatic repulsion**.
It basically is a theory that says that electron-pairs arrange themselves so they are as far away as possible from one another, even the lone pairs.

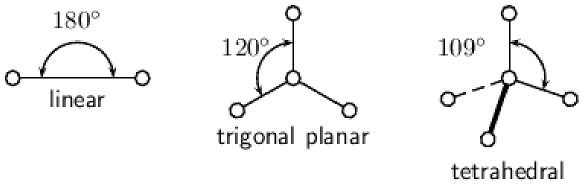
BOND ANGLES

Non-Bonding Pair + Non-Bonding Pair > Non-Bonding Pair + Bonding Pair > Bonding Pair + Bonding Pair

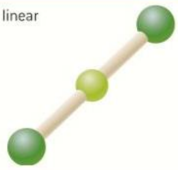
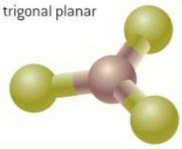
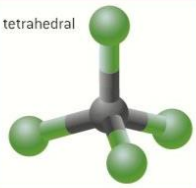
ELECTRON DOMAINS

The space where electrons can occupy are described as **electron domains**. Taking VSEPR into account, the number of electron domains in a compound will influence its shape.

3D SHAPES OF MOLECULES



2 bonding pair, 3 bonding pairs, 4 bonding pairs

Number of electron domains	Molecular geometry	Bond angle	Examples of molecules or ions having this shape
two	linear 	180°	AB_2 $BeCl_2$, CO_2
three	trigonal planar 	120°	AB_3 BF_3, $[NO_3]^-$
four	tetrahedral 	109.5°	AB_4 CH_4, $[NH_4]^+$, $[ClO_4]^-$

These are the geometries when there are **no lone pairs**.

BRINGING IN VSEPR THEORY

There are two ways to describe molecular geometry.

- The **electron domain geometry** (based on the total number of electron domains predicted from VSEPR theory)
- The **molecular geometry** (which gives us the shape of the molecules)

Number of electron domains	Electron domain geometry	Molecular geometry	Bond angle	Examples of molecules or ions having this shape
three	trigonal planar AB_2E	V-shaped (bent)	$<120°$	SO_2, $[NO_2]^-$
four	tetrahedral AB_3E	trigonal pyramidal	$<109.5°$	NH_3, $[SO_3]^{2-}$, $[H_3O]^+$
four	tetrahedral AB_2E_2	V-shaped (bent)	$<109.5°$	H_2O, $[NH_2]^-$

▲ Table 2 Geometries involving lone pairs based on three and four electron domains

A = central atom

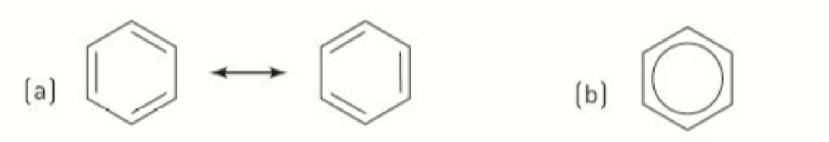
B = Bonds

C = Lone Pairs

As soon as there is a **lone pair**, you can see that the bond angle is **less than** its original.

RESONANCE STRUCTURES

Sometimes it's possible for Lewis structures to have identical arrangements of atoms, but different arrangement of electrons.
These are called **resonance forms**.



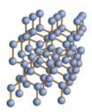
ALLOTROPES

Allotropes of the same element can vary in both physical and chemical properties.

Carbon is a good example as it can exist as **diamond, graphite and fullerene**.

COVALENT NETWORK SOLIDS/LATTICE

Covalent network solids are when the atoms are held together by covalent bonds in a giant 3D lattice structure.



- Diamond – smaller atoms (carbon) so the bonds are tighter and stronger
- Silicon - larger atoms (silicon) so the bonds are further away and weaker
- Silicon dioxide (quartz)

COVALENT LAYER LATTICE

- Graphite
    - Strong layers but only weak forces holding the layers together
    - Layers come off easily (pencil)

COORDINATE COVALENT BONDING

Another type of covalent bonding is called **coordinate covalent bonding**. In coordinate bonding, the shared pair of electrons comes from only one electron; this atom donates both electrons to the shared pair.

A number of species have coordinate covalent bonding. Examples include:

- $[NH_4]^+$
- $[H_3O]^+$
- CO
- Al_2Cl_6
- transition metal complexes (discussed in topic 13).

Ammonium cation, $[NH_4]^+$

When ammonia, NH_3, reacts with an acid, H^+, the lone pair on the nitrogen in NH_3 combines with the proton, H^+, to form the ammonium cation, $[NH_4]^+$:

$$H_3N: + H^+ \rightarrow [NH_4]^+$$