

MSJChem

Tutorials for IB Chemistry

Structure 2.2 HL

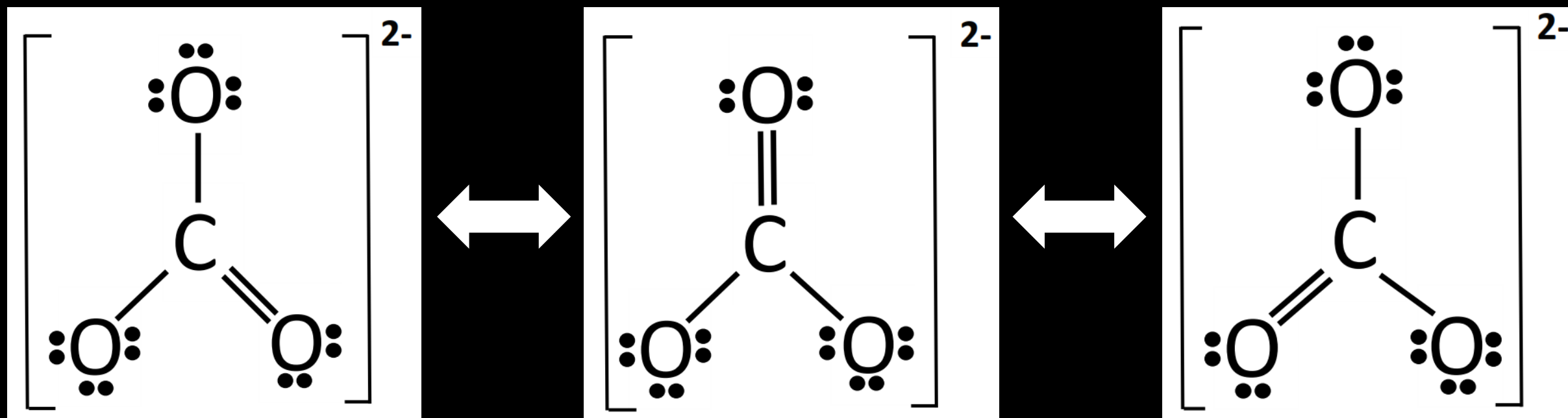
MSJChem

Tutorials for IB Chemistry

**Resonance
structures**

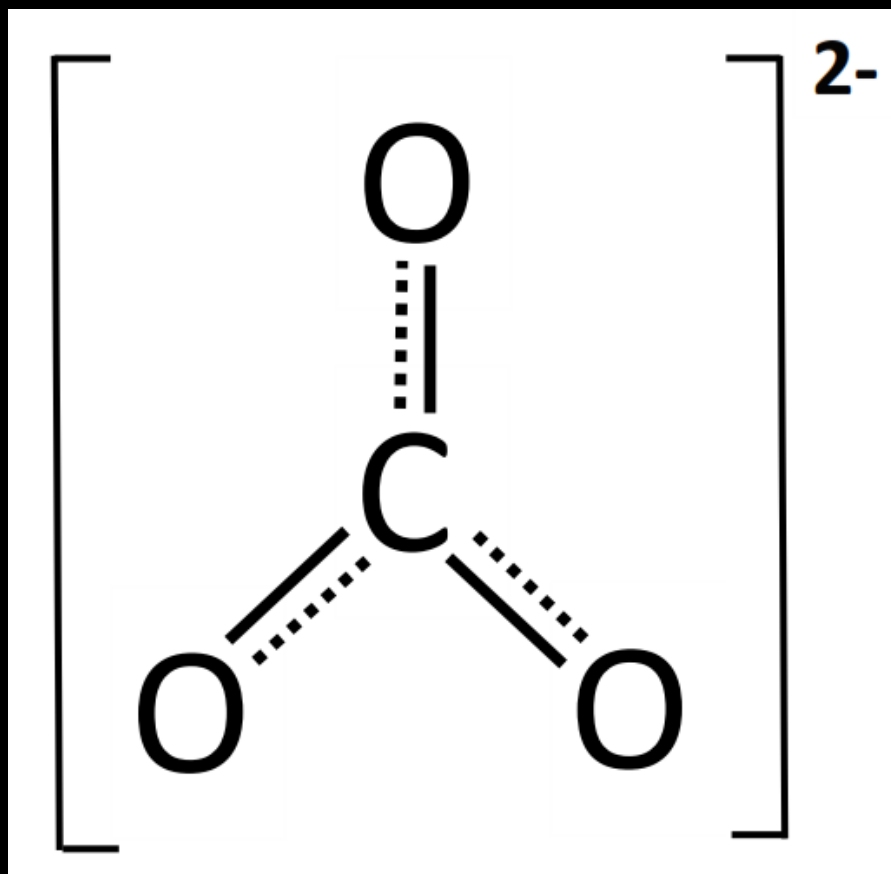
Resonance structures

Resonance structures occur when there is more than one position for a double bond in a molecule.



Resonance structures

The actual structure is a resonance hybrid structure.

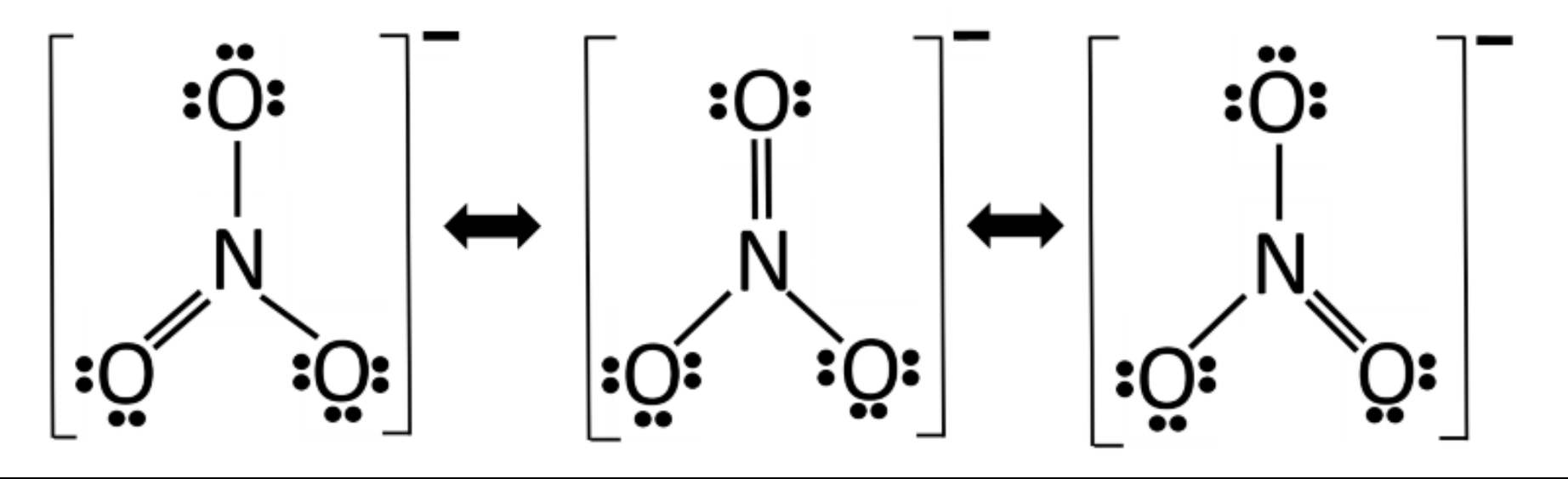


The bond lengths and bond strengths in the carbonate ion are identical.

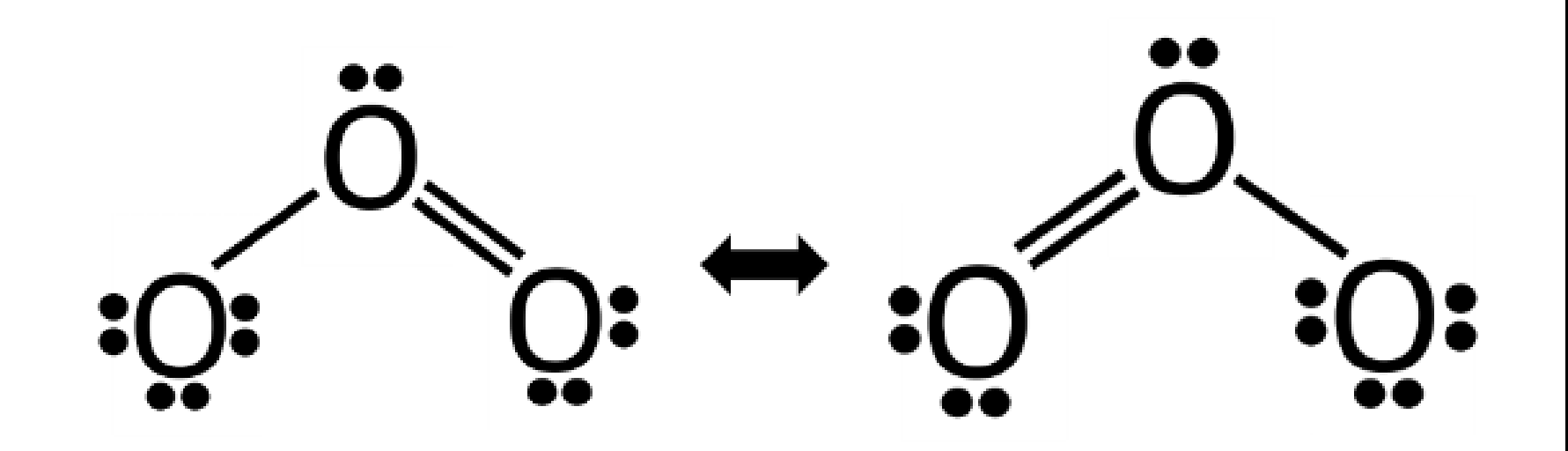
They are intermediate in length and strength between a single and a double bond.

Resonance structures

Nitrate ion NO_3^-

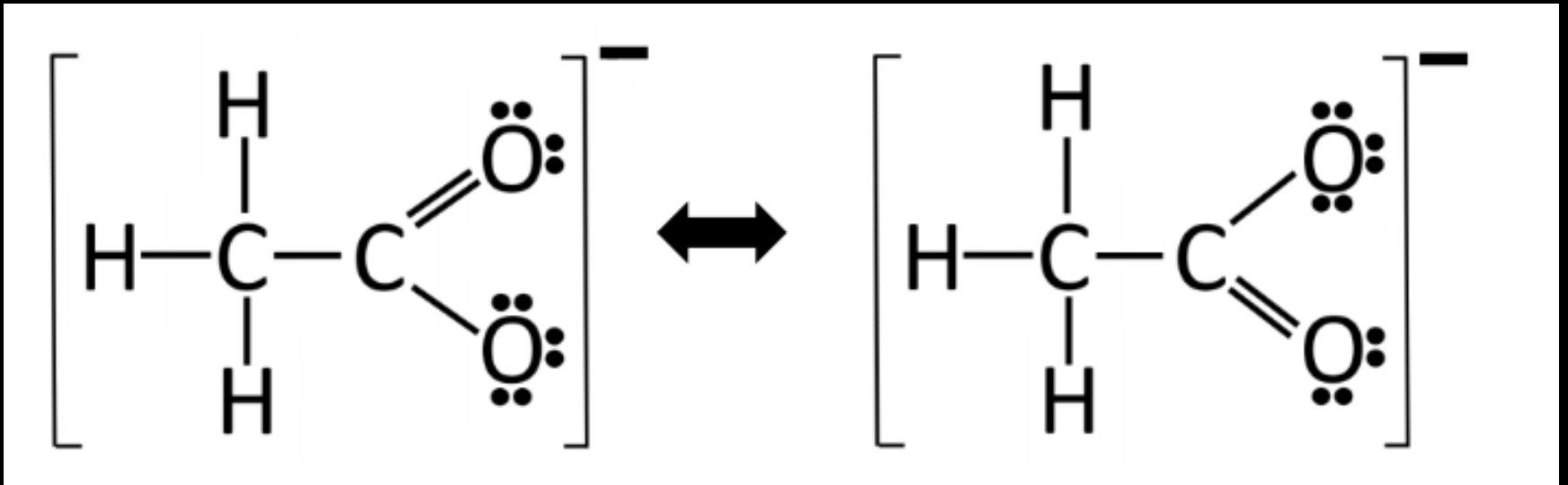


Ozone O_3

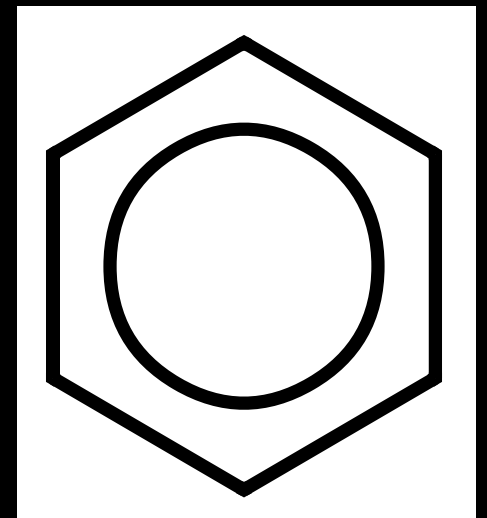
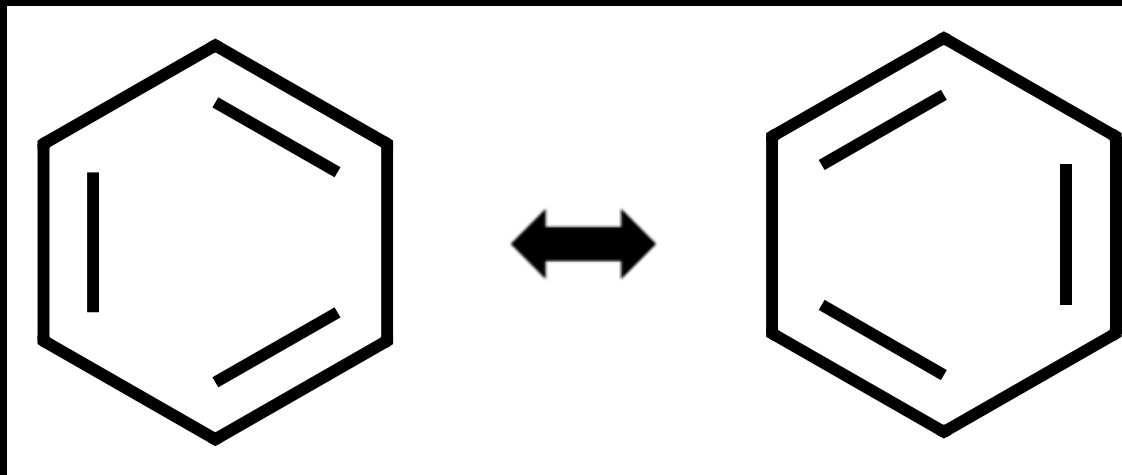


Resonance structures

Ethanoate
ion
 CH_3COO^-



Benzene
 C_6H_6



Resonance structures

Resonance structures occur when there is more than one position for a multiple bond in a molecule or ion – this means that it is possible to draw more than one Lewis structure.

The actual structure of the molecule (or ion) is a resonance hybrid structure in which the bonds are intermediate in length and strength between a single and a double bond.

Resonance structures have delocalised electrons which are shared over more than two nuclei.

MSJChem

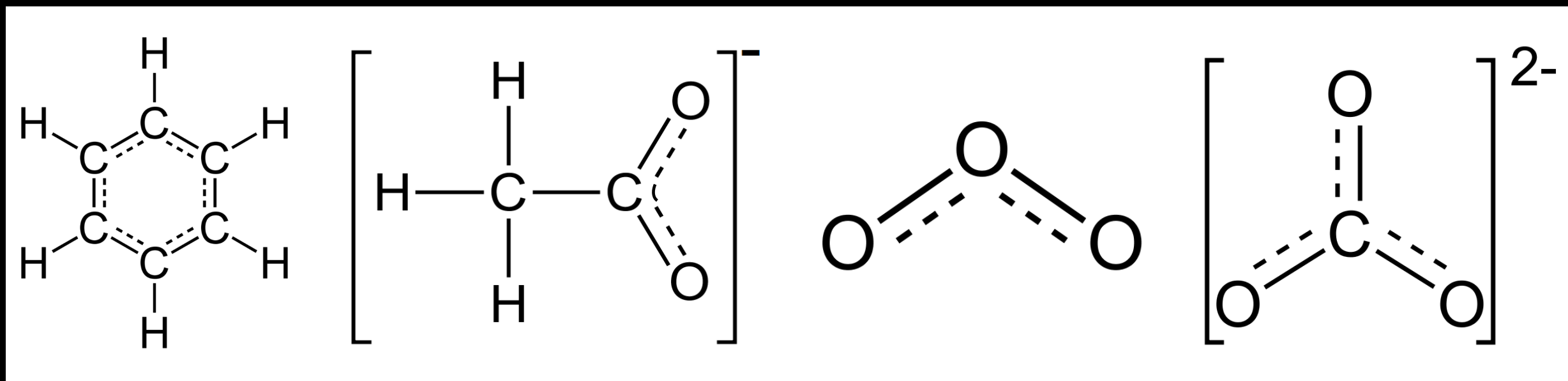
Tutorials for IB Chemistry

**Molecules with
delocalised π electrons**

Delocalised π electrons

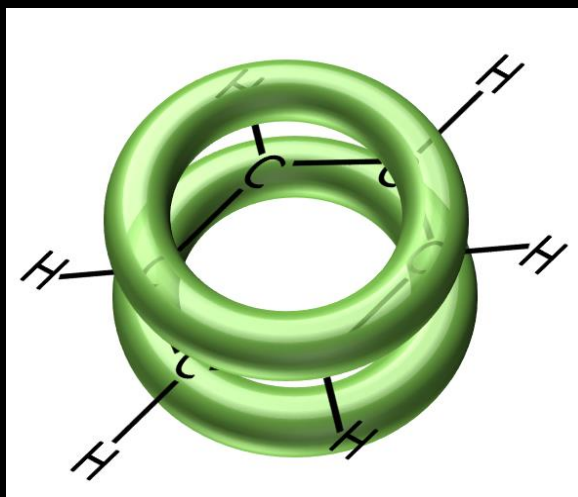
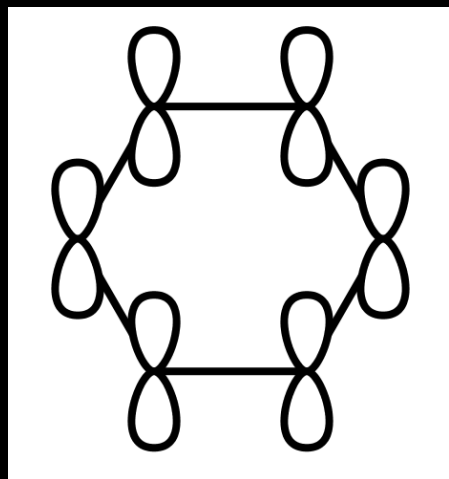
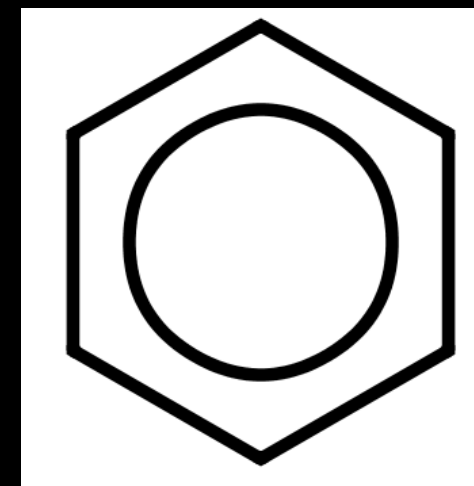
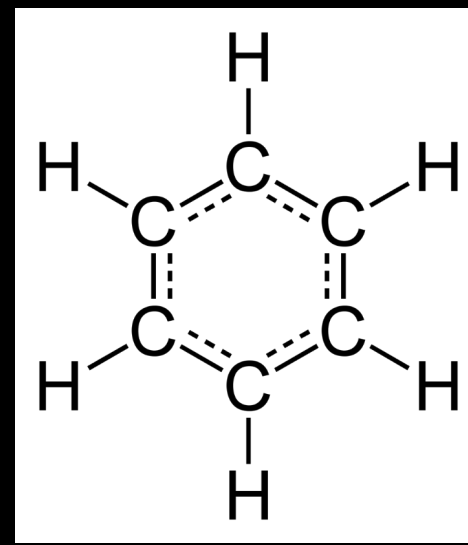
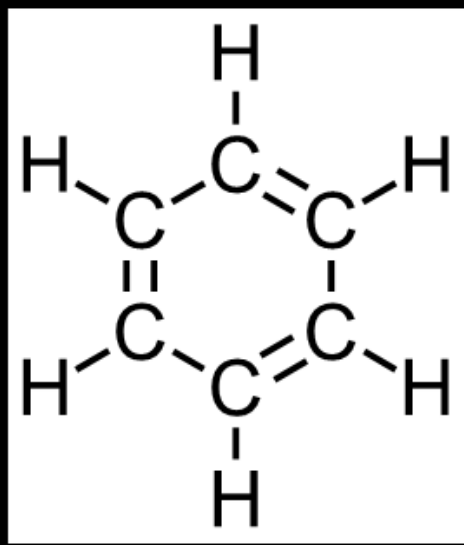
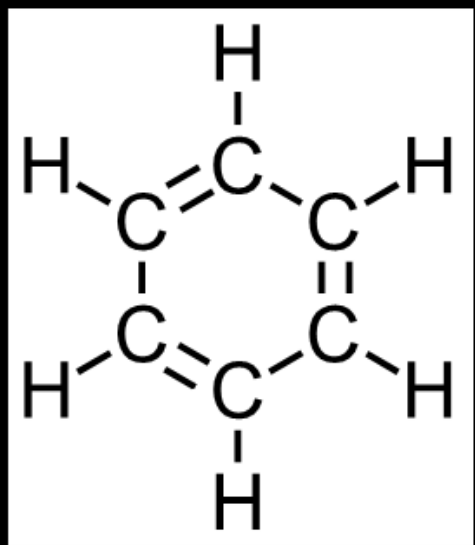
Delocalised π electrons are electrons that are shared between more than two nuclei.

They exist in all molecules or ions for which there is more than one Lewis structure (resonance structures).



Delocalised π electrons

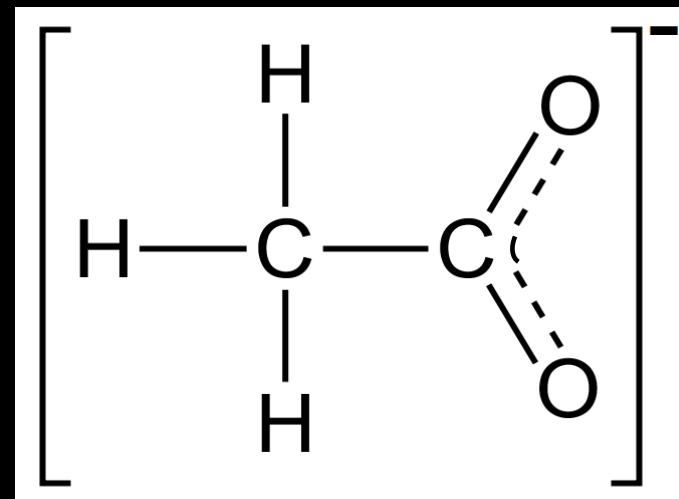
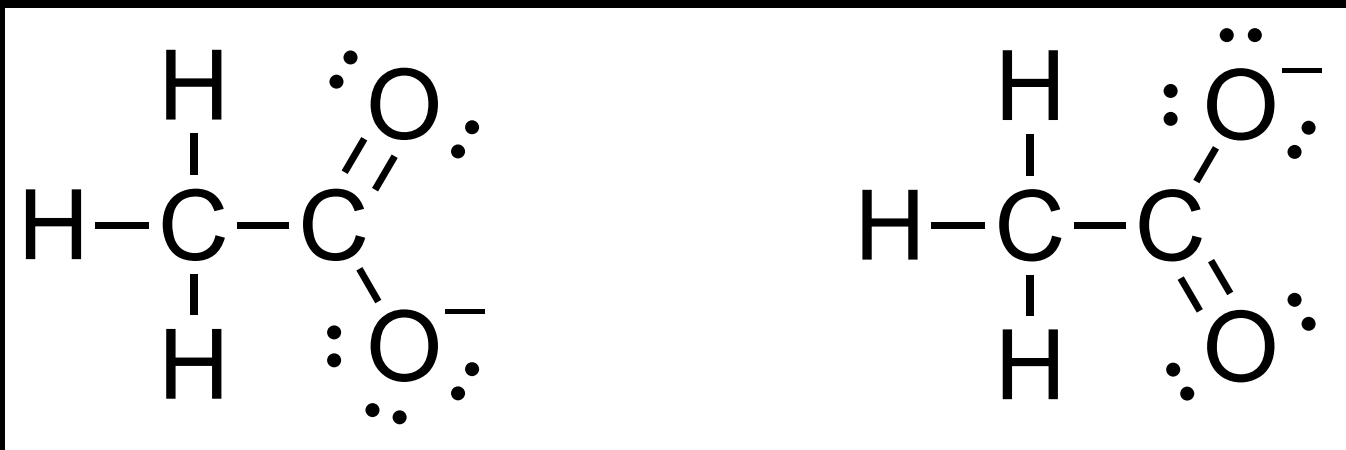
Benzene C_6H_6



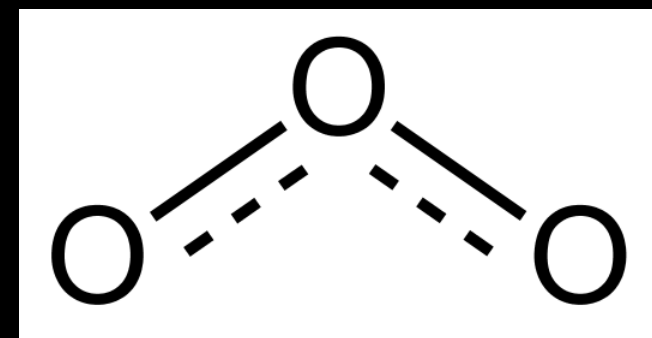
Benzene contains a total of 6 pi electrons - one from each unhybridised p orbital.

Delocalised π electrons

Ethanoate ion CH_3COO^-



Ozone, O_3

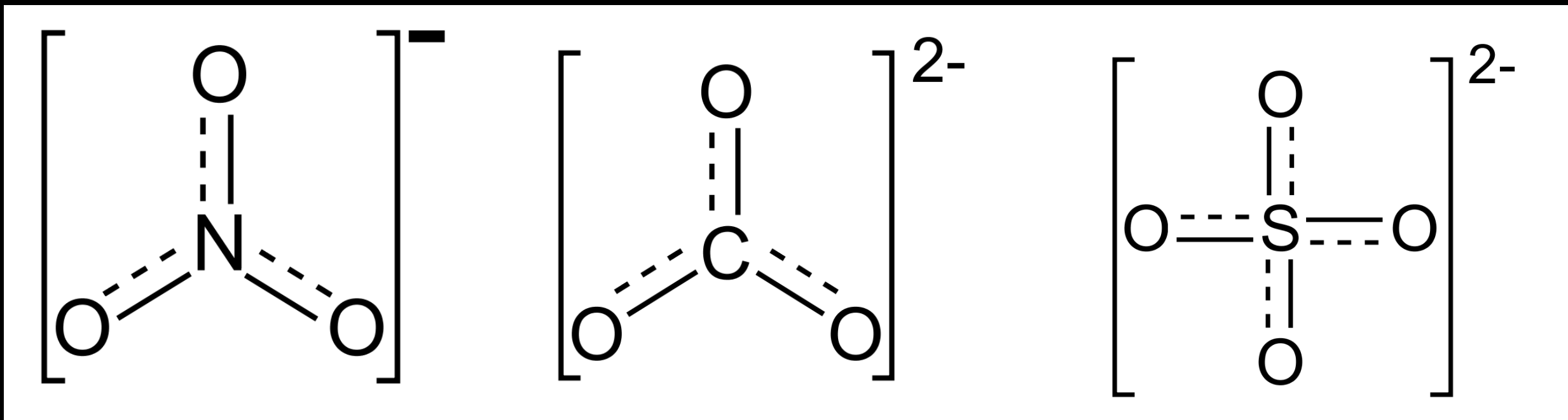


Delocalised π electrons

Nitrate ion NO_3^-

Carbonate ion CO_3^{2-}

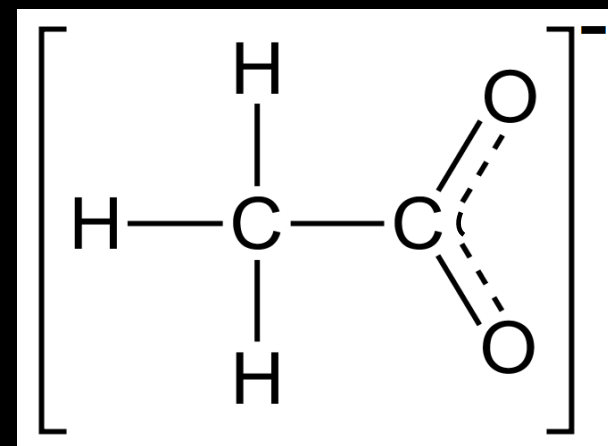
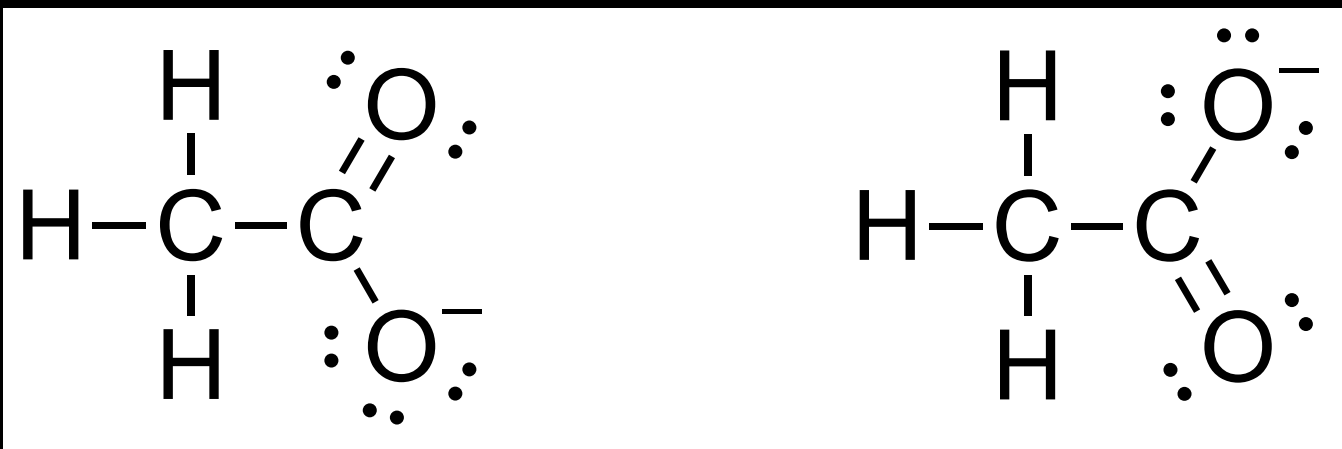
Sulfate ion SO_4^{2-}



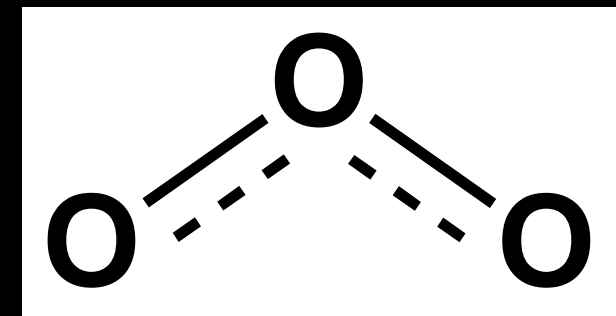
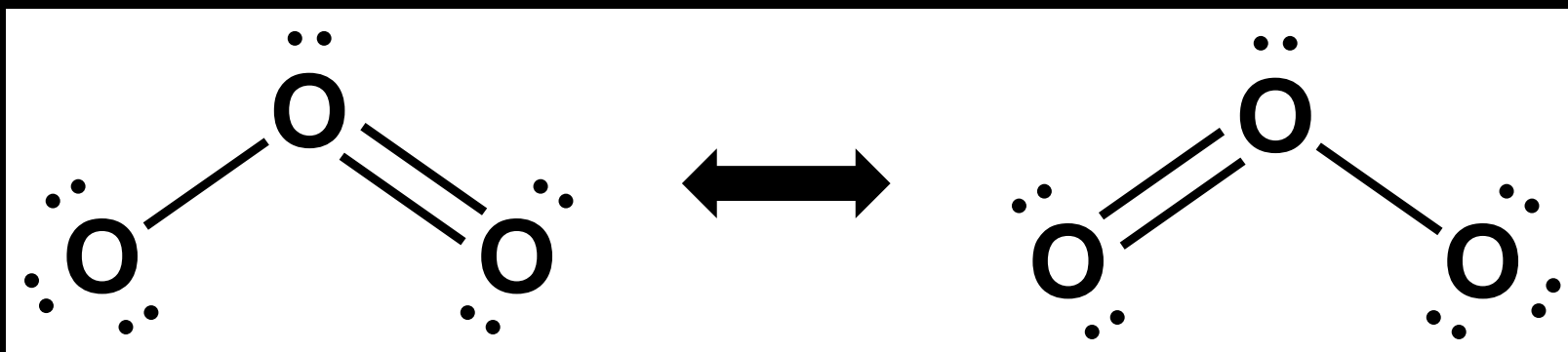
All molecules or ions that have more than one possible Lewis structure (resonance structures) contain delocalised pi electrons shared over more than two nuclei.

Delocalised π electrons

Ethanoate ion CH_3COO^-



Ozone, O_3



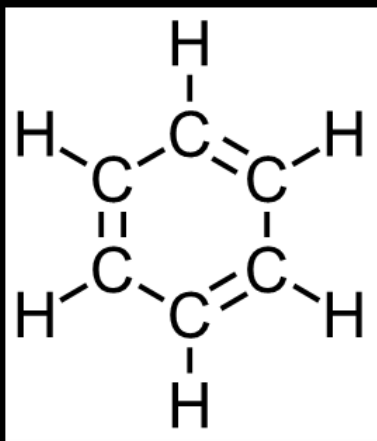
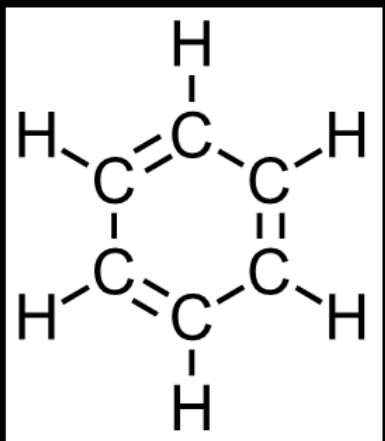
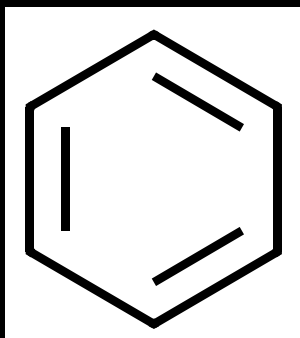
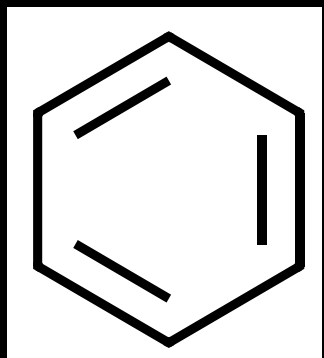
MSJChem

Tutorials for IB Chemistry

**Evidence for the
structure of benzene**

Structure of benzene

The Kekulé structure of benzene consists of alternating single and double carbon to carbon bonds.



All C to C bonds would be different lengths and strengths.

The enthalpy of hydrogenation of benzene would be -360 kJ mol^{-1}

Benzene would undergo addition reactions.

Two possible isomers produced in 1,2-disubstituted benzene compounds.

Structure of benzene

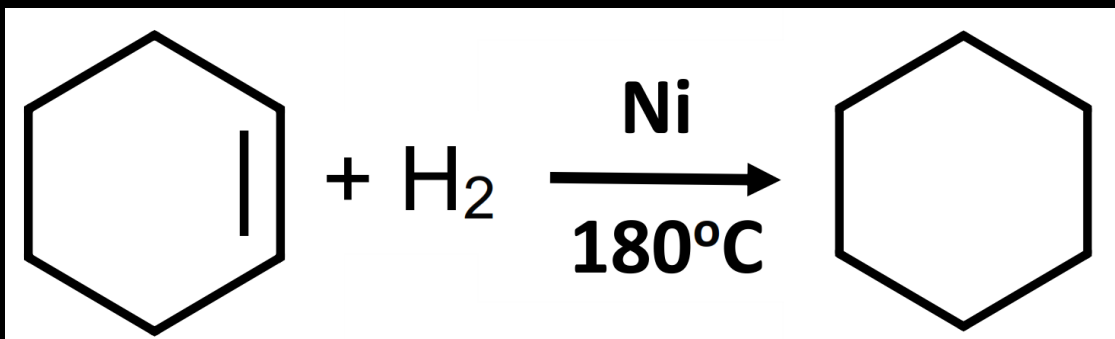
The C to C bonds in benzene are of equal length and equal strength.

Bond	Bond length ($\times 10^{-12}$ m)	Bond strength (kJ mol^{-1})
C-C	154	346
C=C	140	507
C \equiv C	134	614

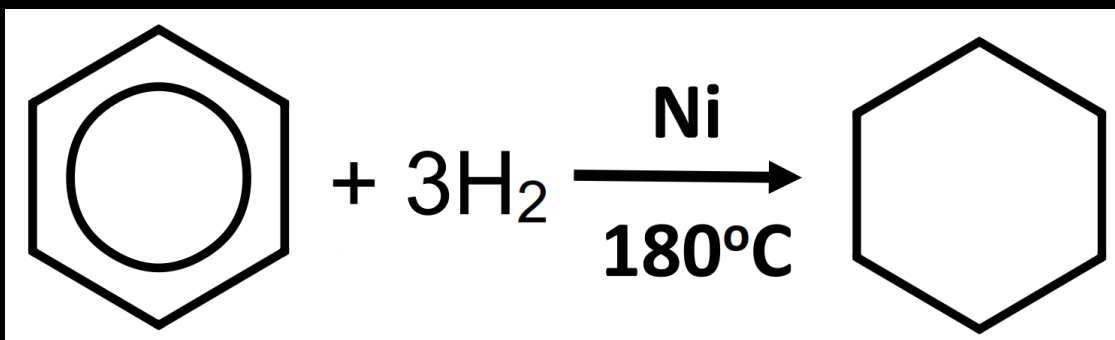
The length and strength of the C to C bonds in benzene are equal - intermediate between a single and a double bond.

Structure of benzene

The enthalpy of hydrogenation of benzene is less than predicted.



$$\Delta H = -120 \text{ kJ mol}^{-1}$$



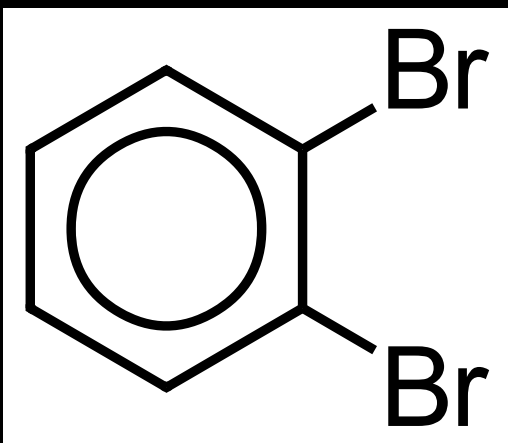
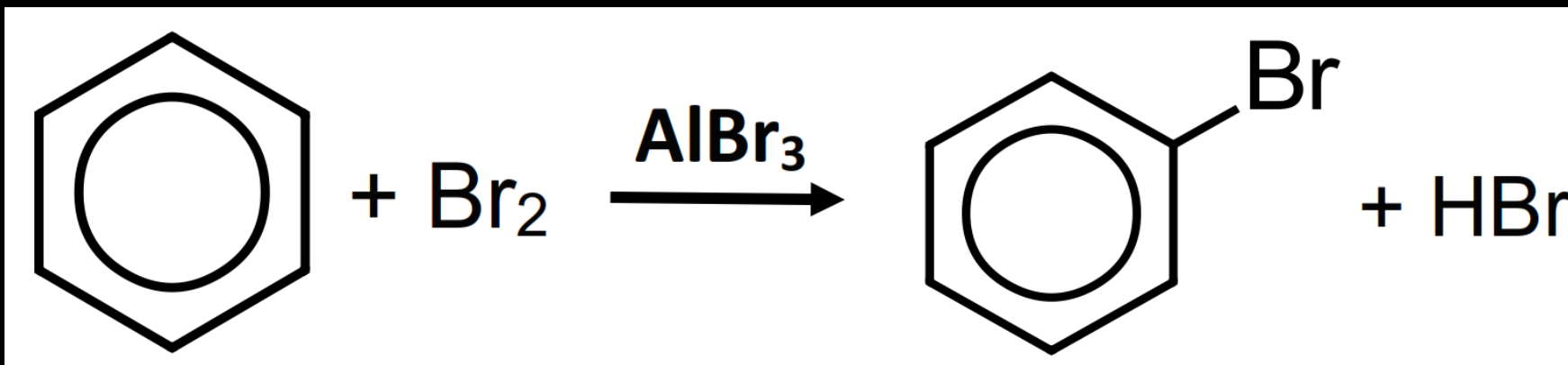
$$\Delta H = -360 \text{ kJ mol}^{-1}$$

$$\Delta H = -210 \text{ kJ mol}^{-1}$$

The difference in energy (-150 kJ mol^{-1}) is known as the resonance energy.

Structure of benzene

Benzene undergoes substitution reactions, rather than addition reactions.



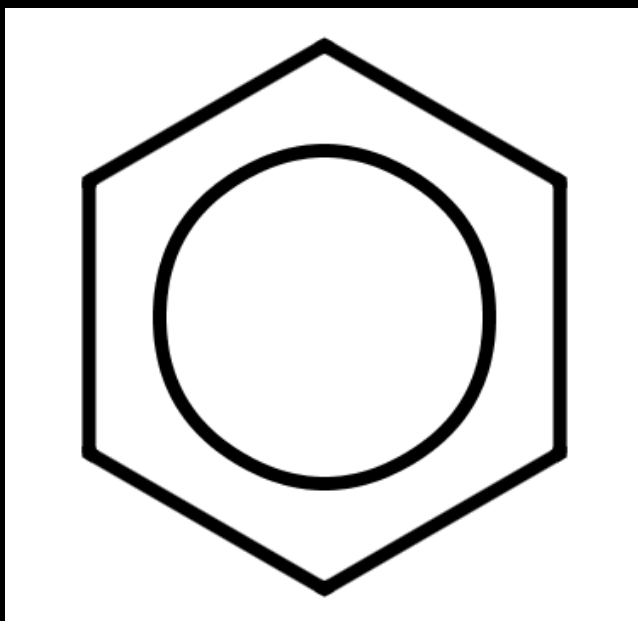
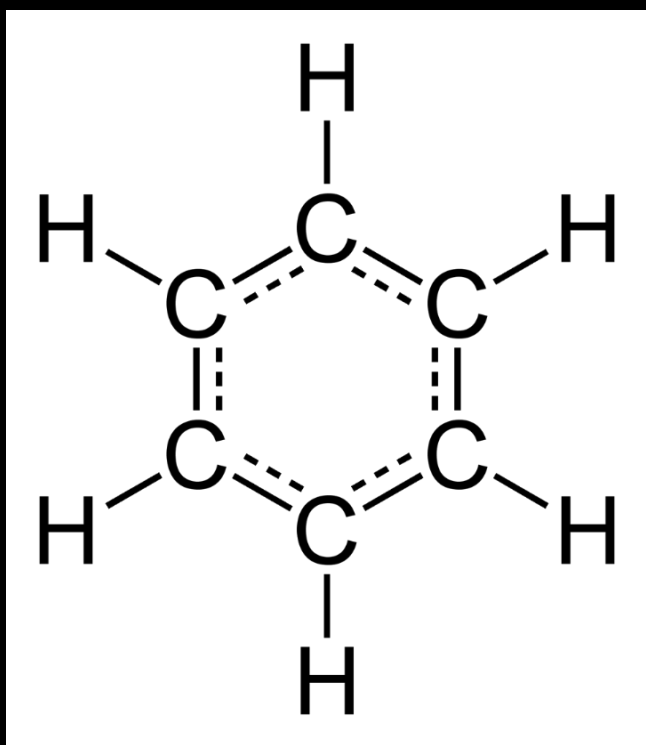
Only one isomer exists for 1,2-disubstituted compounds such as 1,2-dibromobenzene.

Structure of benzene

Kekule structure	Actual structure
Alternating single and double C-C bonds	All C-C bonds are of equal length and equal strength
Enthalpy of hydrogenation is -360 kJ mol^{-1}	Enthalpy of hydrogenation is -210 kJ mol^{-1}
Benzene undergoes addition reactions	Benzene undergoes substitution reactions
Two isomers produced in the reactions with the halogens	Only one isomers exists

Structure of benzene

The actual structure of benzene is a planar regular hexagon (bond angles of 120°).



The ring represents the delocalised electrons within the benzene molecule.

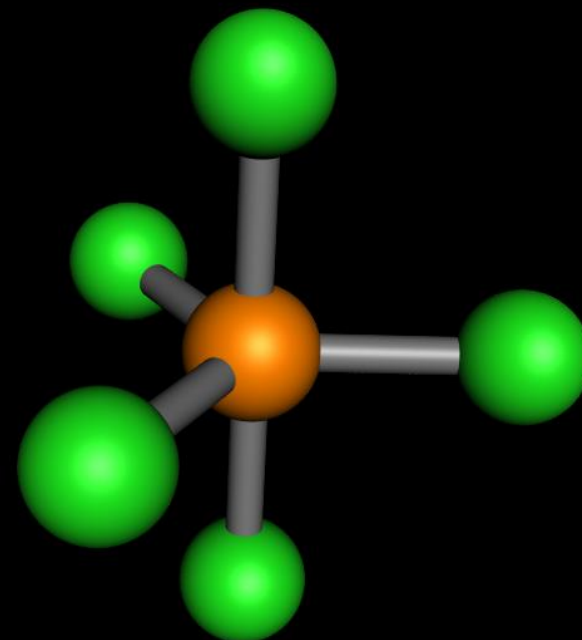
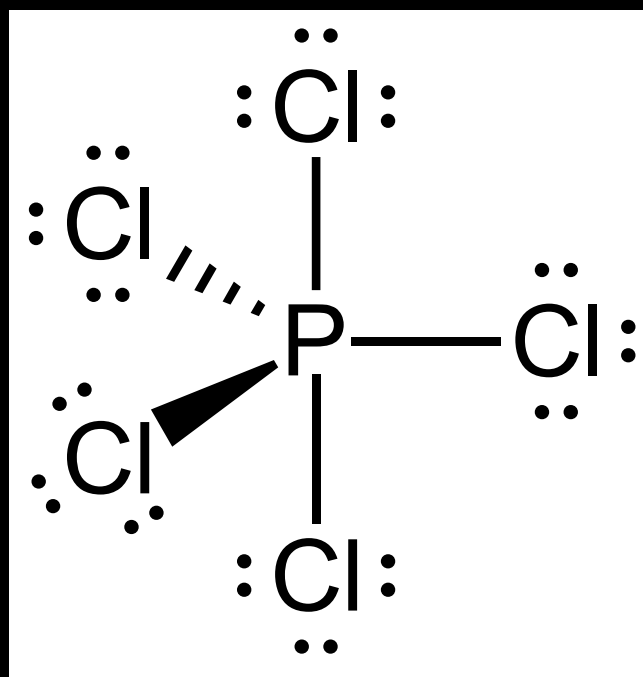
MSJChem

Tutorials for IB Chemistry

Molecular geometry

VSEPR HL

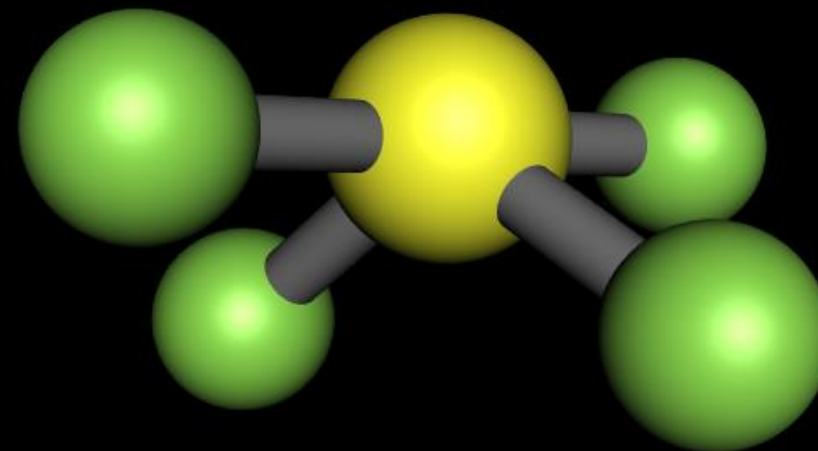
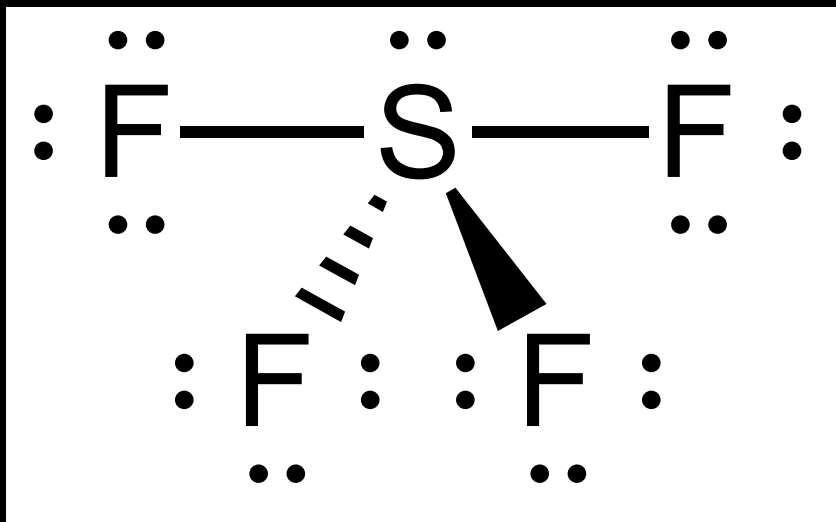
PCl₅
phosphorus
pentachloride



electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
5	5	0	trigonal bipyramidal	trigonal bipyramidal	90° 120°

VSEPR HL

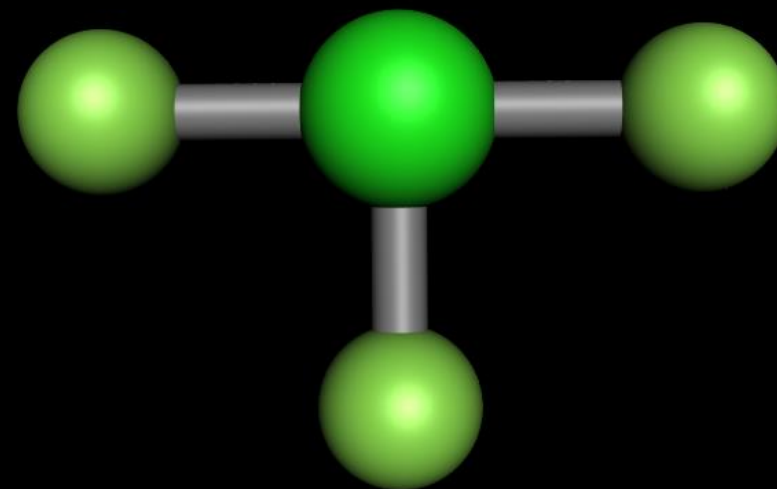
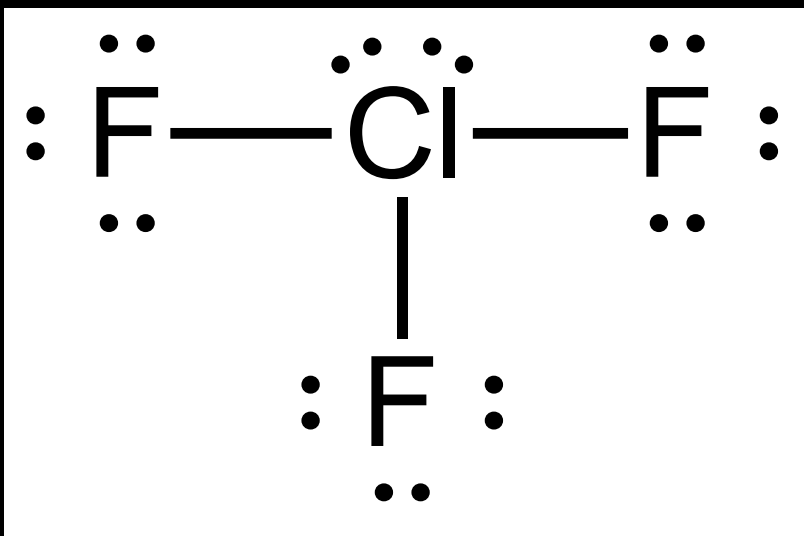
SF₄
sulfur
tetrafluoride



electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
5	4	1	trigonal bipyramidal	see-saw	<90° <120°

VSEPR HL

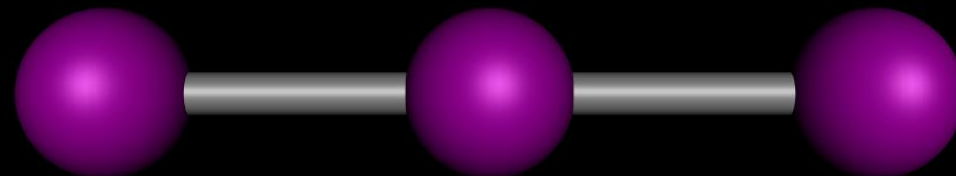
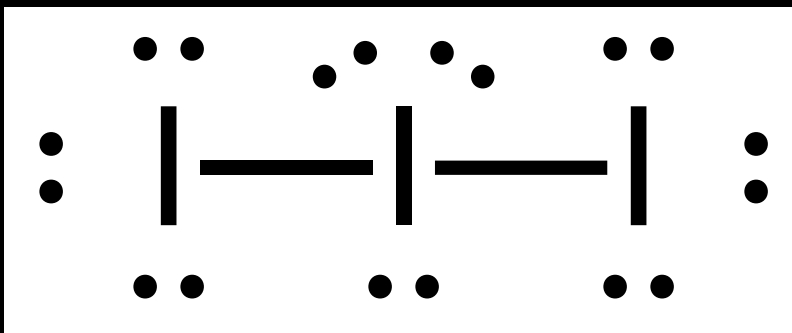
ClF₃
chlorine
trifluoride



electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
5	3	2	trigonal bipyramidal	T-shaped	<90°

VSEPR HL

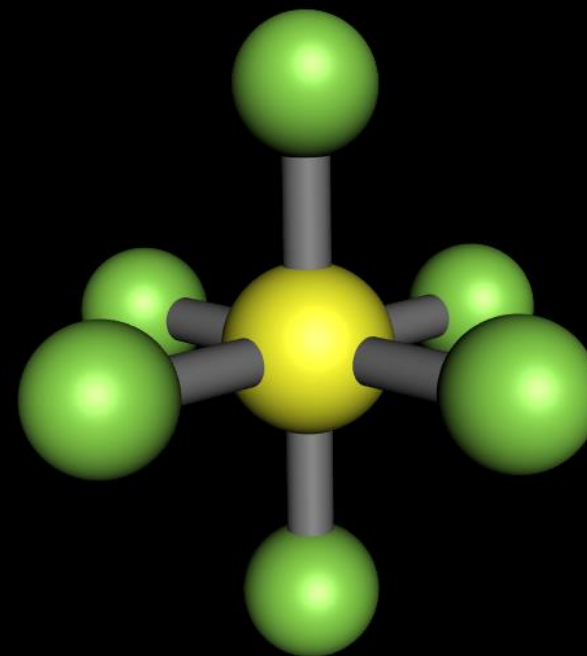
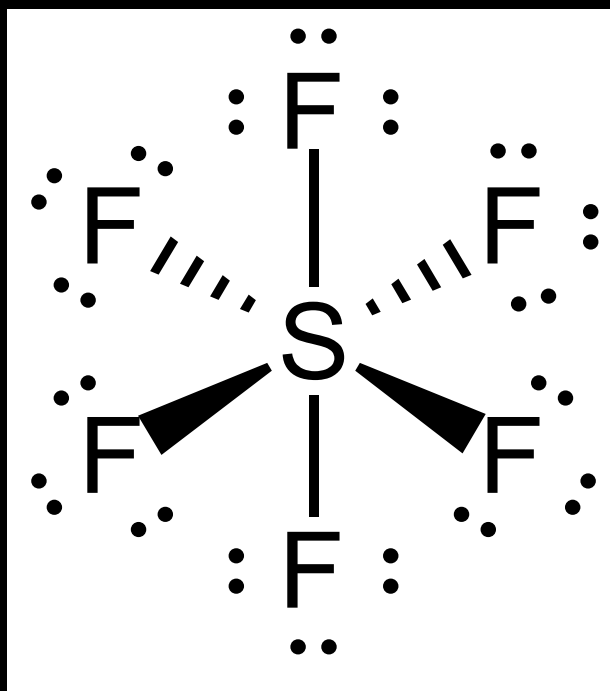
I_3^-
triiodide ion



electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
5	2	3	trigonal bipyramidal	linear	180°

VSEPR HL

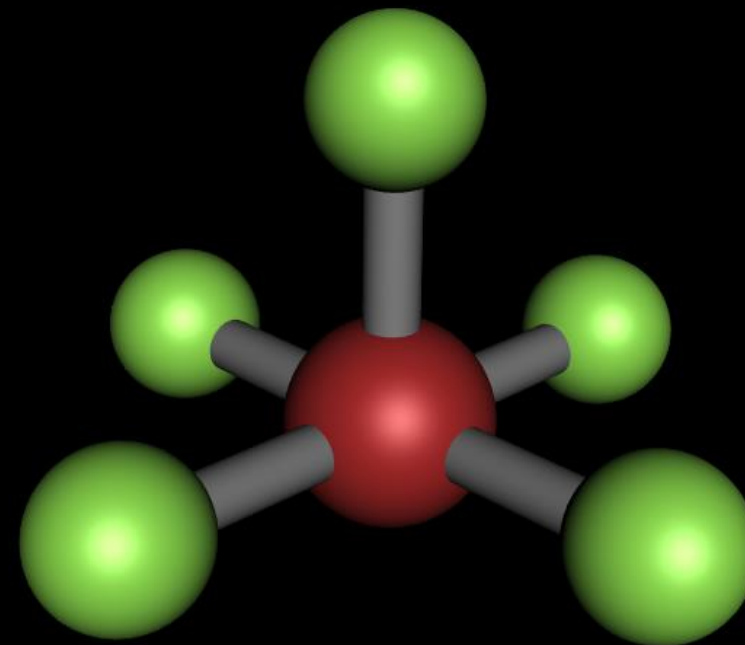
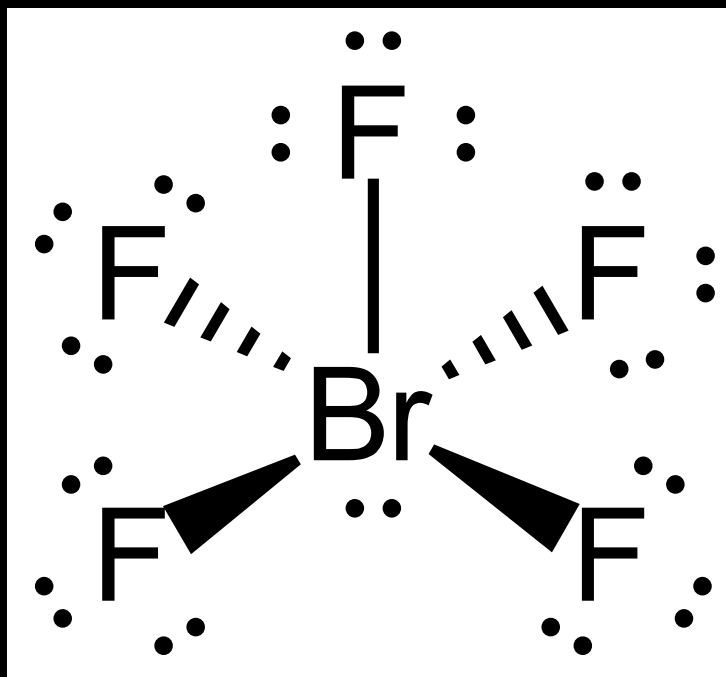
SF₆
sulfur
hexafluoride



electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
6	6	0	octahedral	octahedral	90°

VSEPR HL

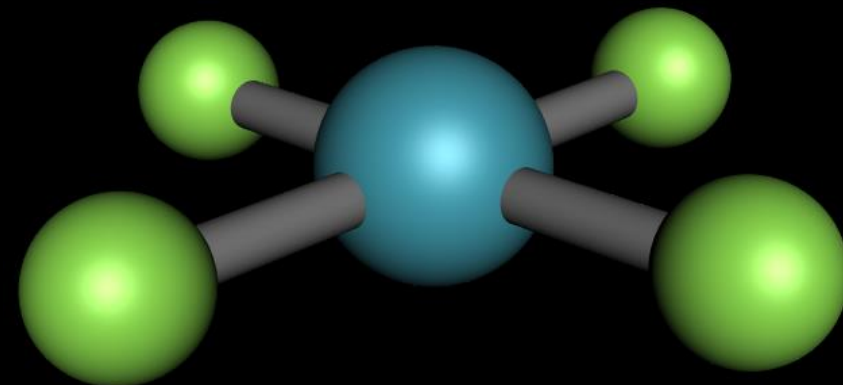
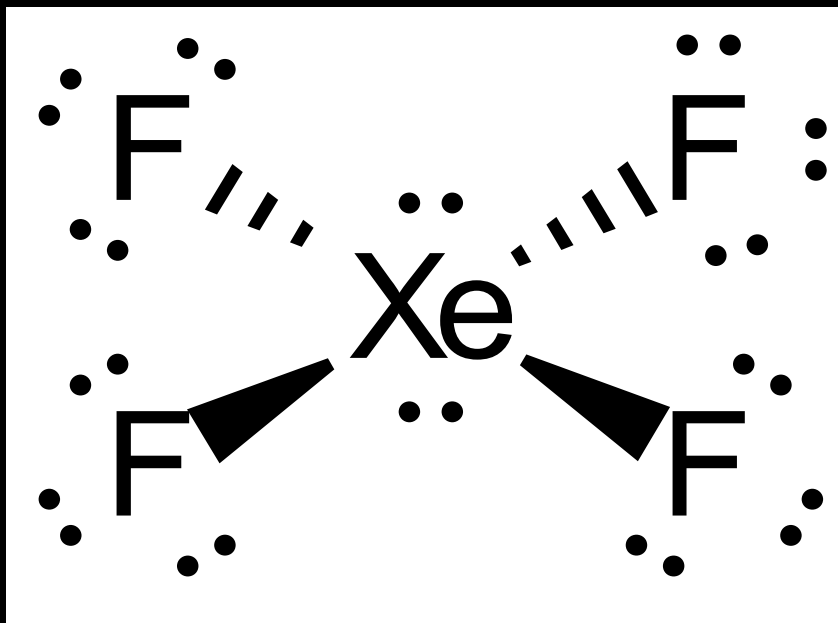
BrF₅
bromine
pentafluoride



electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
6	5	1	octahedral	square pyramidal	<90°

VSEPR HL

XeF₄
xenon
tetrafluoride



electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
6	4	2	octahedral	square planar	90°

MSJChem

Tutorials for IB Chemistry

Formal charge

Formal charge

Formal charge is used to determine which Lewis structure is preferred when more than one is possible.

The formal charge is the charge an atom would have if all the atoms in a molecule had the same electronegativity.

The preferred Lewis structure is the one where the individual atoms have a formal charge that is closest to zero.

Formal charge

The formal charge of an atom in a compound is calculated using the following equation:

Number of
valence
electrons

—

Number of
non-bonding
electrons

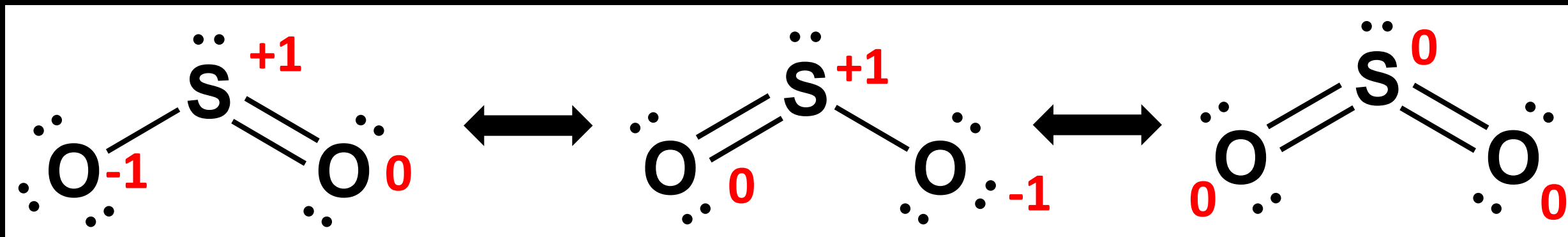
—

number of
 $\frac{1}{2}$ bonding
electrons

$$FC = V - N - \frac{1}{2} B$$

Formal charge

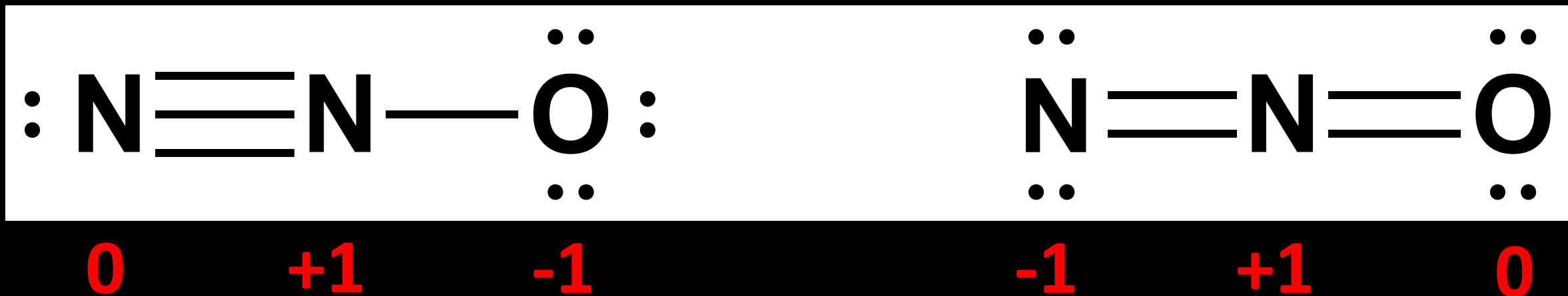
Three possible Lewis structures for SO_2 are shown below.



The preferred Lewis structure is the one where the individual atoms have a formal charge closest to zero, therefore the structure on the right is the preferred one.

Formal charge

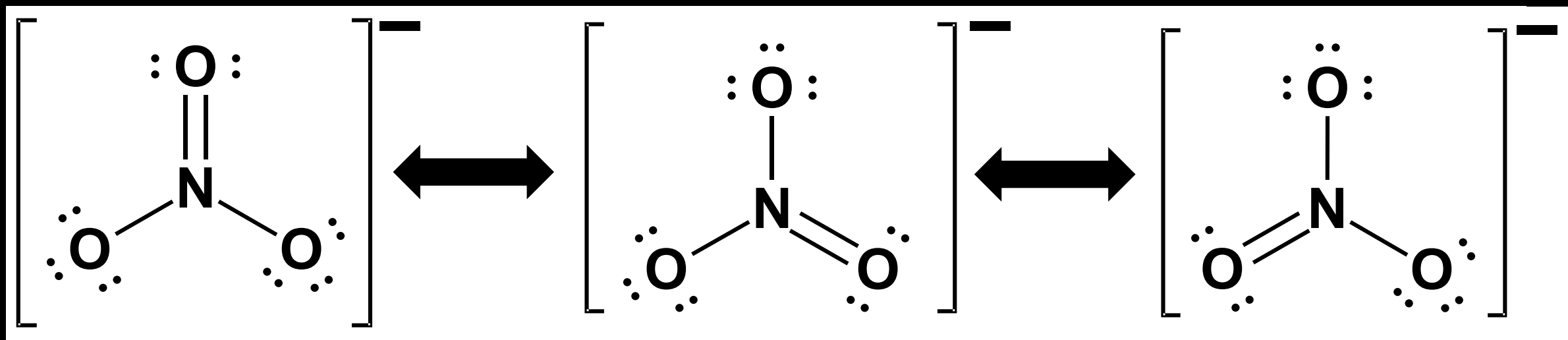
Two possible Lewis structures for N_2O are shown below.



The structure on the left has the negative formal charge on the more electronegative atom (oxygen), therefore it is the preferred Lewis structure.

Formal charge

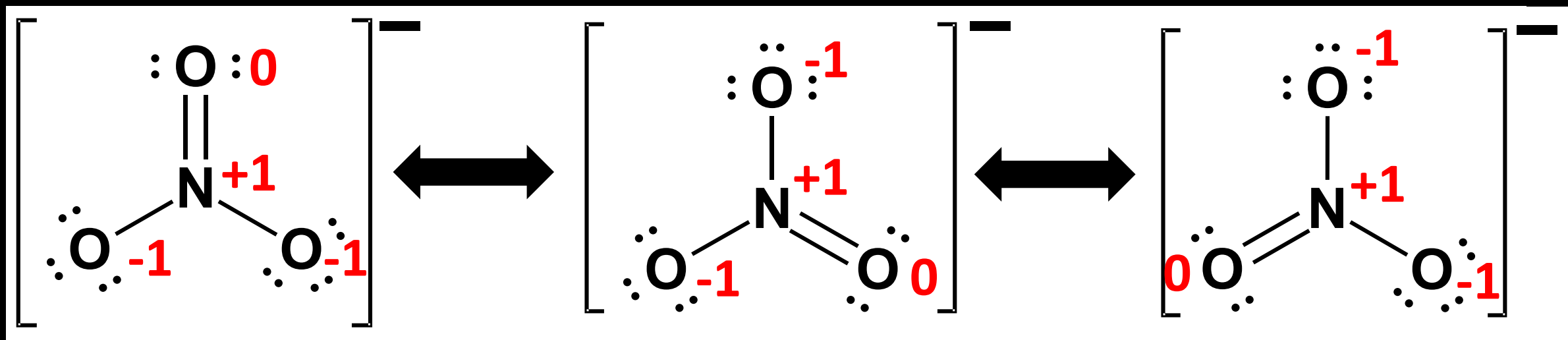
Three possible Lewis structures for the nitrate ion (NO_3^-) are shown below.



For ions, the sum of the formal charges must be equal to the overall charge on the ion.

Formal charge

Three possible Lewis structures for the nitrate ion (NO_3^-) are shown below.



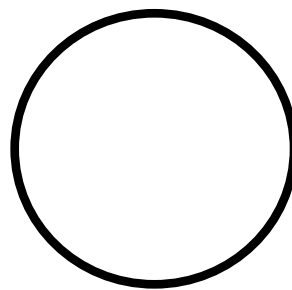
For ions, the sum of the formal charges must be equal to the overall charge on the ion.

25 Mn Manganese 54.938045	16 S Sulfur 32.065	J	6 C Carbon 12.0107	2 He Helium 4.002602	25 Mn Manganese 54.938045
---	------------------------------------	----------	------------------------------------	--------------------------------------	---

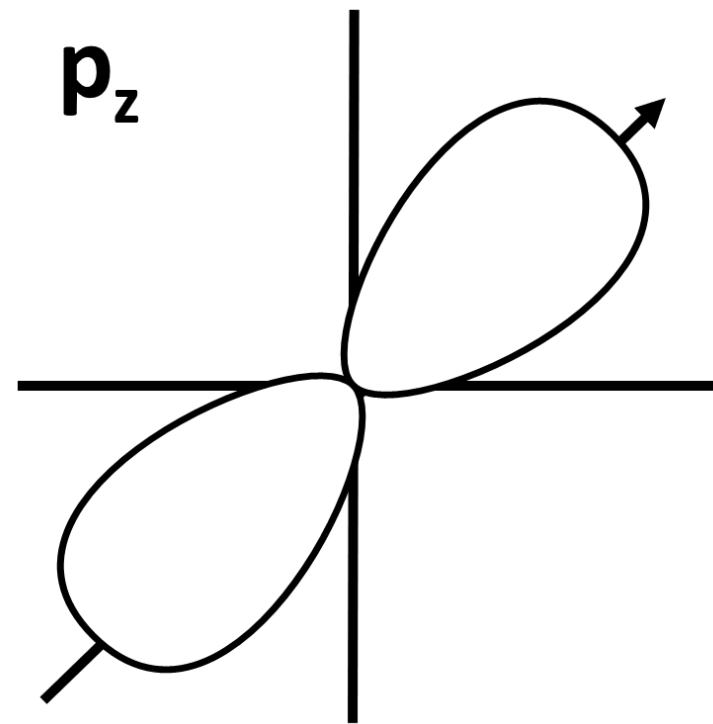
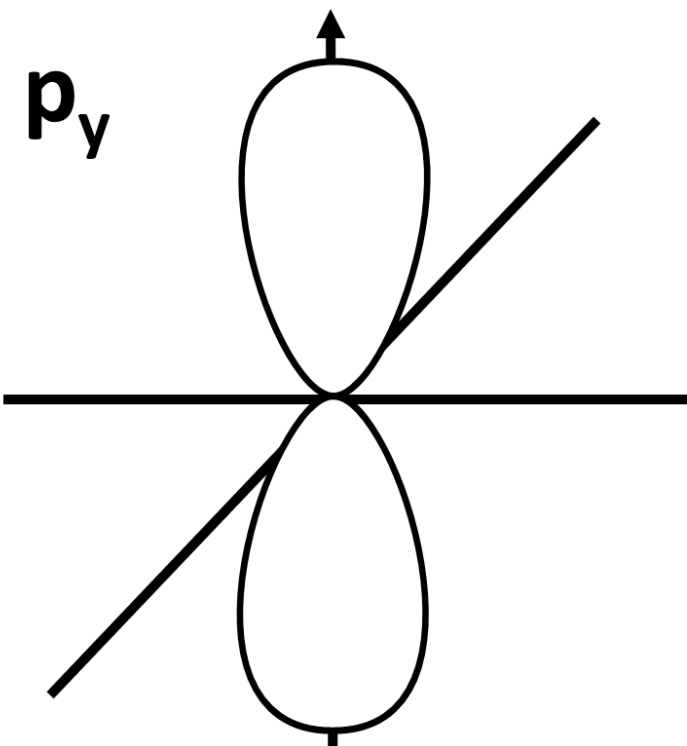
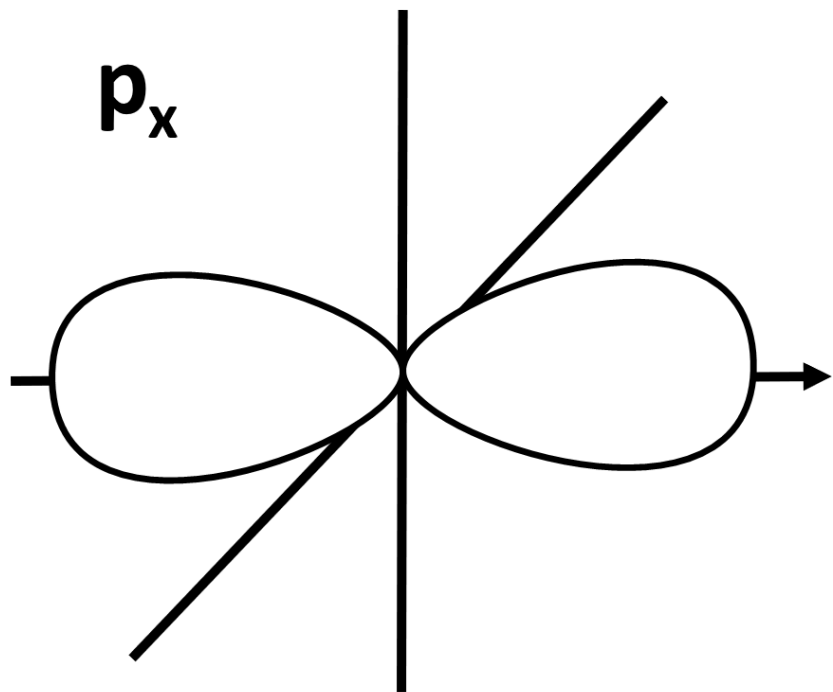
**sigma (σ) and
pi (π) bonds**

sigma (σ) and pi (π) bonds

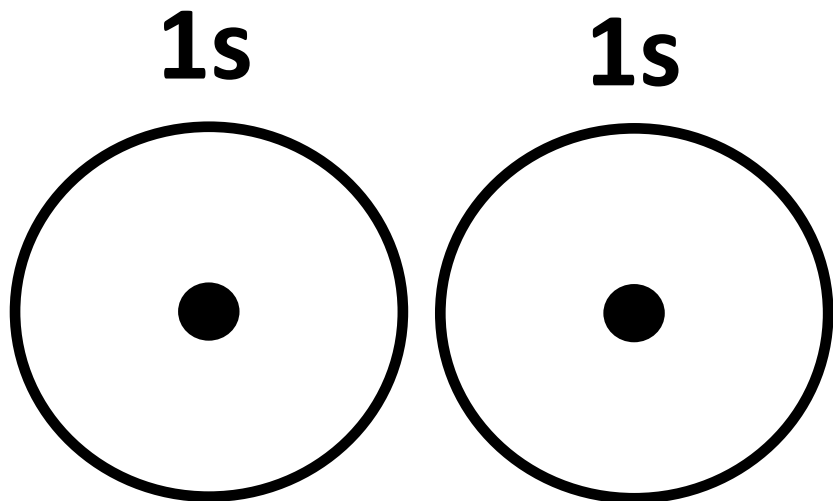
s orbitals are spherical.



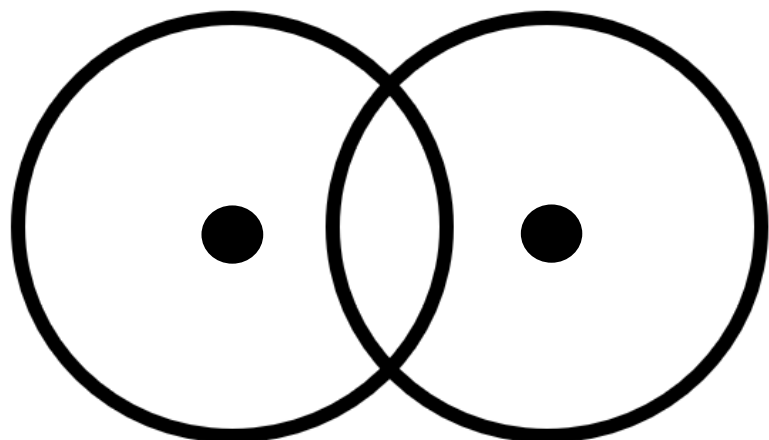
p orbitals are dumbbell shaped.



sigma (σ) and pi (π) bonds



σ bond

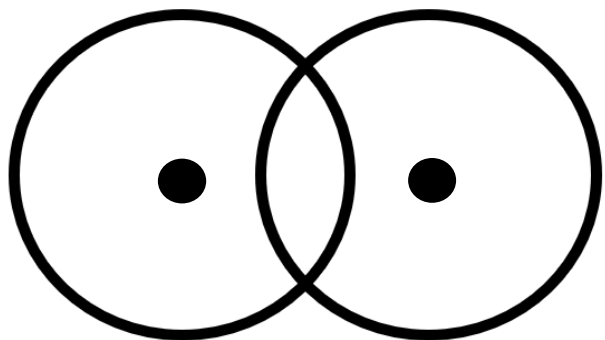


A sigma bond is formed by the head-on overlap of atomic orbitals.

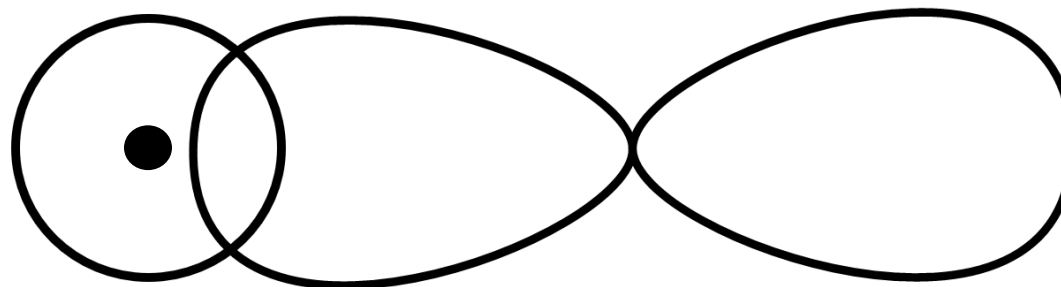
The electron density is concentrated between the nuclei of the bonding atoms.

sigma (σ) and pi (π) bonds

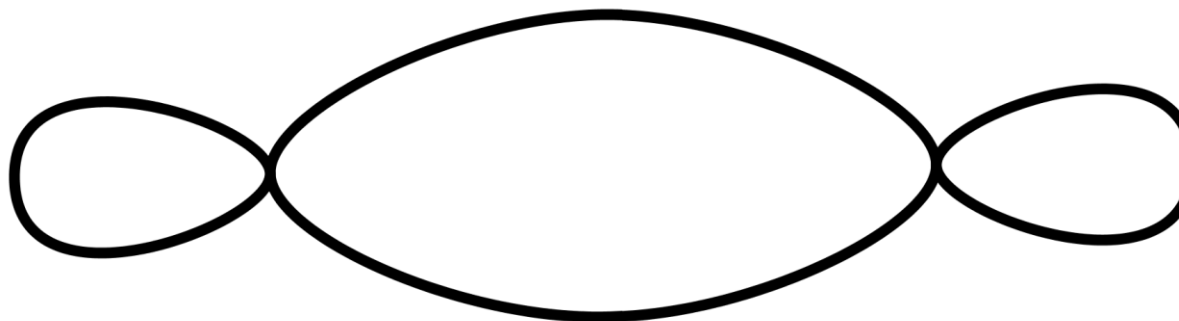
**Two s orbitals
overlap head-on
(s-s)**



**s orbital overlaps head-on
with p orbital (s-p)**

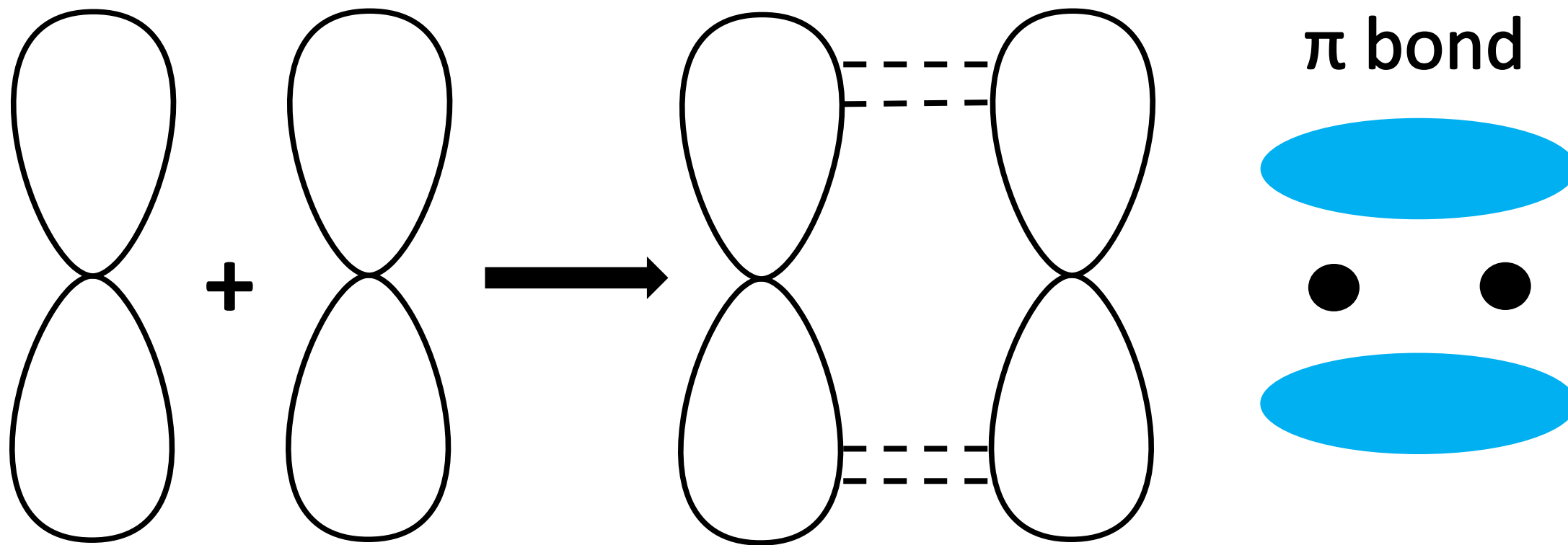


Two p orbitals overlap head-on (p-p)



sigma (σ) and pi (π) bonds

A pi bond is formed by sideways overlap of atomic orbitals. This results in electron density above and below the plane of the nuclei of the bonding atoms.

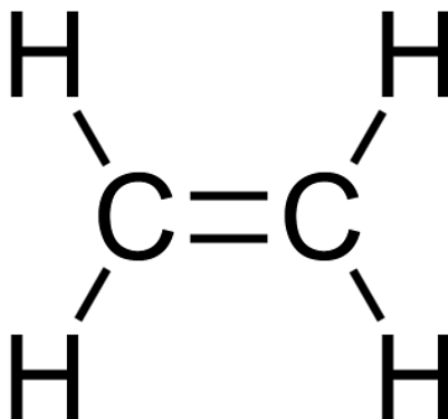
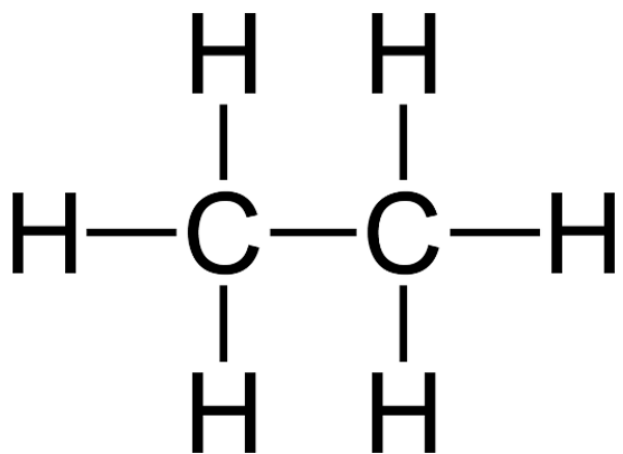


sigma (σ) and pi (π) bonds

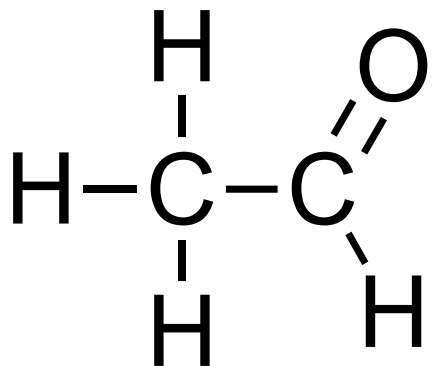
Type of overlap	Type of bond formed
s-s head-on (axial)	sigma (σ)
s-p head-on (axial)	sigma (σ)
p-p head-on (axial)	sigma (σ)
p-p sideways (lateral)	pi (π)

sigma (σ) and pi (π) bonds

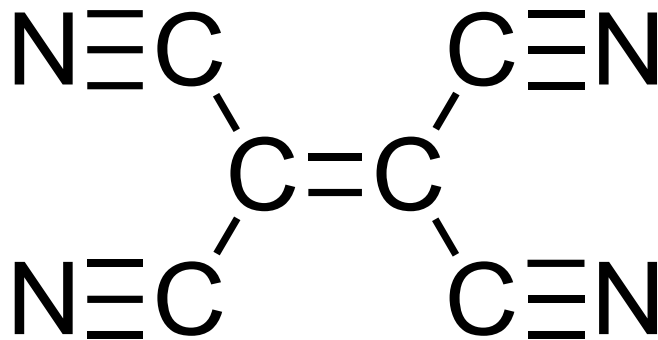
Type of bond	sigma (σ)	pi (π)
Single covalent	1	0
Double covalent	1	1
Triple covalent	1	2



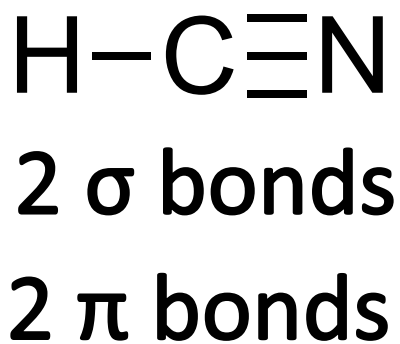
sigma (σ) and pi (π) bonds



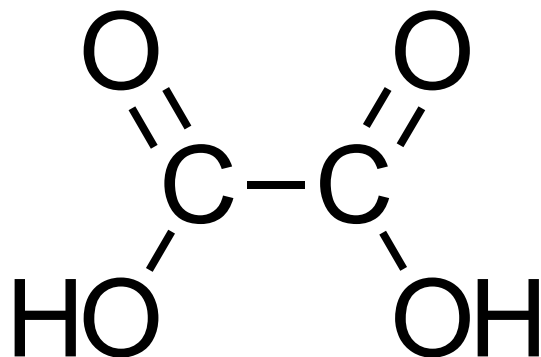
6 σ bonds
1 π bond



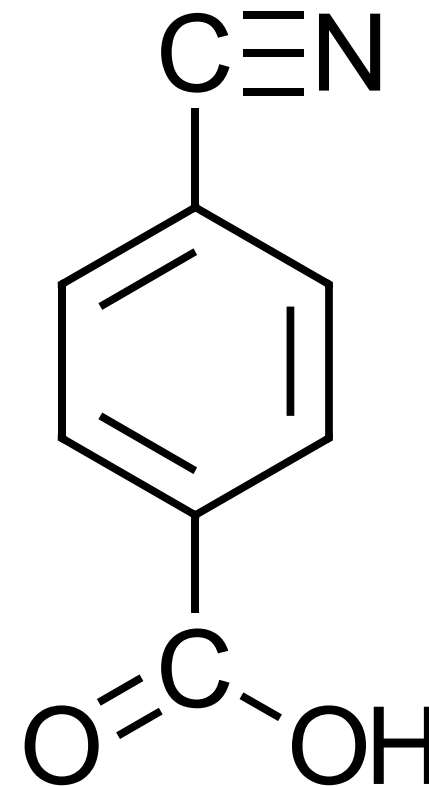
9 σ bonds
9 π bonds



2 σ bonds
2 π bonds



7 σ bonds
2 π bonds



16 σ bonds
6 π bonds

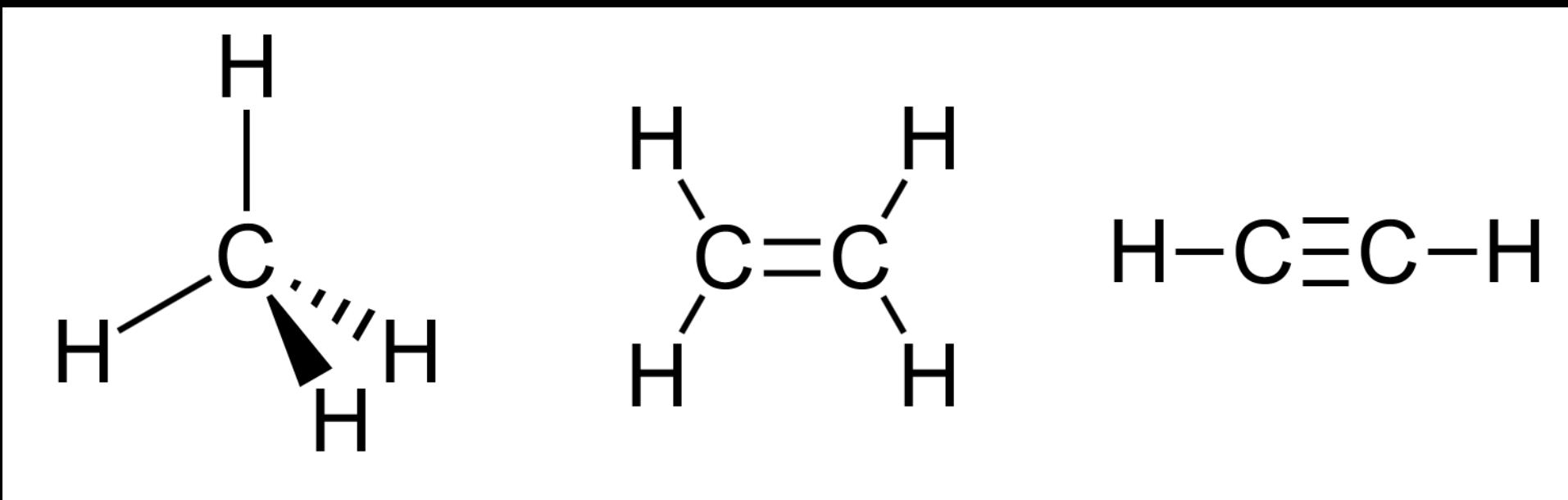
MSJChem

Tutorials for IB Chemistry

Hybridisation

Hybridisation

Hybridisation is the mixing of atomic orbitals to produce hybrid orbitals used for bonding.



Methane

sp³ hybridisation

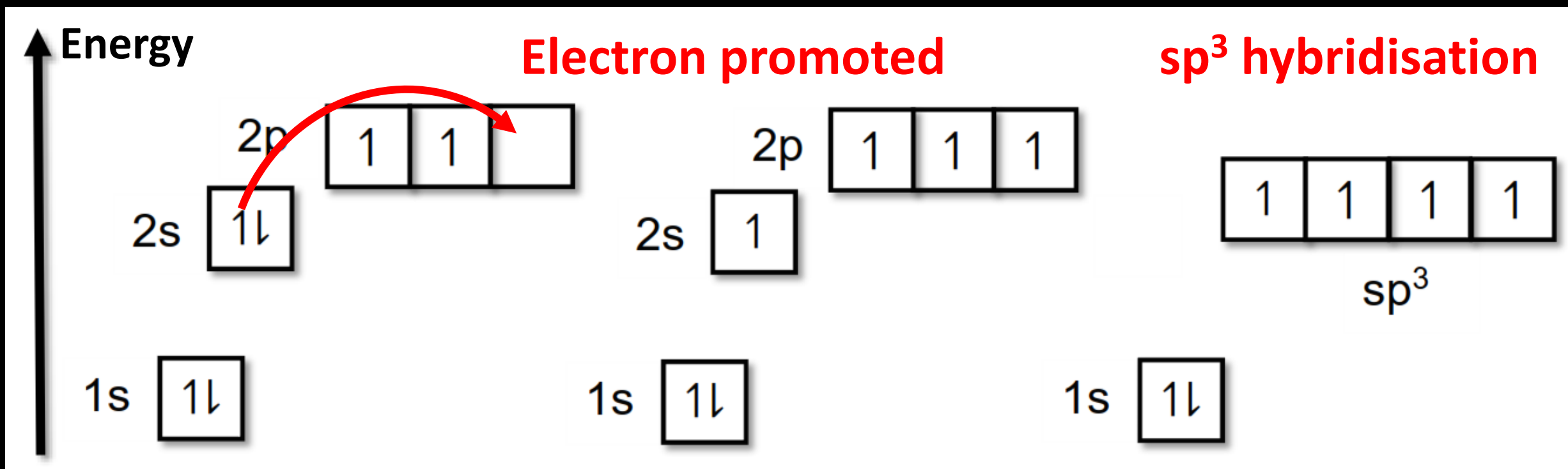
Ethene

sp² hybridisation

Ethyne

sp hybridisation

sp^3 hybridisation

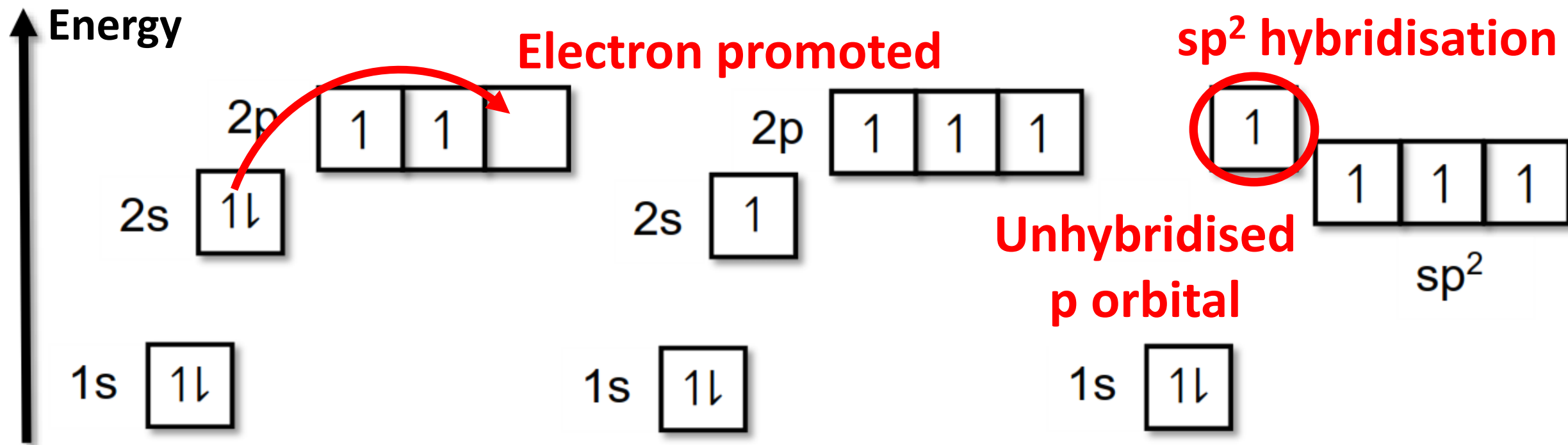


Carbon atom in
its ground state

Carbon atom in
its excited state

Four sp^3 hybrid
orbitals

sp^2 hybridisation

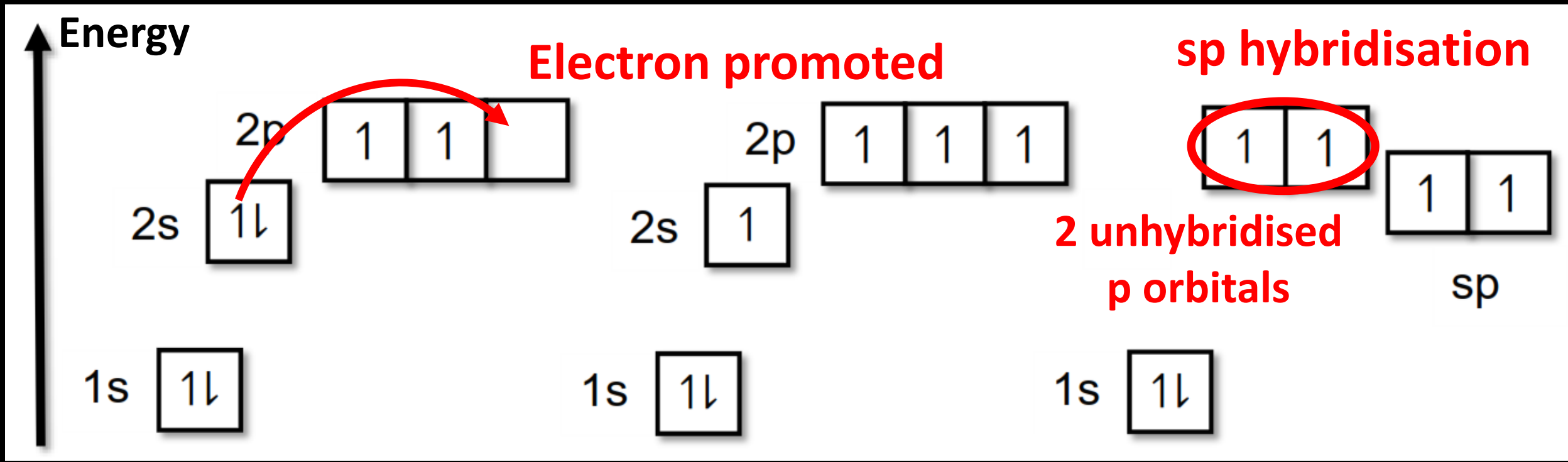


Carbon atom in its ground state

Carbon atom in its excited state

Three sp^2 hybrid orbitals

sp hybridisation



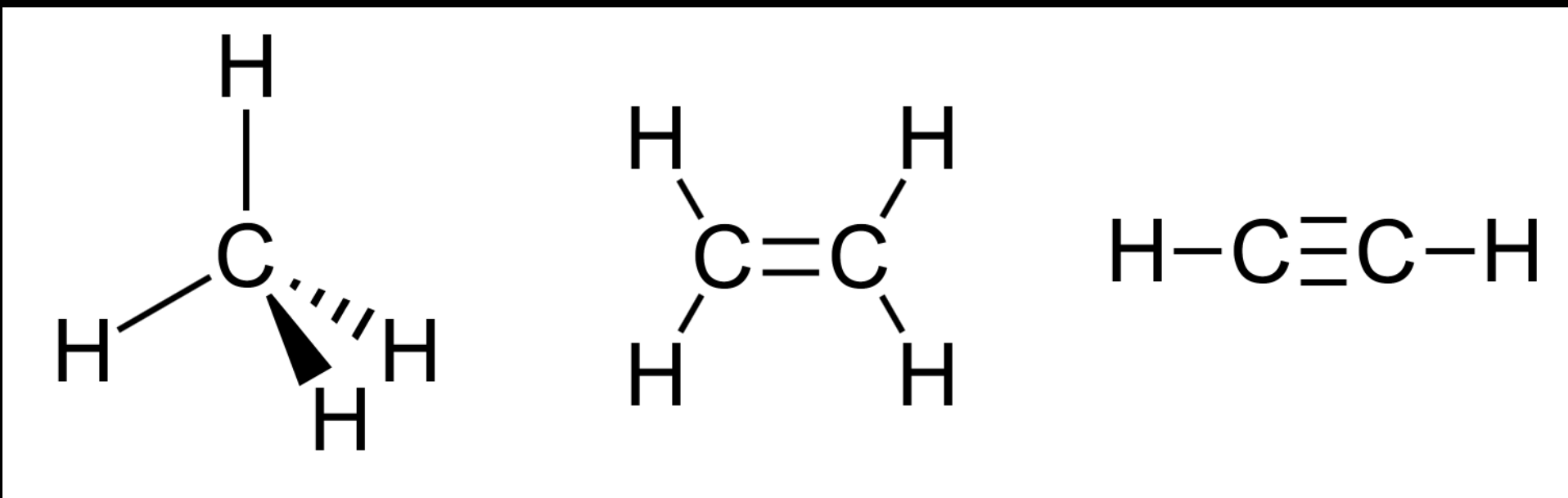
Carbon atom in its ground state

Carbon atom in its excited state

Two sp hybrid orbitals

Hybridisation

Hybridisation is the mixing of atomic orbitals to produce hybrid orbitals used for bonding.



Methane

sp³ hybridisation

Ethene

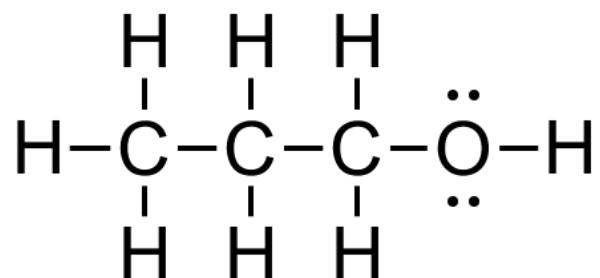
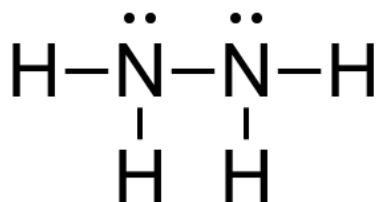
sp² hybridisation

Ethyne

sp hybridisation

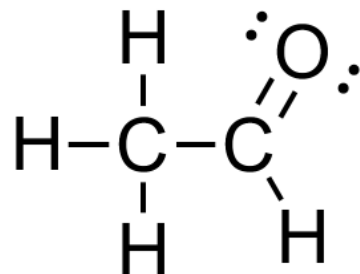
Number of electron domains	Hybridisation	Electron domain geometry	Molecular geometry	Bond angle	Examples
2	sp	Linear	Linear	180°	CO ₂ C ₂ H ₂
3	sp ²	Trigonal planar	Trigonal planar	120°	C ₂ H ₄ BF ₃
4	sp ³	Tetrahedral	Tetrahedral, bent, trigonal pyramidal	≤ 109.5°	CH ₄ H ₂ O NH ₃

Hydrazine

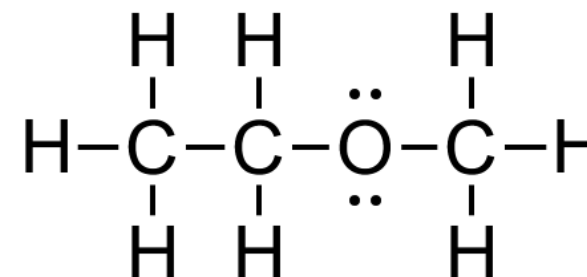


Propan-1-ol

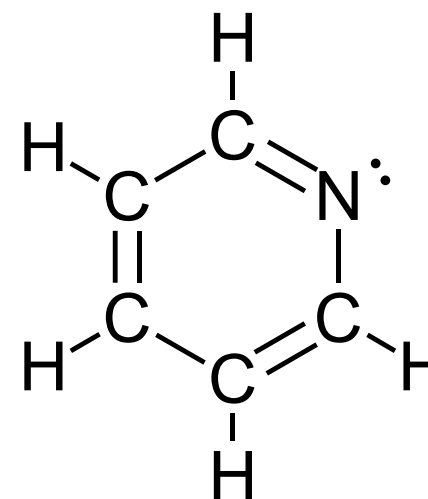
Ethanal



Methoxyethane



Pyridine



Ethanenitrile

