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VIDEO TUTORIALS FOR IB CHEMISTRY

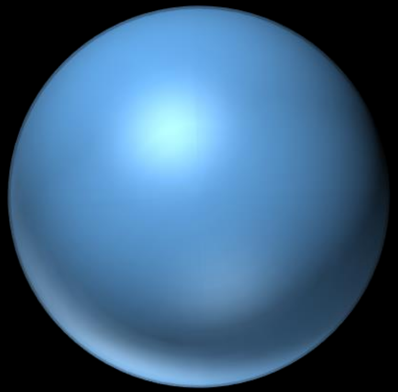
sigma and pi bonds

Covalent bonding

- Covalent bonds are formed by the overlapping of atomic orbitals to form molecular orbitals.
- There are two types of covalent bond – sigma (σ) and pi (π)

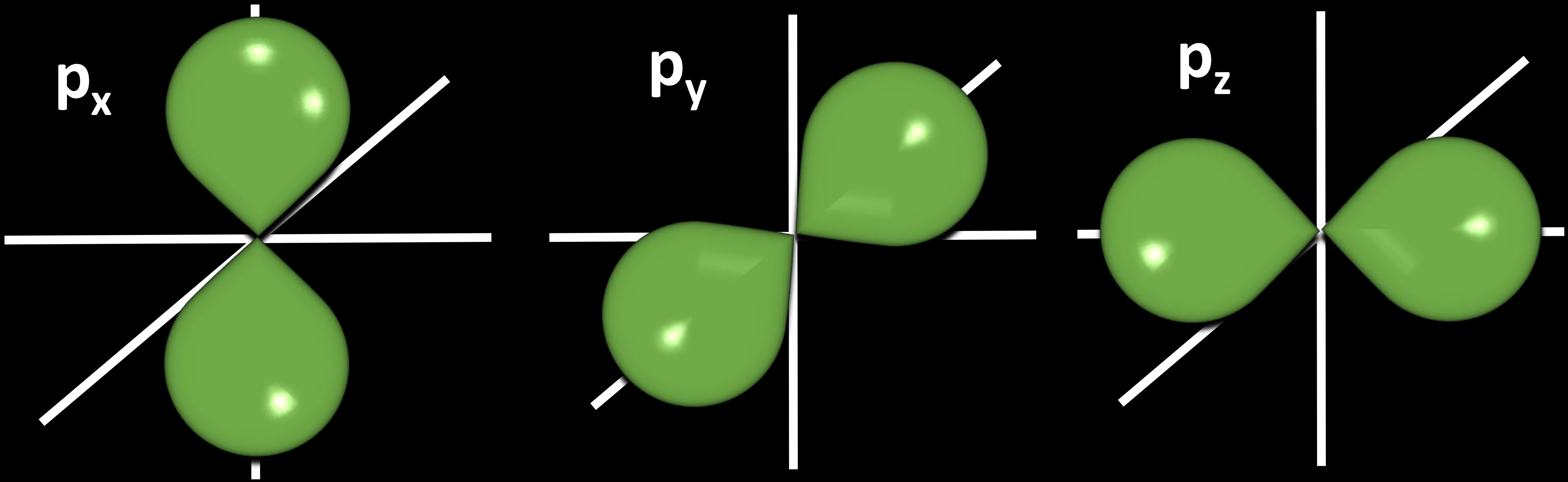
s atomic orbitals

s orbitals are spherical

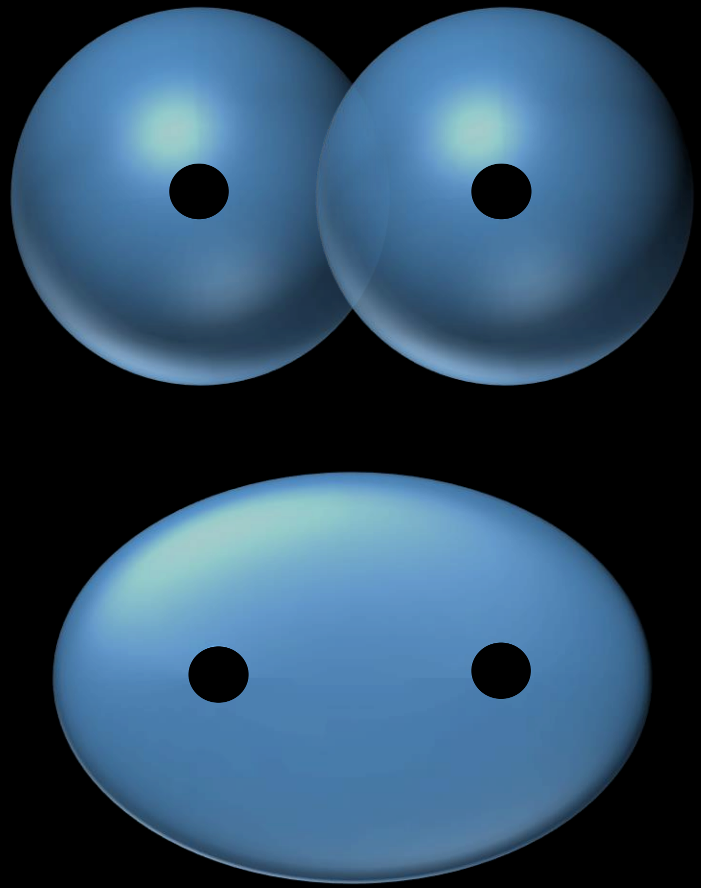


p atomic orbitals

p orbitals are dumbbell shaped



sigma (σ) bonds

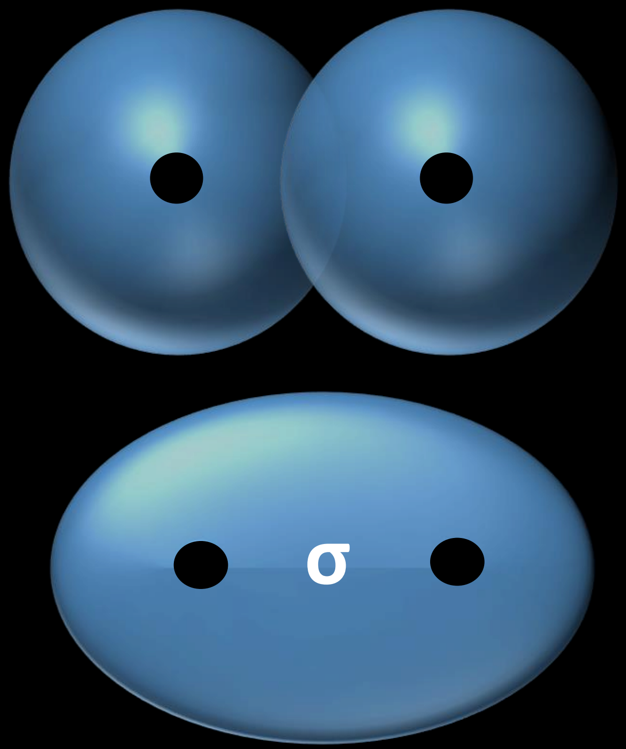


A sigma bond is formed by the head on overlap of atomic orbitals.

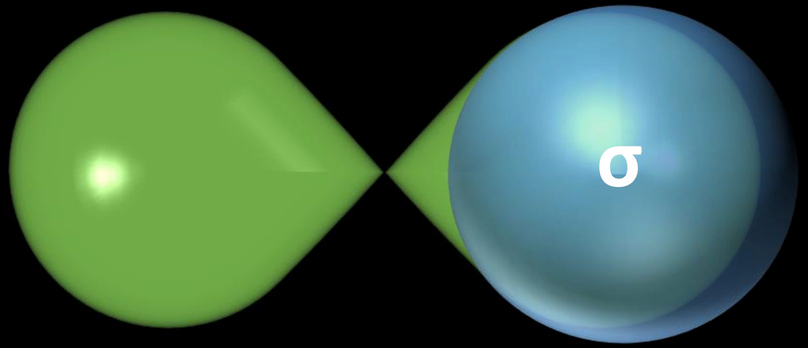
This results in electron density concentrated between the nuclei of the bonding atoms.

sigma (σ) bonds

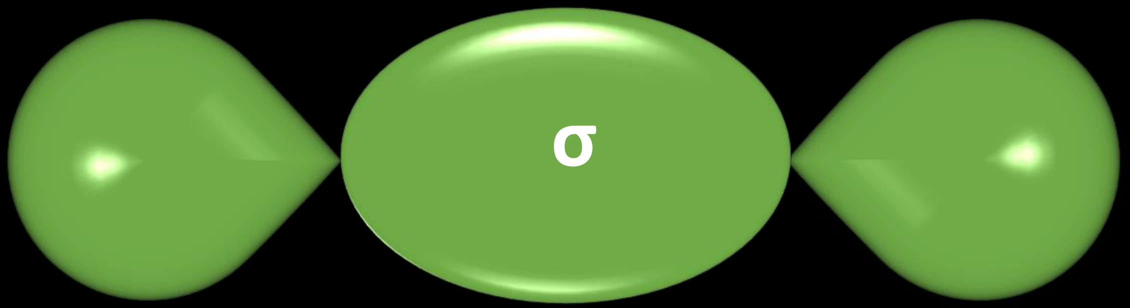
Two s orbitals overlap



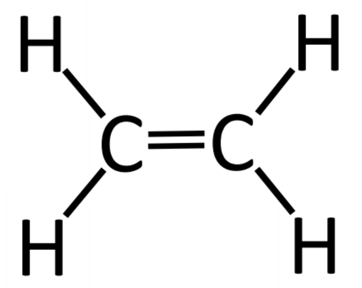
s orbital overlaps with p orbital



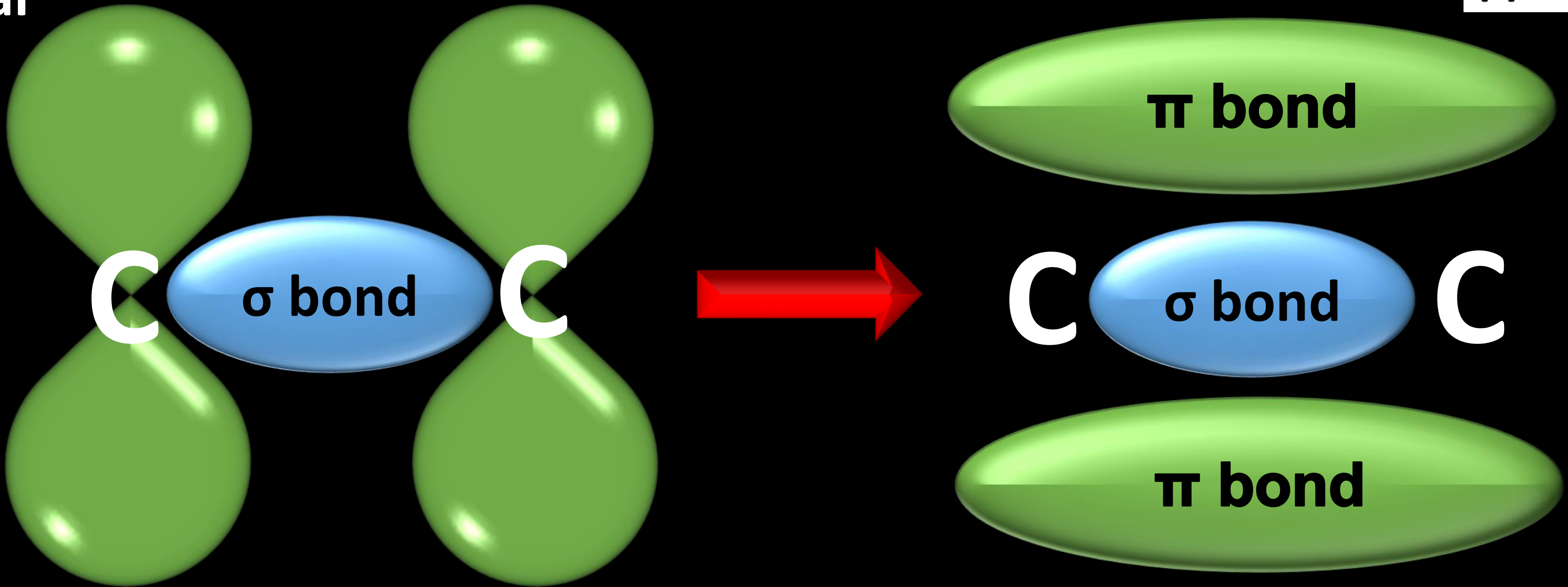
Two p orbitals overlap head on



pi (π) bonds



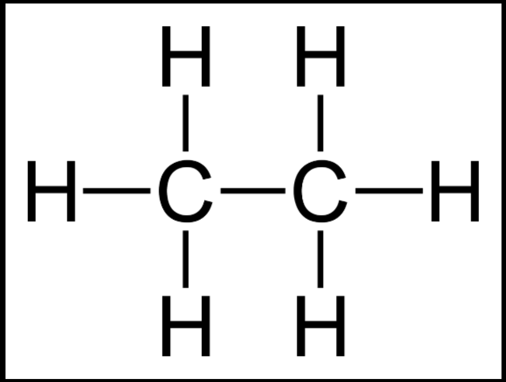
Unhybridised p orbital

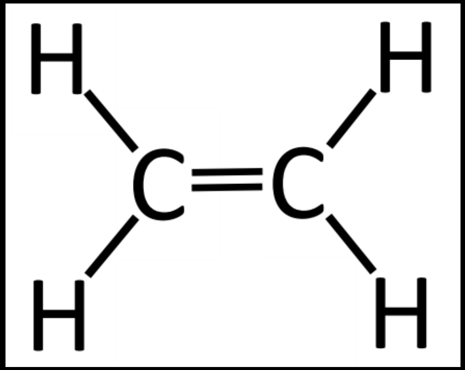


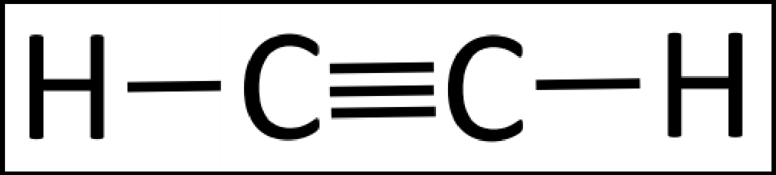
A pi bond is formed by sideways overlap of atomic orbitals. This results in electron density above and below the plane of the nuclei of the bonding atoms.

sigma and pi bonds

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







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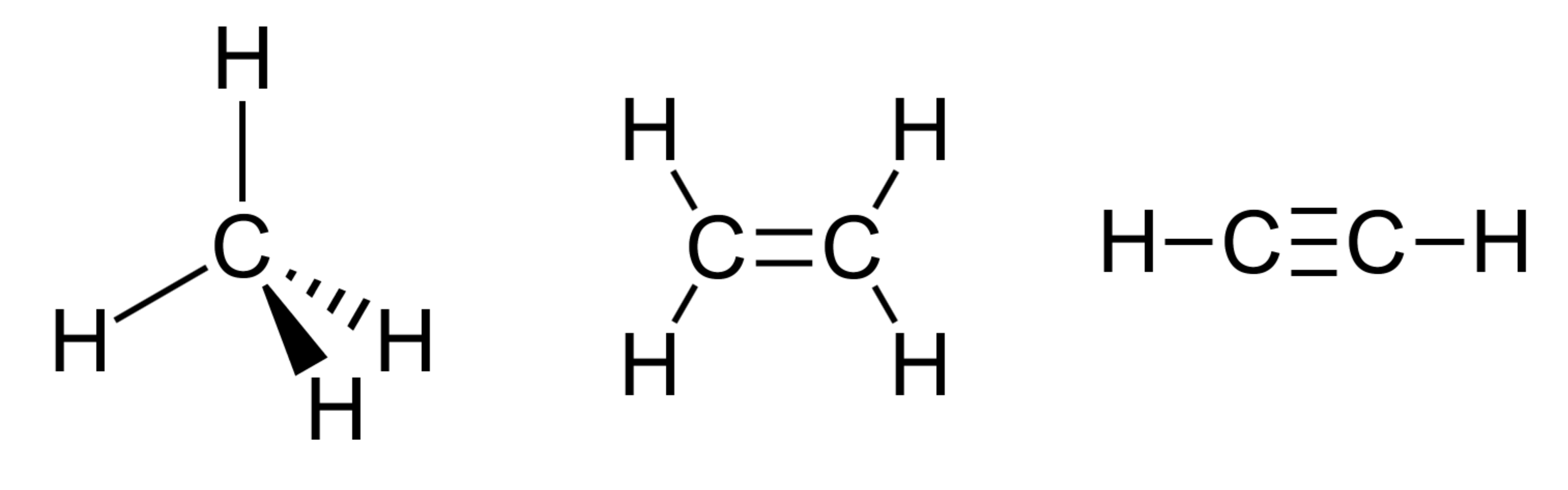
Hybridisation

Hybridisation

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



Methane
sp^3 hybridisation

Ethene
sp^2 hybridisation

Ethyne
sp hybridisation

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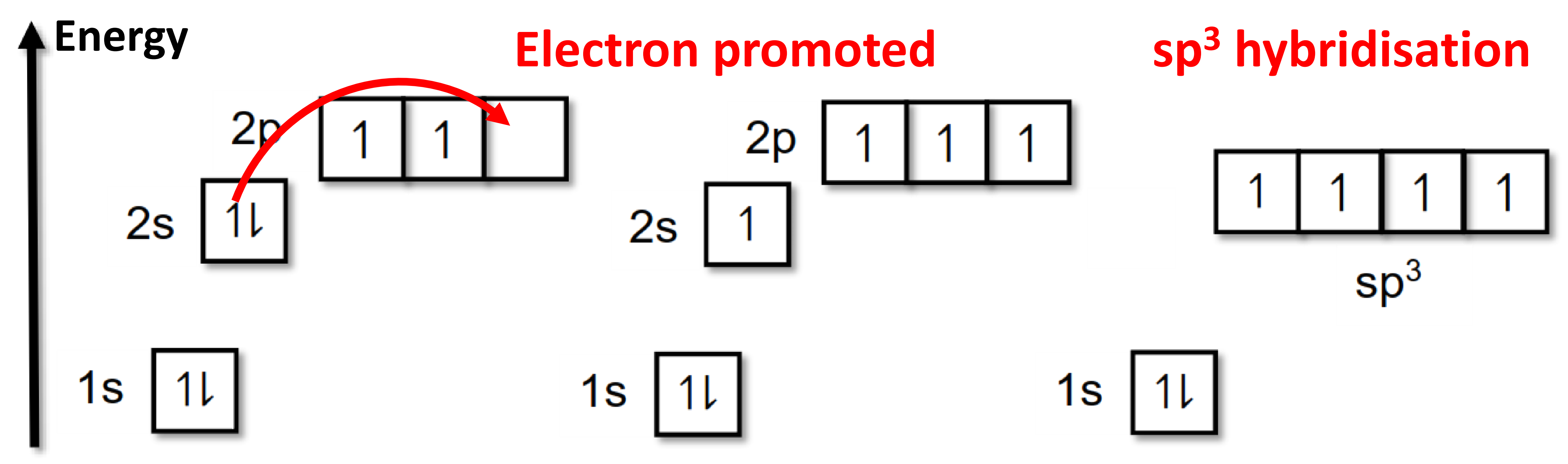
sp^3 hybridisation

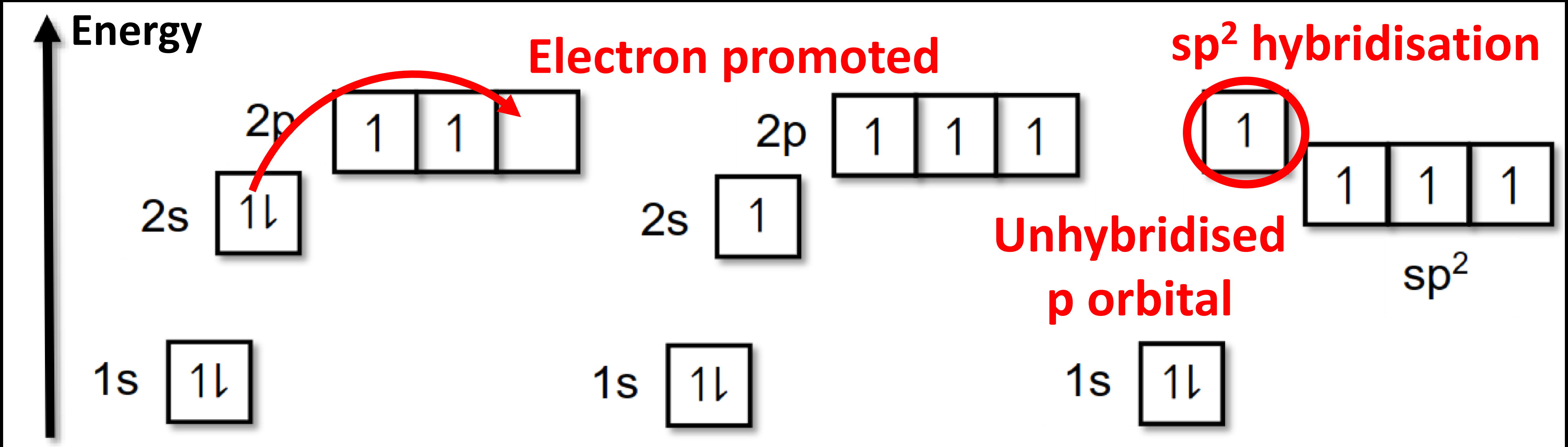


Carbon atom in its ground state

Carbon atom in its excited state

Four sp^3 hybrid orbitals

sp^2 hybridisation

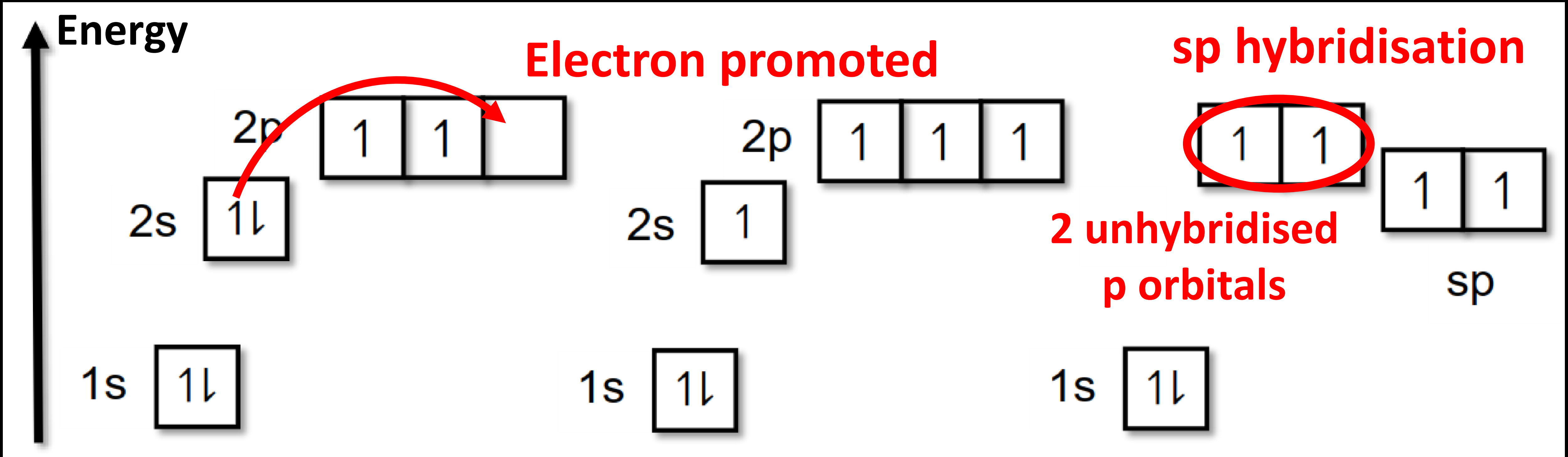


Carbon atom in its ground state

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

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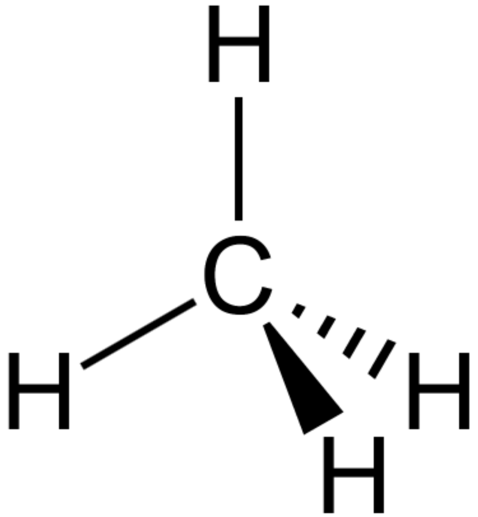

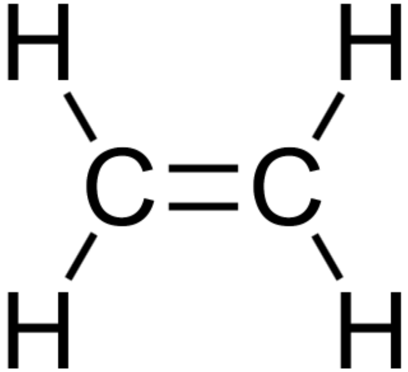

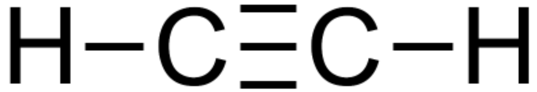

Methane
sp^3 hybridisation

Ethene
sp^2 hybridisation

Ethyne
sp hybridisation

Hybridisation and molecular geometry

Number of electron domains	Hybridisation	Electron domain geometry	Molecular geometry	Bond angle	Examples
2	sp	Linear	Linear	180°	CO_2 C_2H_2
3	sp^2	Trigonal planar	Trigonal planar	120°	C_2H_4 BF_3
4	sp^3	Tetrahedral	Tetrahedral, bent, trigonal pyramidal	≤ 109.5°	CH_4 H_2O NH_3

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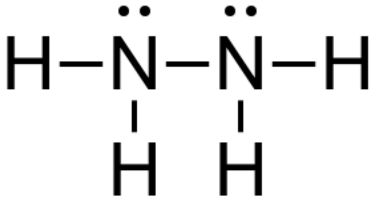
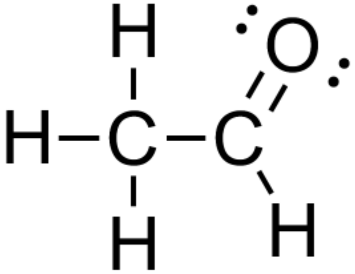
Hybridisation and molecular geometry

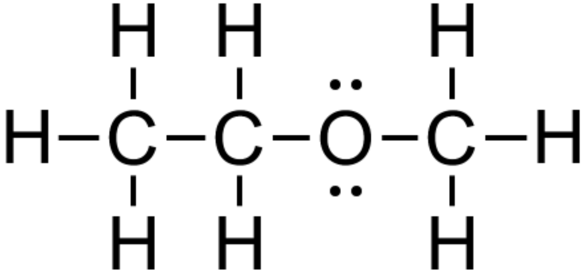
Hydrazine

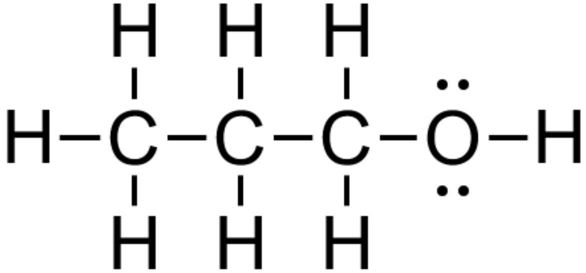


Ethanal

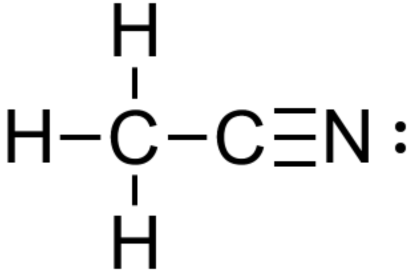


Methoxyethane



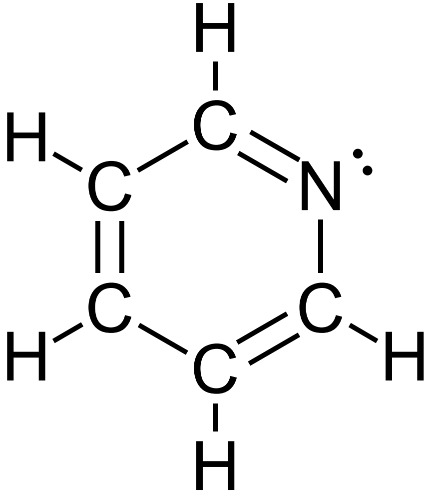


Propan-1-ol



Ethanenitrile

Pyridine



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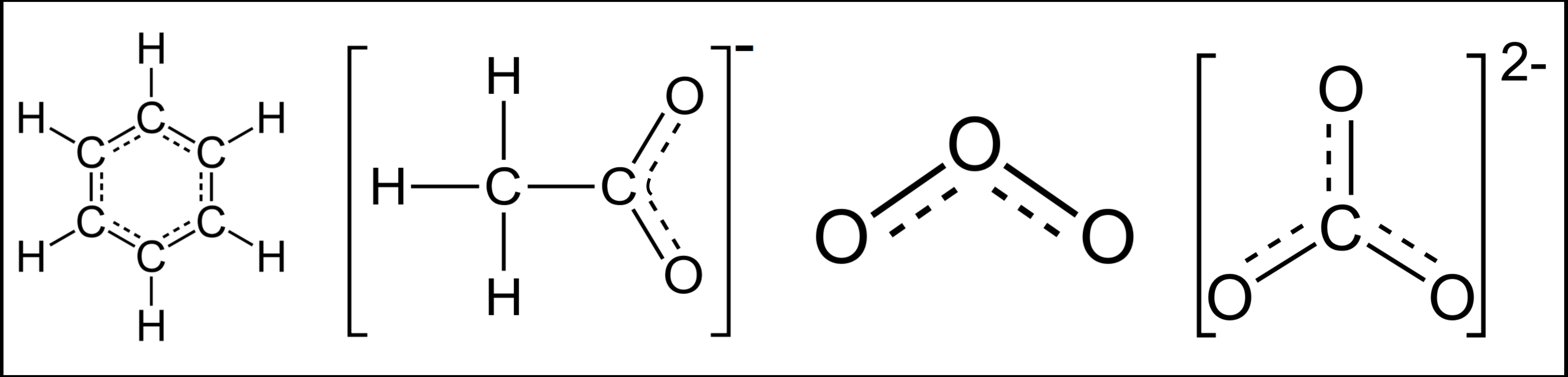
Molecules with delocalised π electrons

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).



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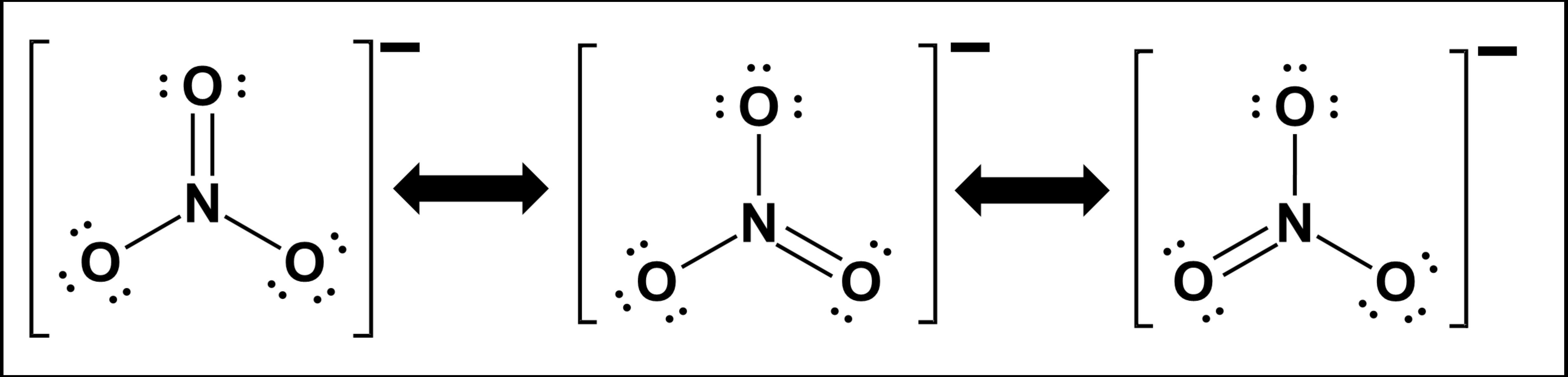

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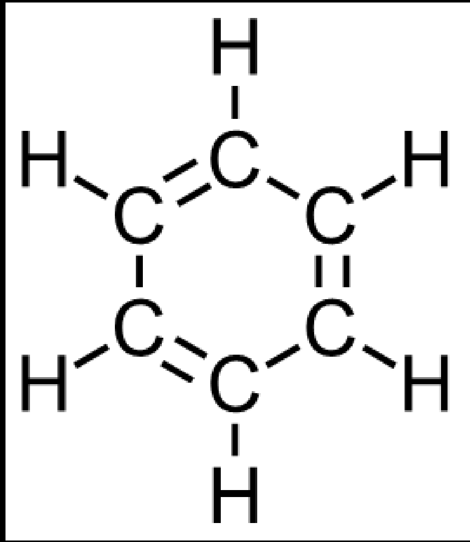
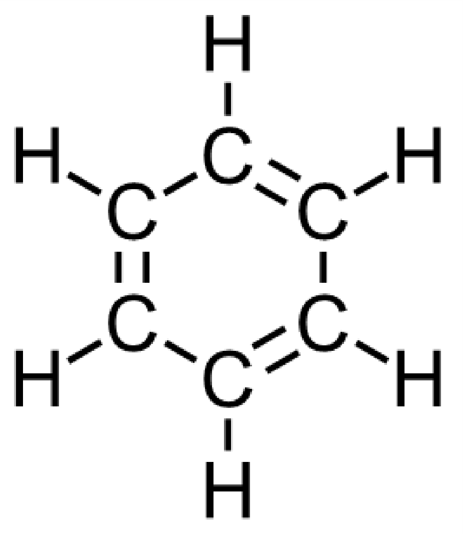
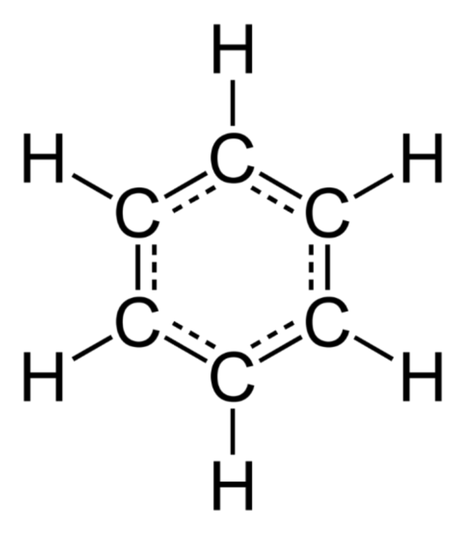
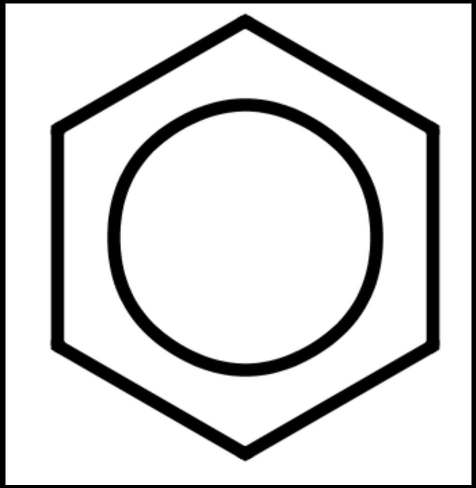
Delocalised π electrons

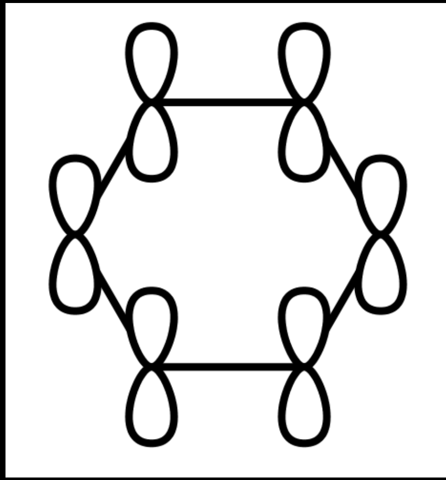
Benzene C_6H_6

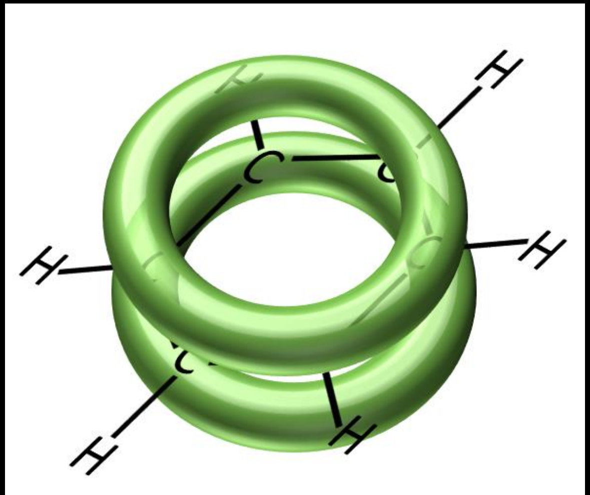












Benzene contains a total of 6 pi electrons - one from each unhybridised p orbital.

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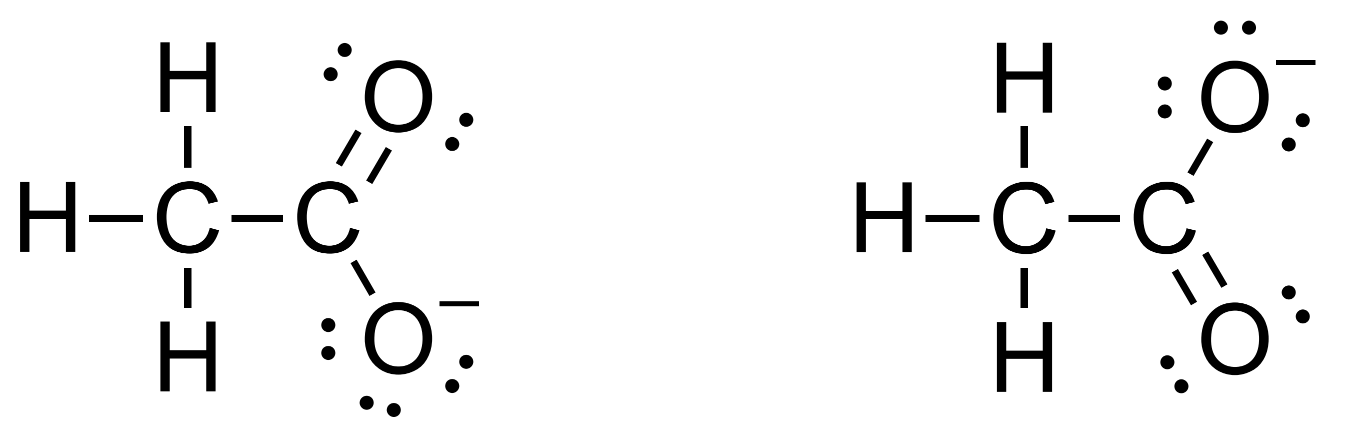
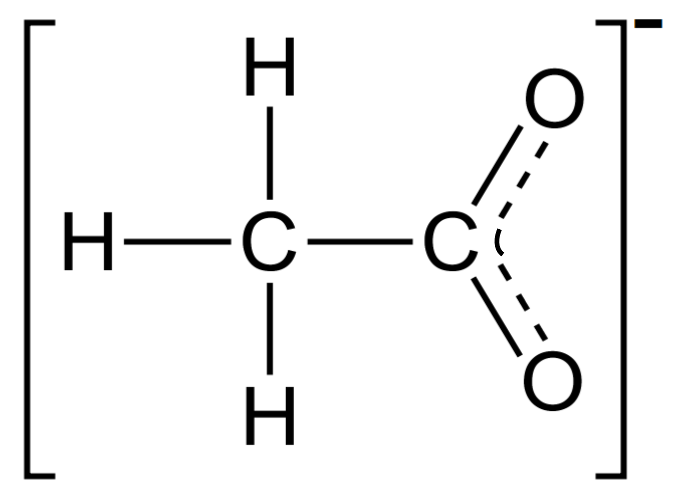
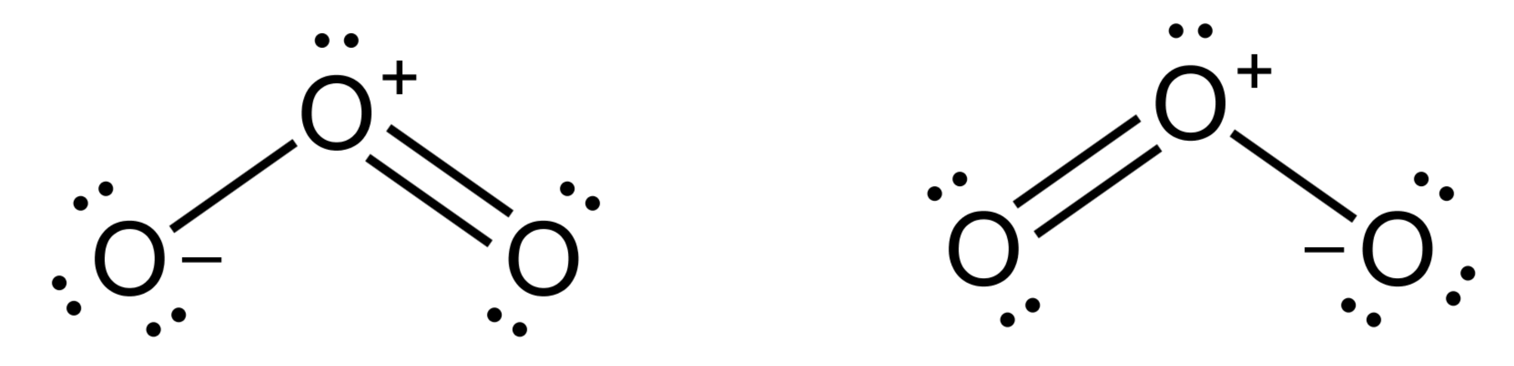
Delocalised π electrons

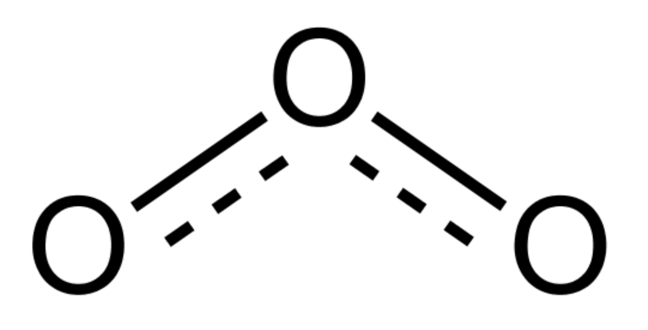
Ethanoate ion CH_3COO^-





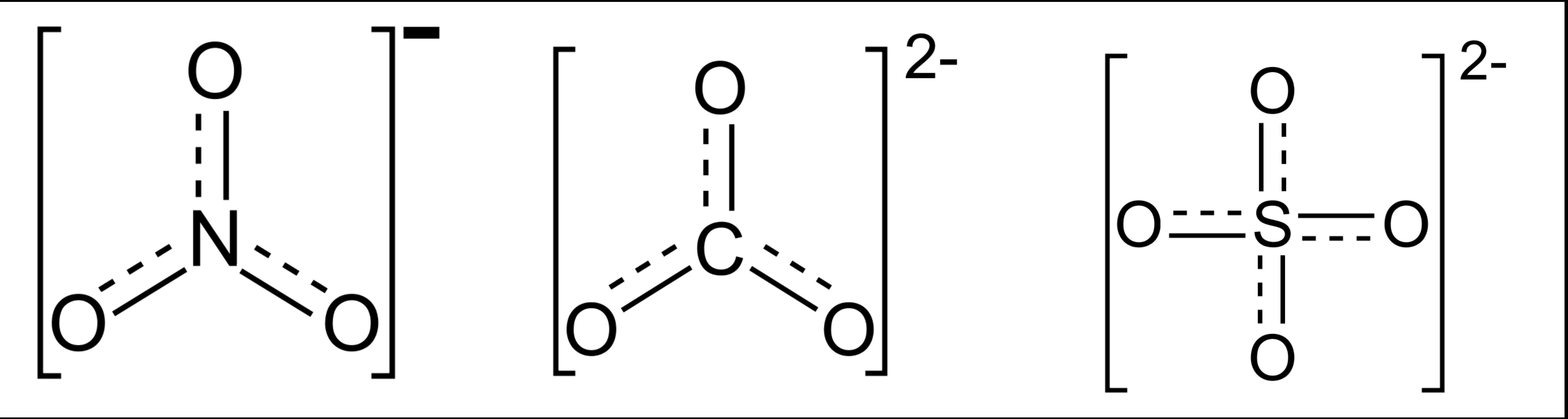
Ozone, O_3





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

Pi (π) electrons are electrons located in pi bonds in a double or triple bond, or in a conjugated system.

Type of bond	sigma (σ)	pi (π)	Number of π electrons
Single	1	0	0
Double	1	1	2
Triple	1	2	4

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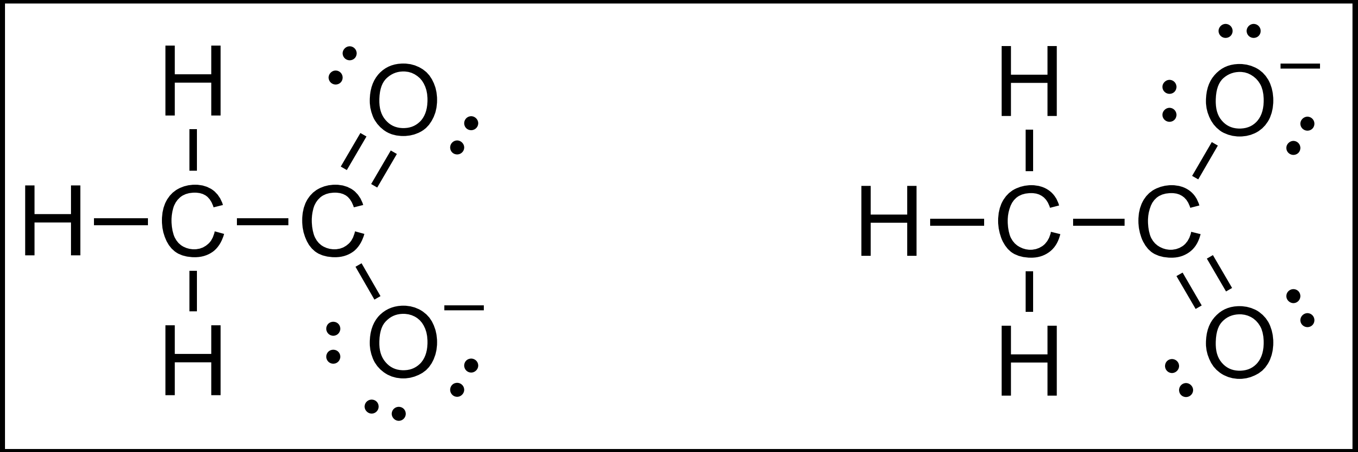
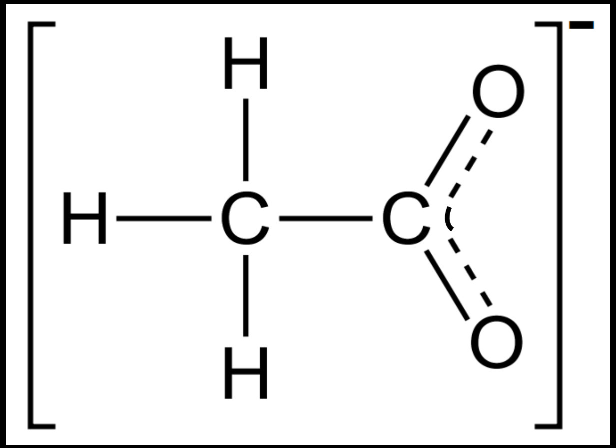
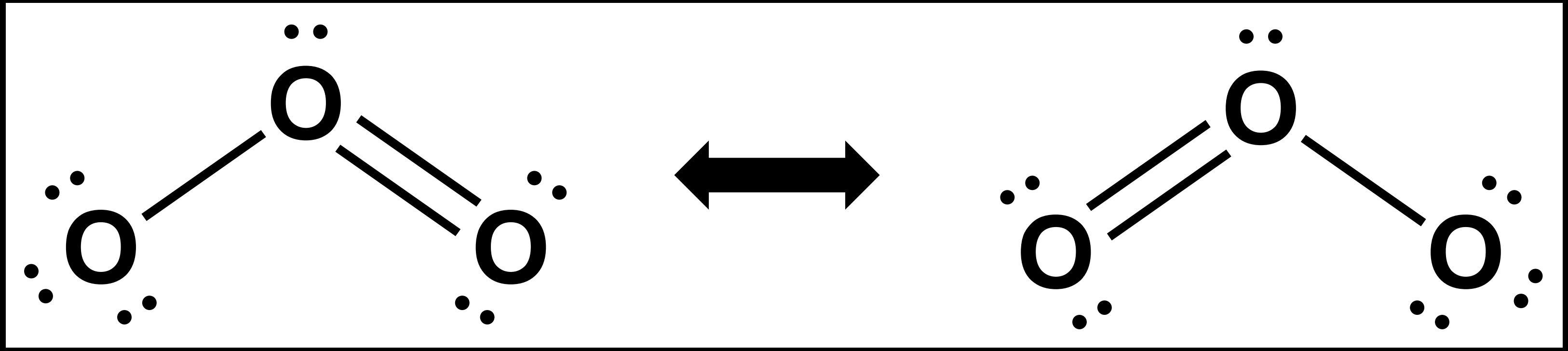
Delocalised π electrons

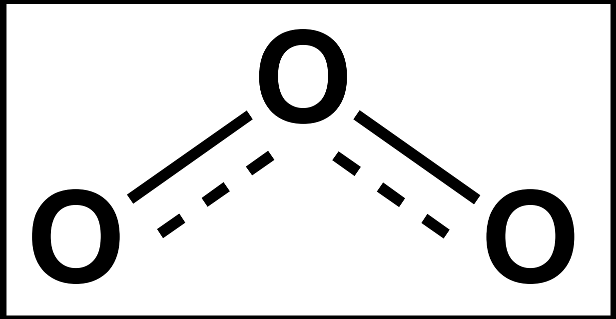
Ethanoate ion CH_3COO^-





Ozone, O_3





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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

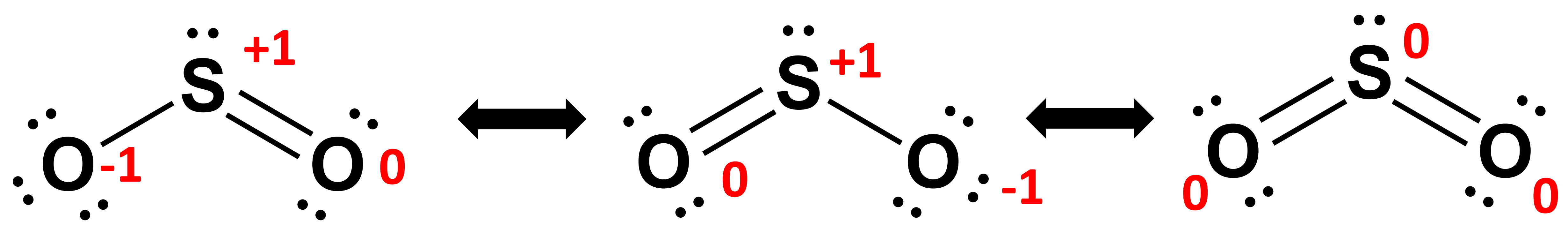
The formal charge of an atom in a compound is calculated using the following equation:

Number of valence electrons – Number of non-bonding electrons – ½ number of 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.

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Formal charge

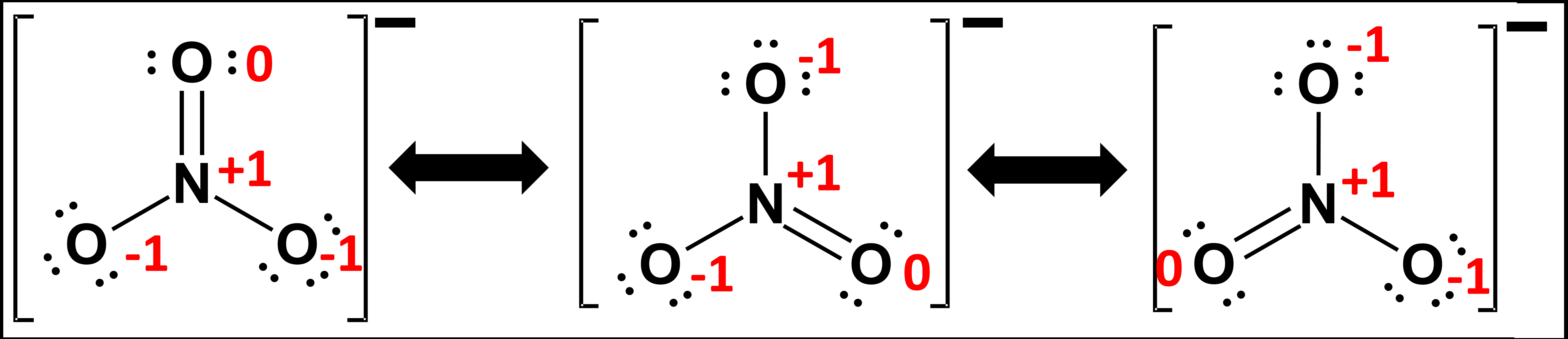
Two possible Lewis structures for N_2O are shown below.

0 +1 -1 -1 +1 0

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.

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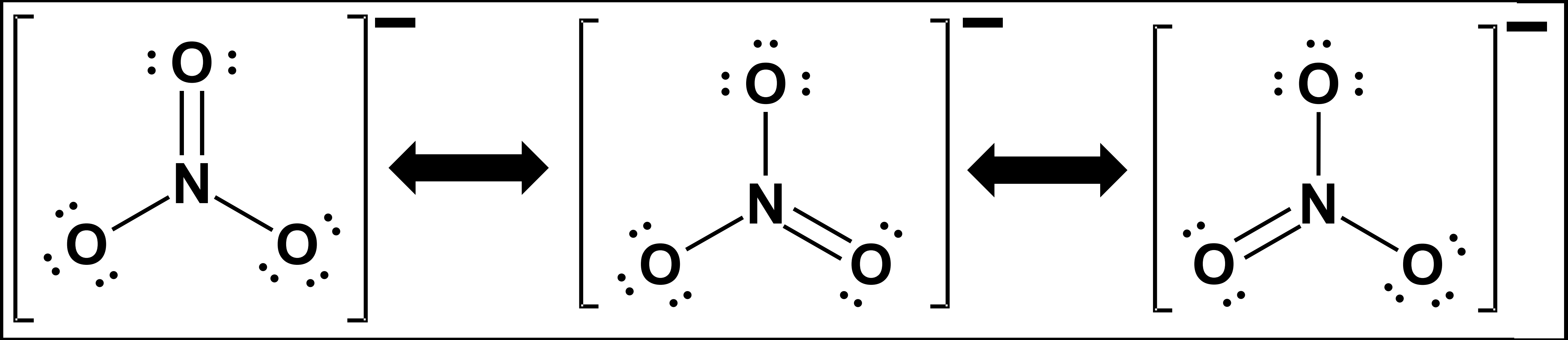

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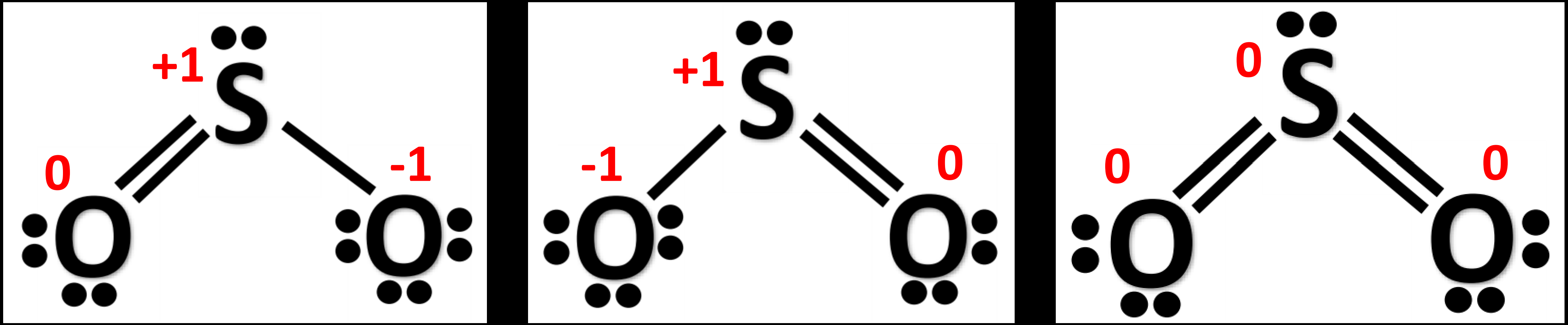

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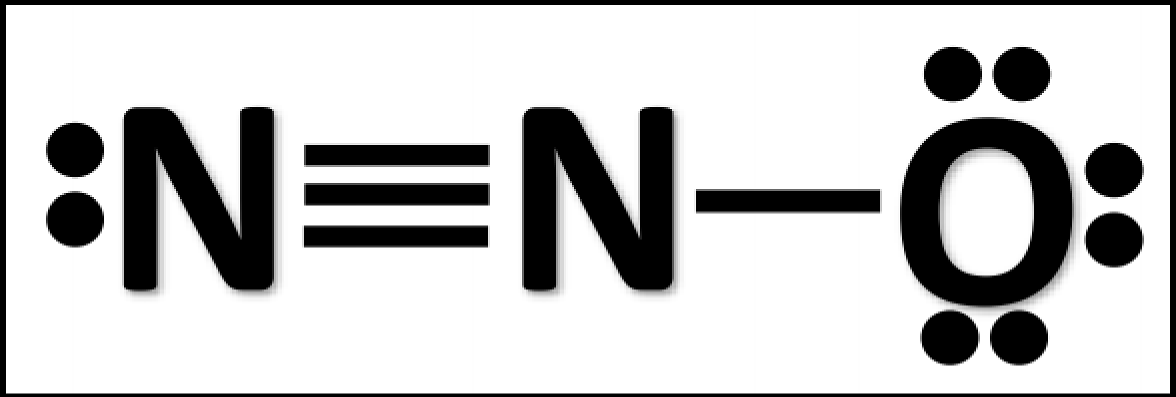
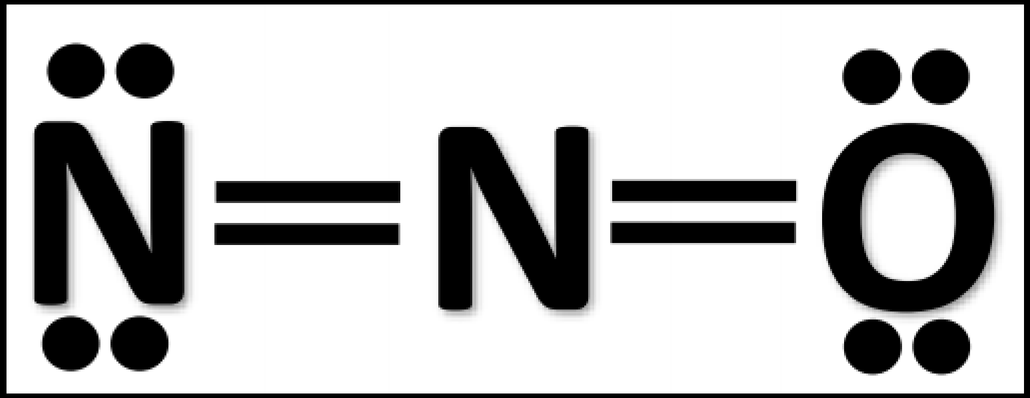


0 +1 -1



-1 +1 0

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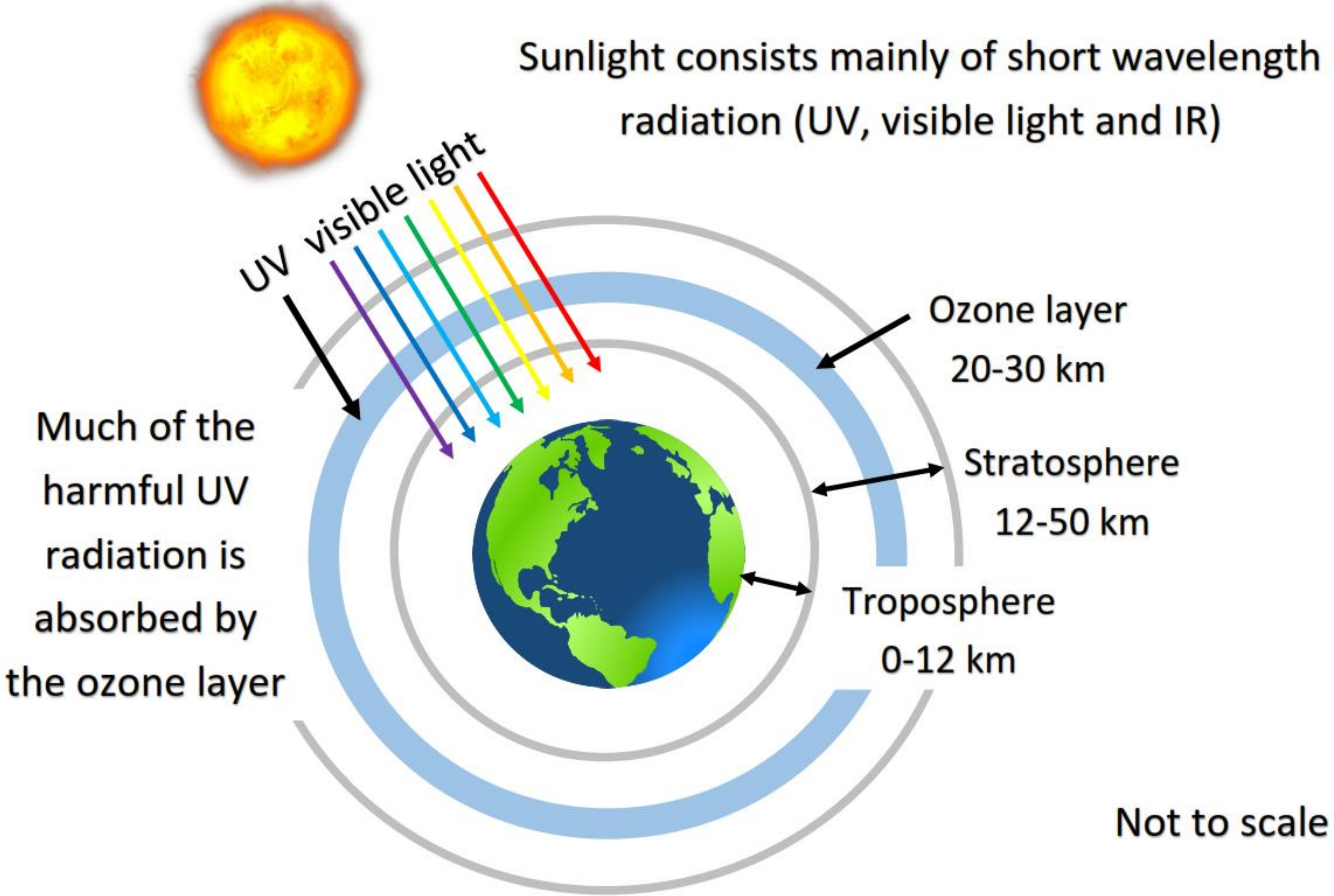
Formation and destruction of ozone


Sunlight consists mainly of short wavelength radiation (UV, visible light and IR)
UV
visible light
Ozone layer
20-30 km
Stratosphere
12-50 km
Troposphere
0-12 km
Much of the harmful UV radiation is absorbed by the ozone layer
Not to scale

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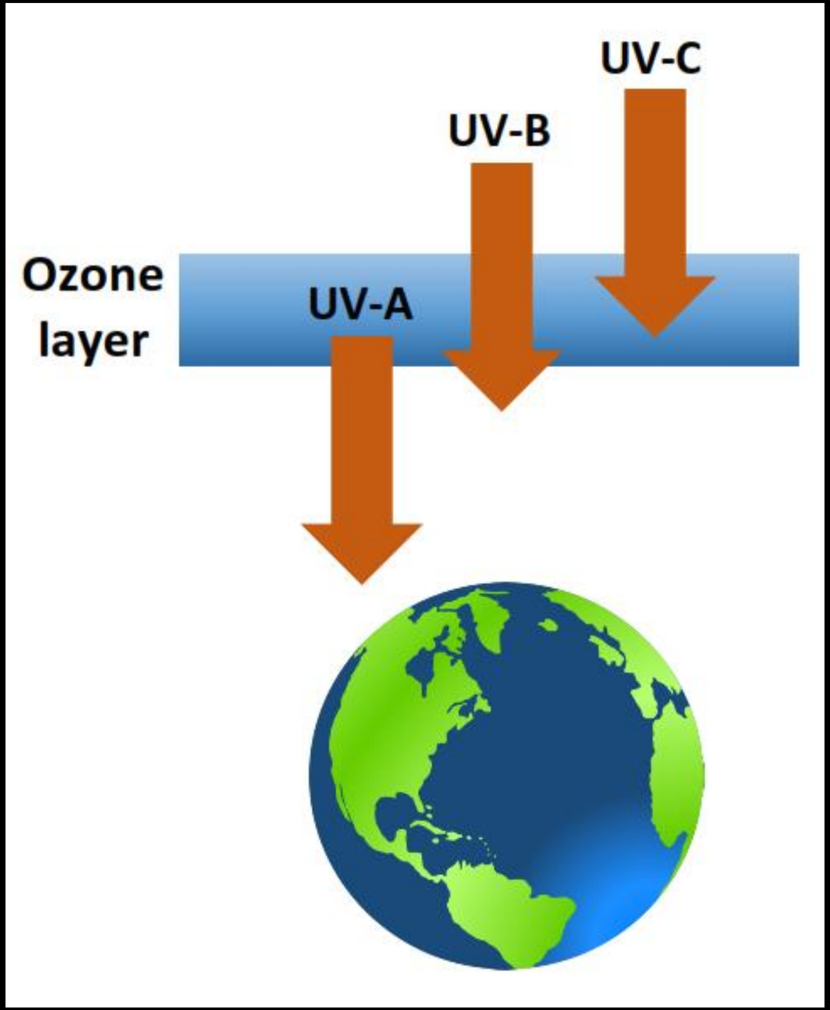
Ozone



Ozone absorbs UV radiation in the range of 200nm-315nm. This corresponds to the higher energy UV radiation (UV-B and UV-C) which can cause damage to living tissue.

Formation of ozone (O_3)

$$O_{2(g)} \xrightarrow[<242nm]{UV} O\bullet_{(g)} + O\bullet_{(g)}$$

$$O\bullet_{(g)} + O_{2(g)} \longrightarrow O_{3(g)}$$

The oxygen molecule dissociates in the presence of high energy UV radiation to form two oxygen free radicals. The free radicals then react with molecular oxygen to form ozone.

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Destruction of ozone (O_3)

$$O_{3(g)} \xrightarrow[<330\,nm]{UV} O_{2(g)} + O\bullet_{(g)}$$

$$O_{3(g)} + O\bullet_{(g)} \rightarrow 2O_{2(g)}$$

The ozone molecule dissociates in the presence of low energy UV radiation to form O_2 and an oxygen free radical. The free radical then reacts with ozone to form molecular oxygen.

Formation and destruction of ozone

The rate of formation of ozone is equal to the rate of the destruction of ozone (steady state).

In this process, harmful high energy UV radiation is absorbed.

Human pollutants such NO_x and CFCs can disrupt this process and lead to holes in the ozone layer.

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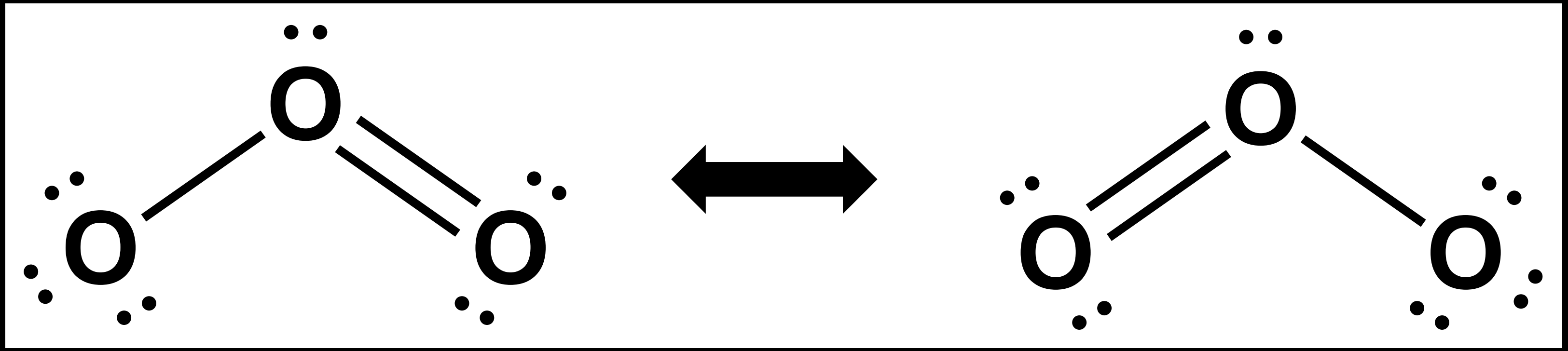
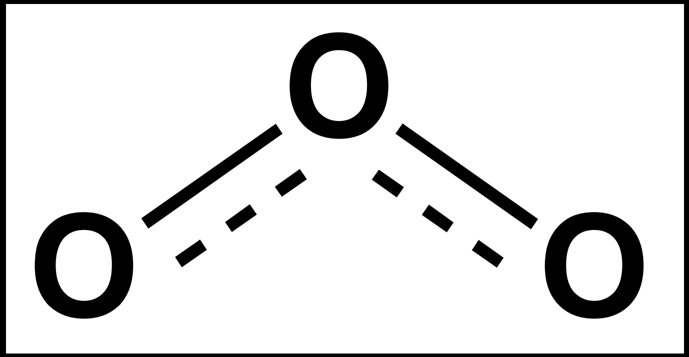
Bonding in oxygen and ozone

Ozone (O_3)

The bonds in ozone are intermediate in strength and length between a single and a double bond (bond order 1.5).





The bonds in O_3 are broken by UV radiation with a wavelength of < 330 nm.

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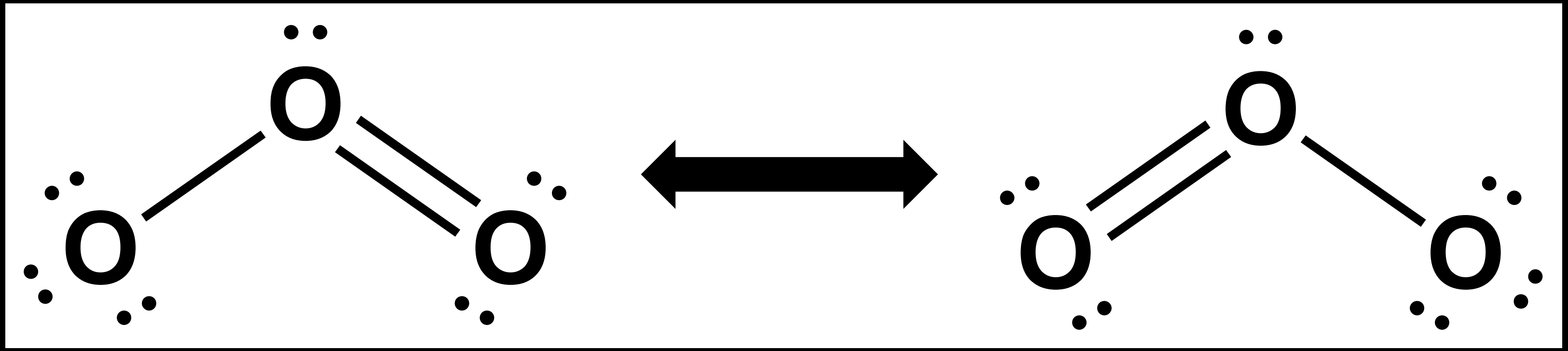

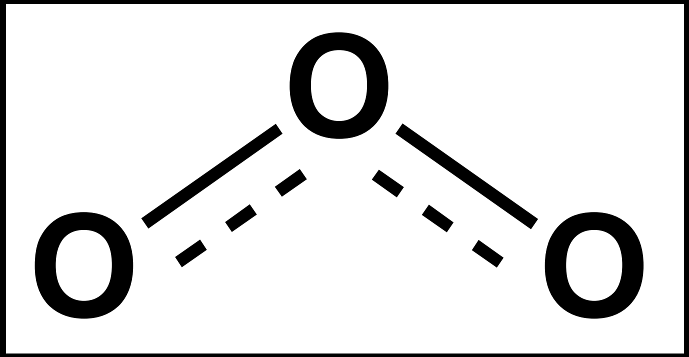

The bonds in O_3 are broken by UV radiation with a wavelength of < 330 nm.

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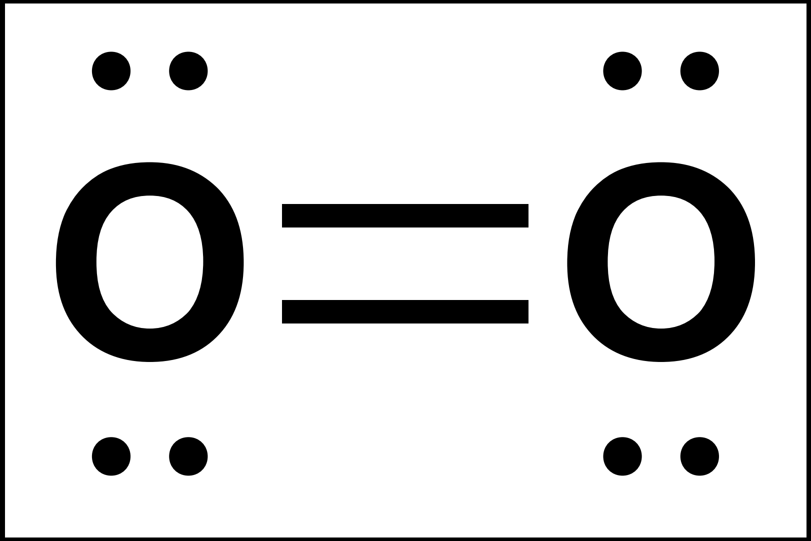
Oxygen (O_2)

The oxygen molecule has a double covalent bond between the oxygen atoms (bond order 2).



The double covalent bond in O_2 is broken by UV radiation with a wavelength of < 242 nm.

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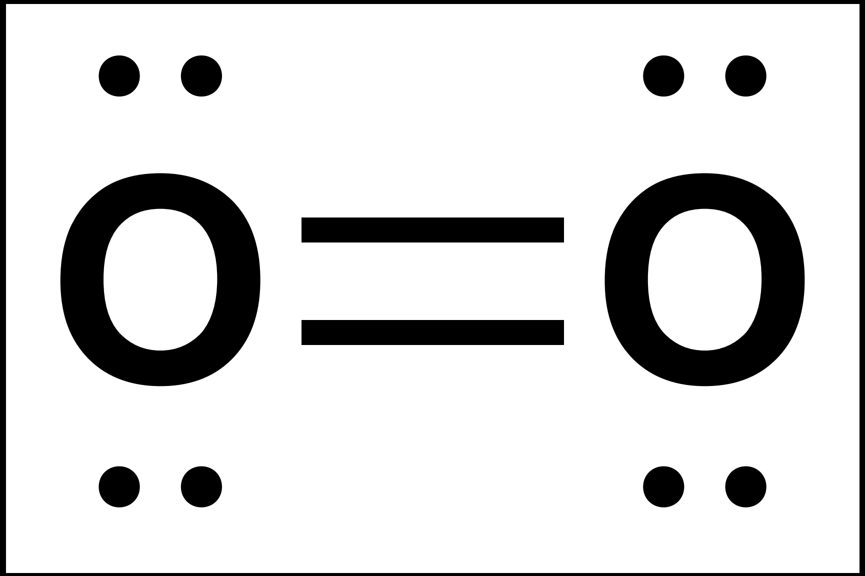
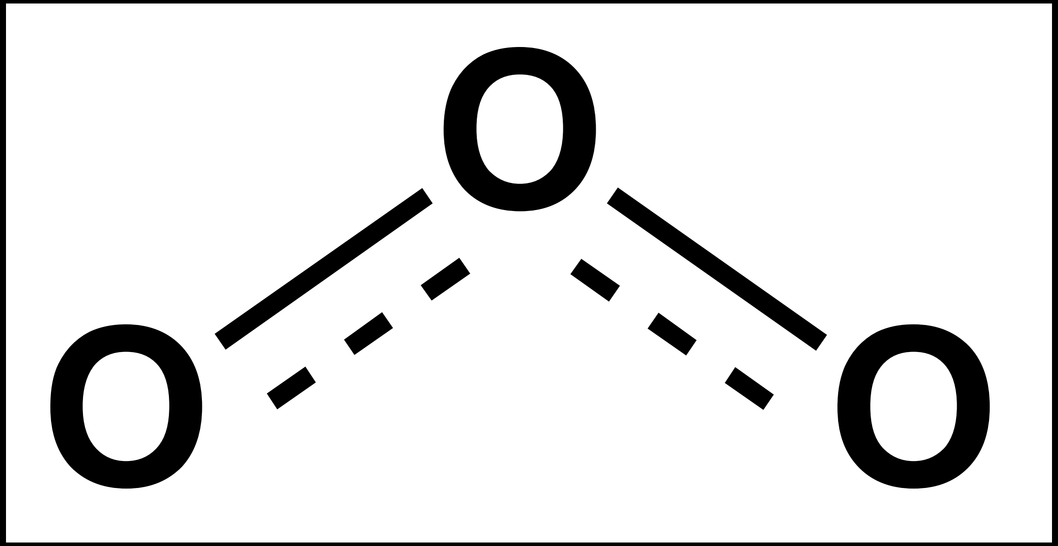
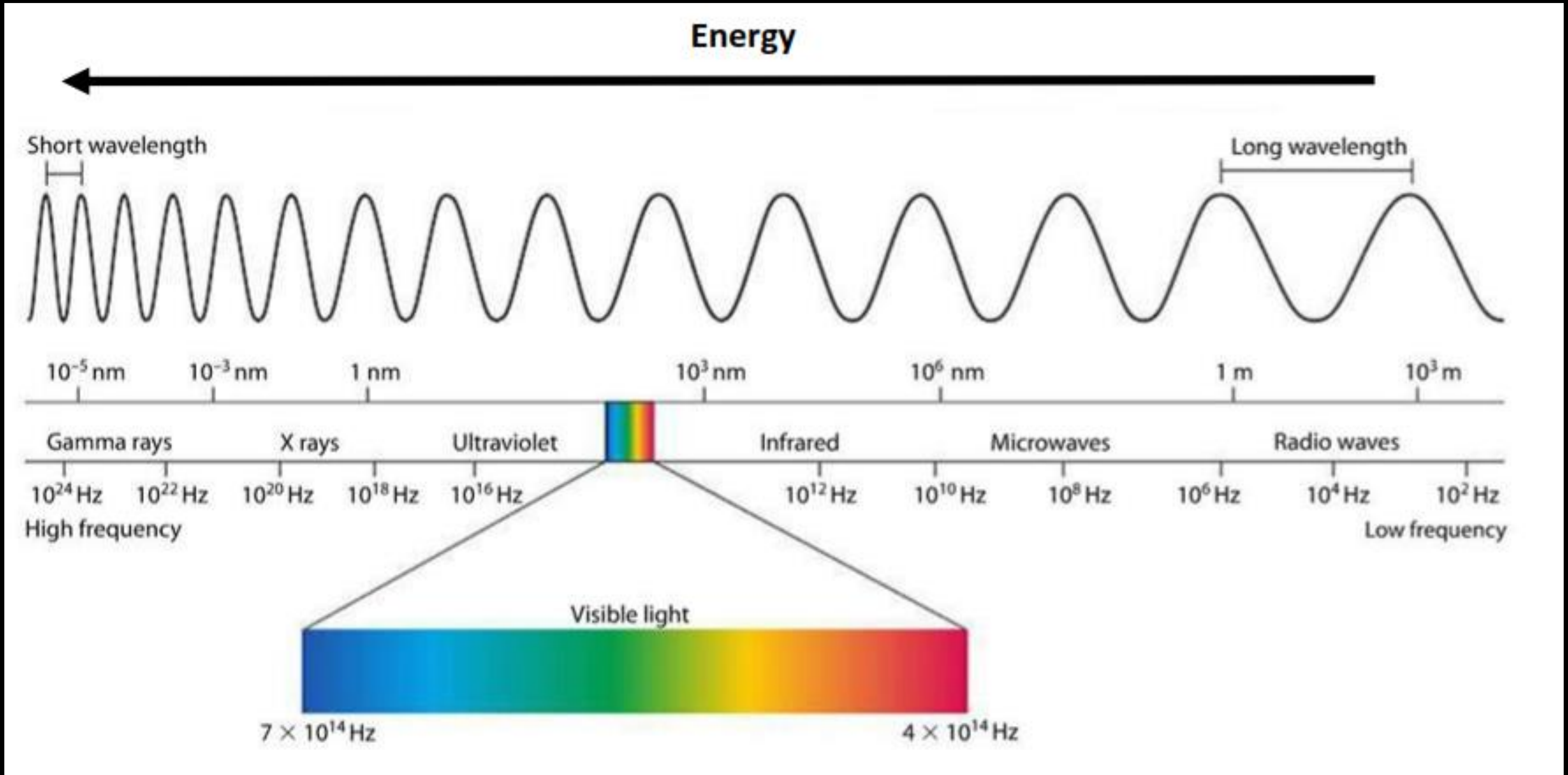
Bond strength in O_2 and O_3





The double bond in O_2 is stronger than the bonds in O_3 – it requires more energy to break the bond in O_2 than in O_3

Energy and wavelength



Higher energy = shorter wavelength = higher frequency

Lower energy = longer wavelength = lower frequency

Bond strength in O_2 and O_3

Molecule	Bond order	λ UV radiation (nm)
O_2	2	< 242
O_3	1.5	< 330

The stronger double bond in O_2 requires higher energy UV radiation (shorter wavelength) to break. The weaker bonds in O_3 require lower energy UV radiation (longer wavelength) to break.

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O_2 bond dissociation

$$O_{2(g)} \xrightarrow{UV} O\cdot_{(g)} + O\cdot_{(g)}$$

The double bond in O_2 is broken by UV radiation with a wavelength of <242nm forming two oxygen free radicals.

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O_3 bond dissociation

$$O_{3(g)} \xrightarrow{UV} O_{2(g)} + O\bullet_{(g)}$$

The bond in O_3 is broken by UV radiation with a wavelength of <330nm forming an oxygen molecule and an oxygen free radical

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Catalytic destruction of ozone (NO and CFCs)

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Nitrogen monoxide (NO)

NO is produced in internal combustion engines by the direct combination of nitrogen and oxygen at high temperatures.

$$N_{2(g)} + O_{2(g)} \rightarrow 2NO\bullet_{(g)}$$

Destruction of ozone (NO)

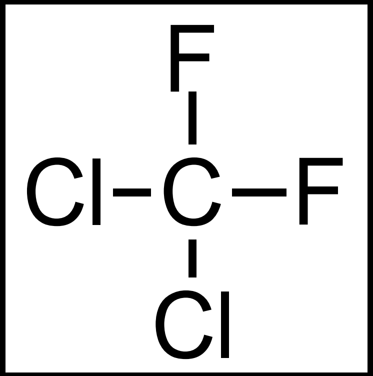
$$NO\bullet_{(g)} + O_{3(g)} \longrightarrow NO_{2(g)} + O_{2(g)}$$

$$NO_{2(g)} + O\bullet_{(g)} \longrightarrow NO\bullet_{(g)} + O_{2(g)}$$

$$O_{3(g)} + O\bullet_{(g)} \longrightarrow 2O_{2(g)}$$

Chlorofluorocarbons (CFCs)

Freon-12



CFCs were widely used in aerosols, refrigerants, solvents, and plastics due to their low toxicity, low flammability and lack of reactivity.

In 1987, it was decided that their use should be phased out because of their ozone depleting ability.

The Cl atoms in CFCs act as catalysts to convert ozone to molecular oxygen.

$$CCl_2F_{2(g)} \xrightarrow{UV} CClF_{2(g)} + Cl\bullet_{(g)}$$

Destruction of ozone (CFCs)

$$Cl\bullet_{(g)} + O_{3(g)} \longrightarrow ClO\bullet_{(g)} + O_{2(g)}$$

$$ClO\bullet_{(g)} + O\bullet_{(g)} \longrightarrow O_{2(g)} + Cl\bullet_{(g)}$$

$$O_{3(g)} + O\bullet_{(g)} \longrightarrow 2O_{2(g)}$$

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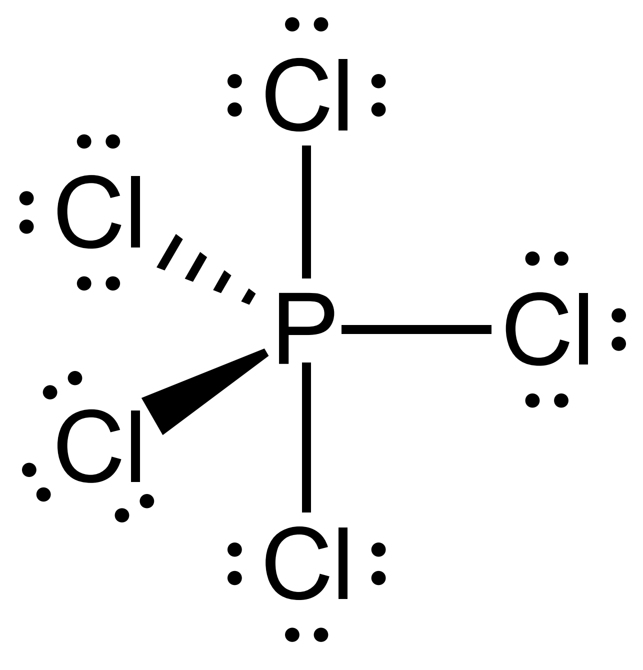
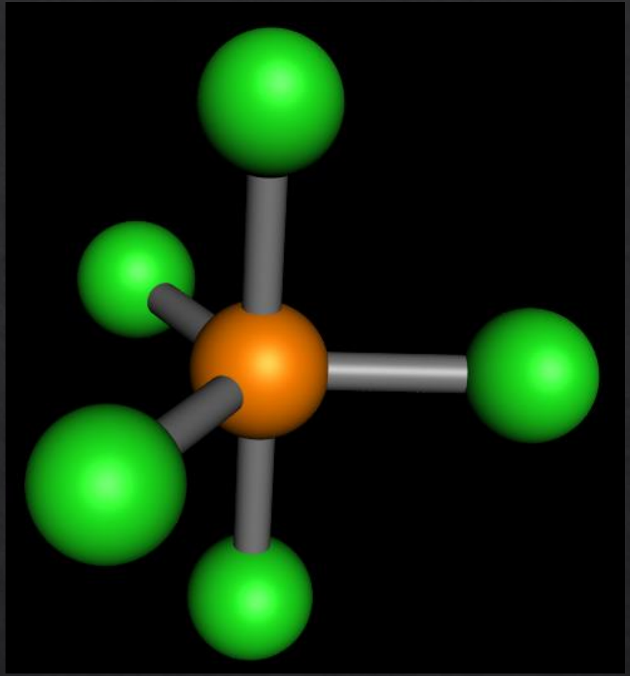
Molecular geometry (HL)

VSEPR HL

PCl_5
phosphorus pentachloride

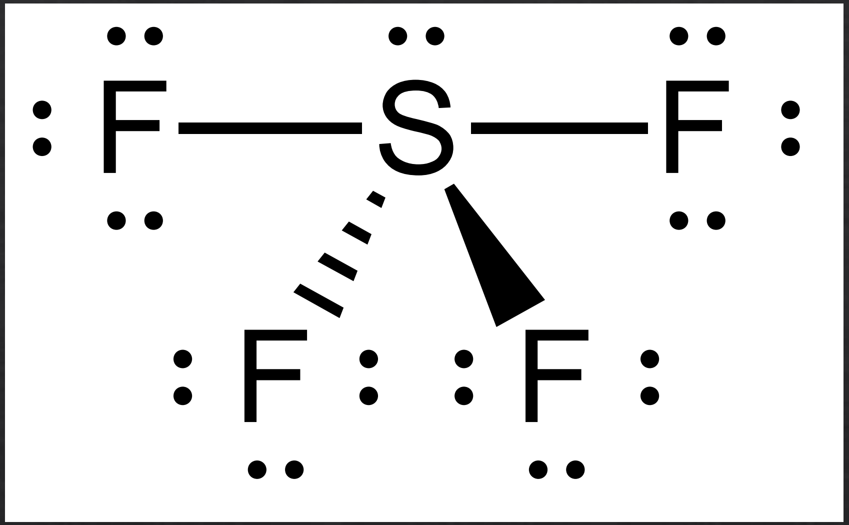


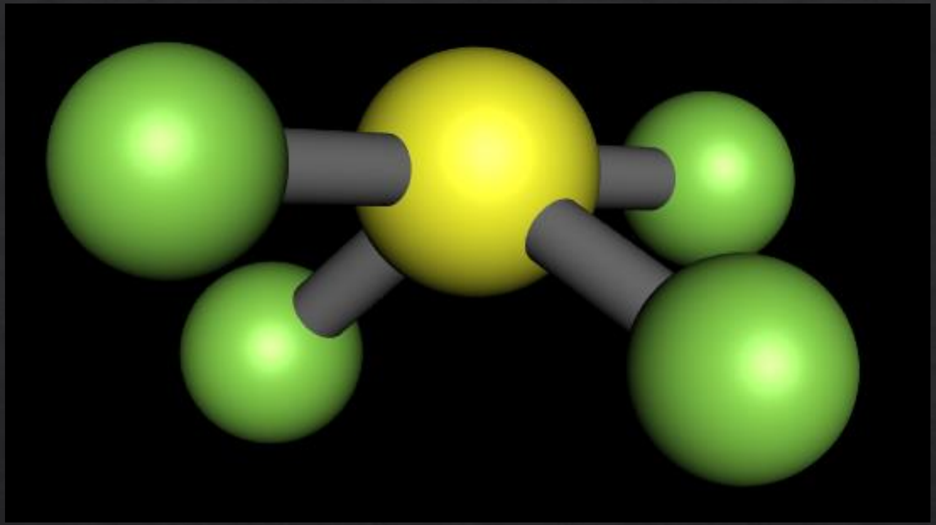


electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
5	5	0	trigonal bipyramidal	trigonal bipyramidal	90º 120º

VSEPR HL

SF_4
sulfur tetrafluoride

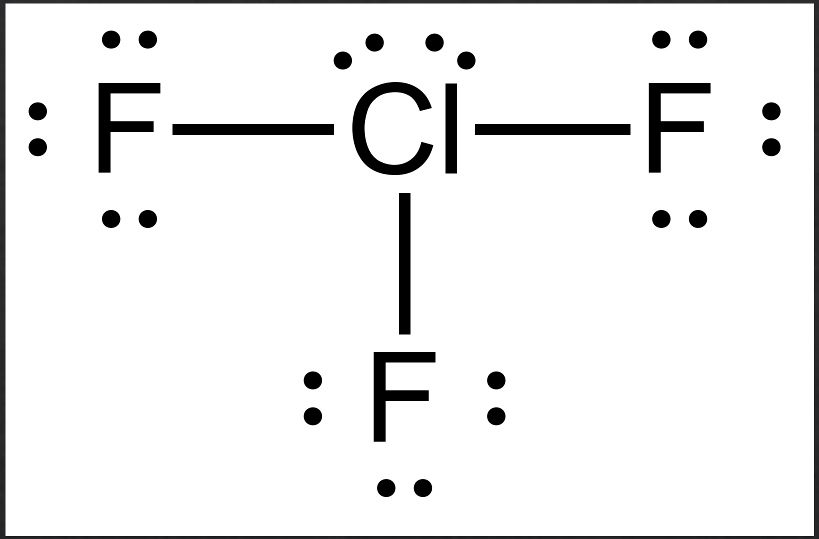


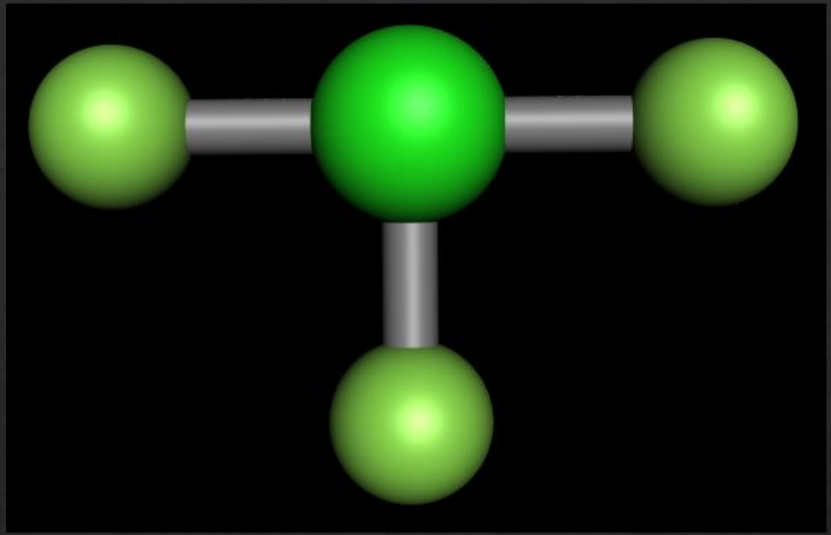


electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
5	4	1	trigonal bipyramidal	see-saw	<90º <120º

VSEPR HL

ClF_3
chlorine trifluoride





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

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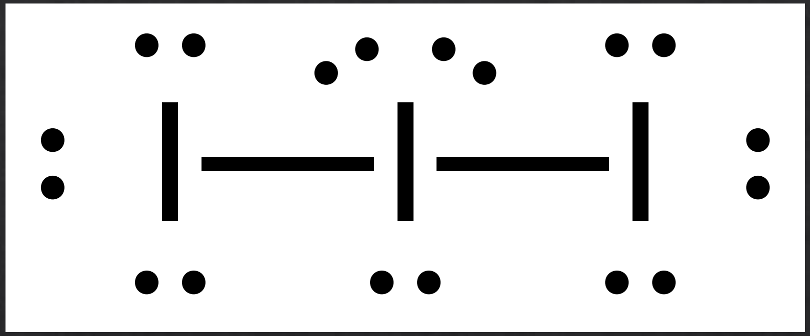
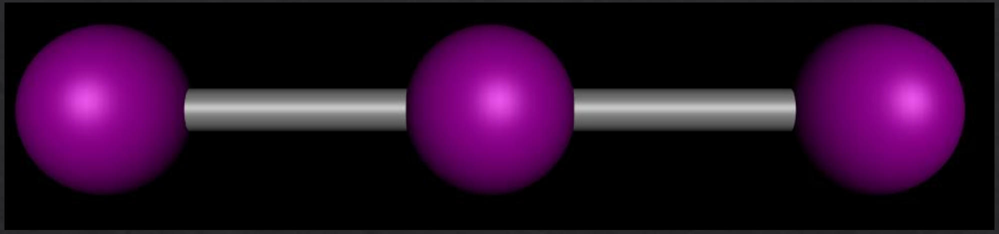
VSEPR HL

I_3^-
triiodide ion





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

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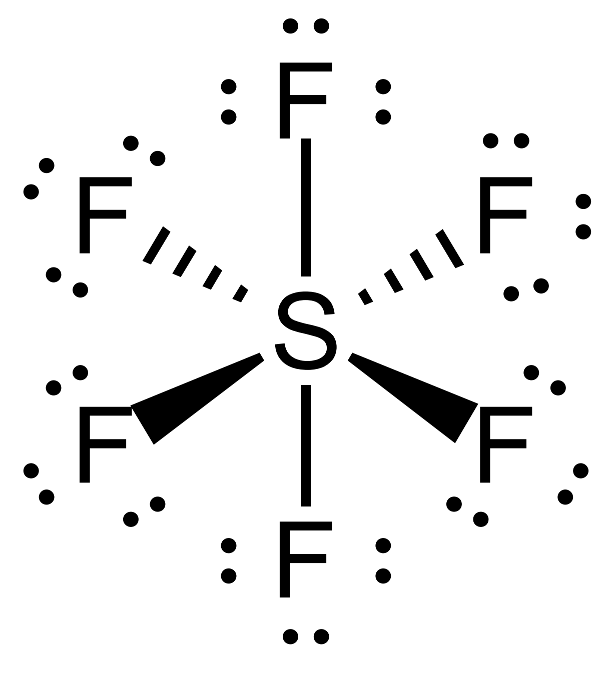
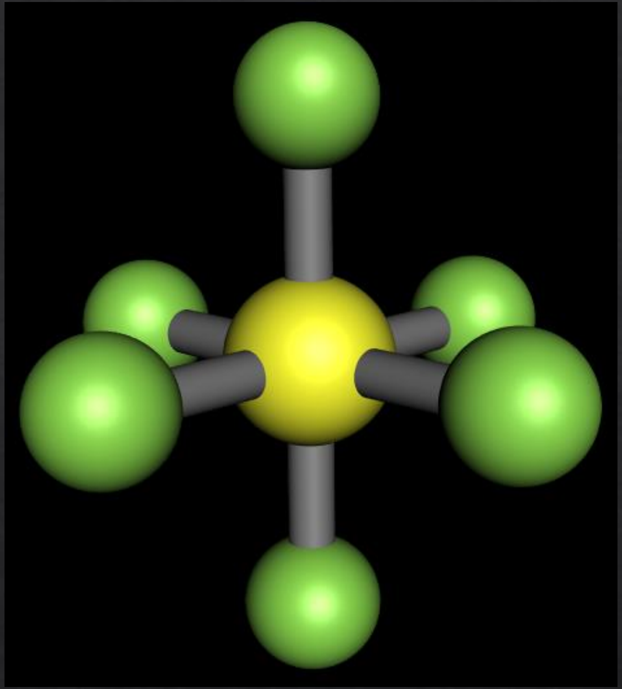
VSEPR HL

SF_6
sulfur hexafluoride

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

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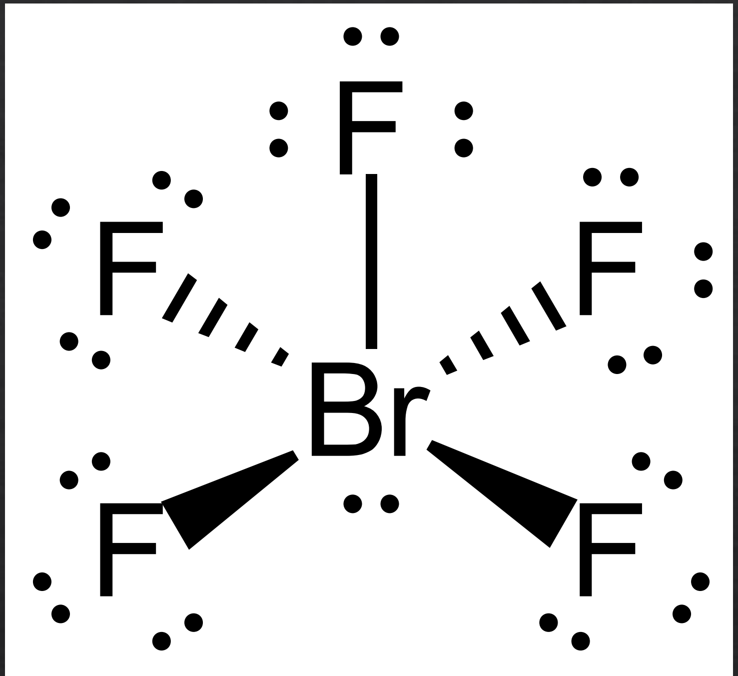
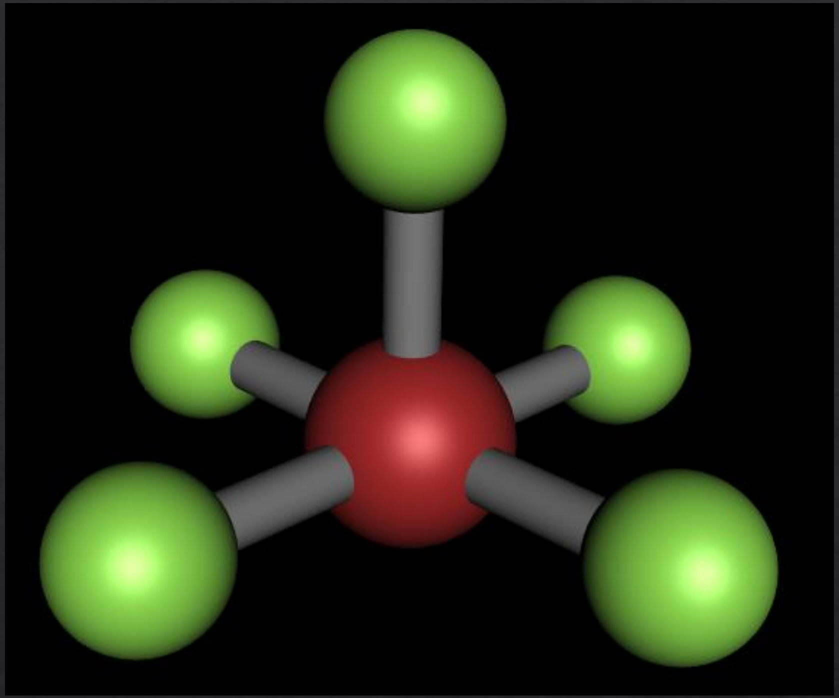
VSEPR HL

BrF_5
bromine
pentafluoride

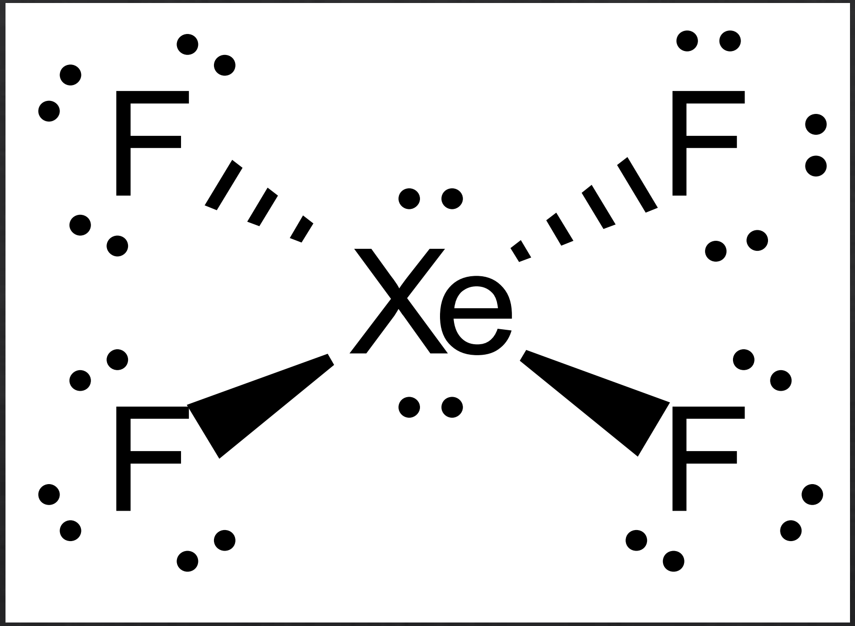


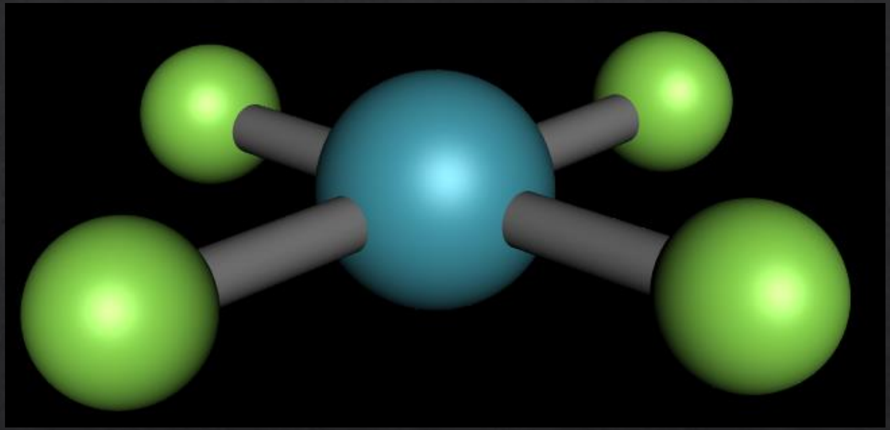


electron domains	bonding domains	lone pairs	electron domain geometry	molecular geometry	bond angle
6	5	1	octahedral	square pyramidal	<90º

VSEPR HL

XeF_4
xenon tetrafluoride





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