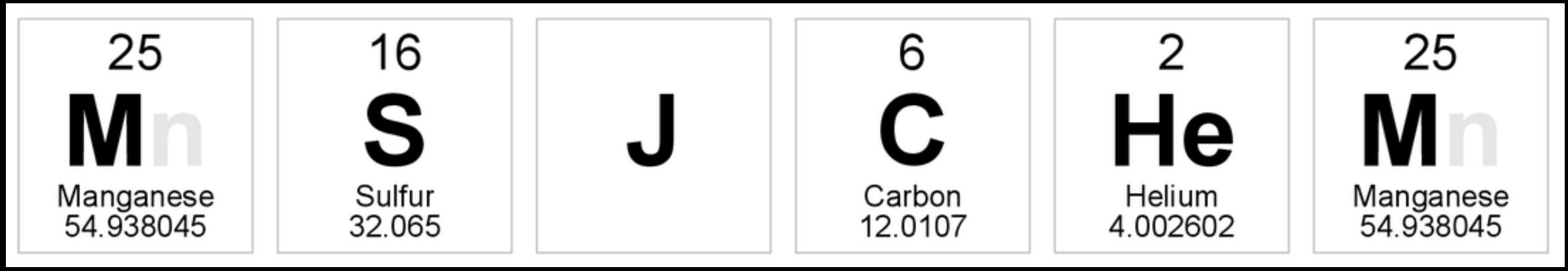
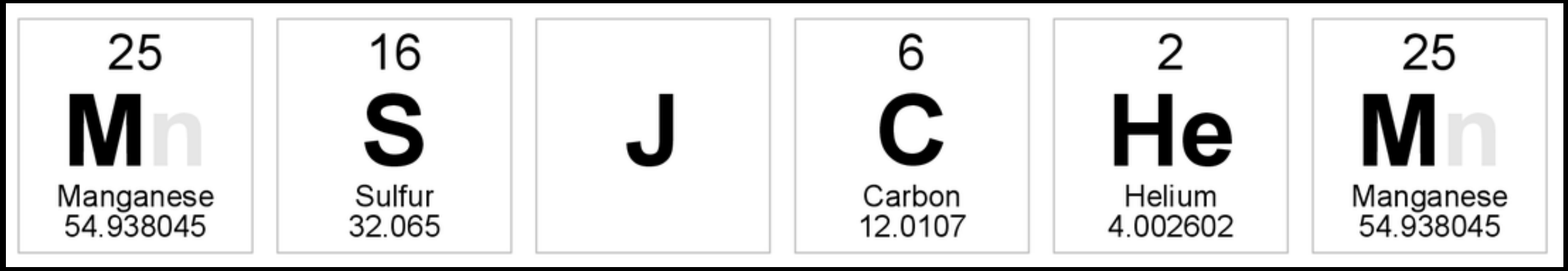


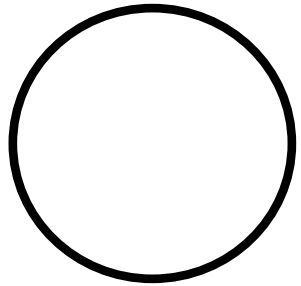
Topic 14
Bonding HL



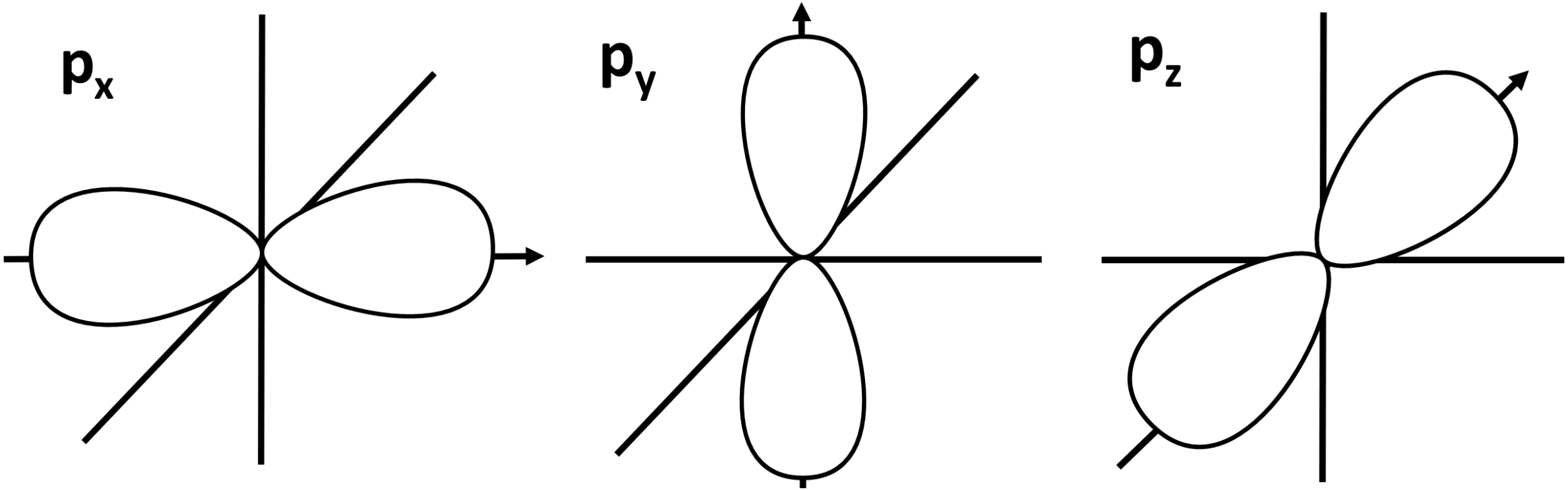
sigma (σ) and pi (π) bonds

sigma (σ) and pi (π) bonds

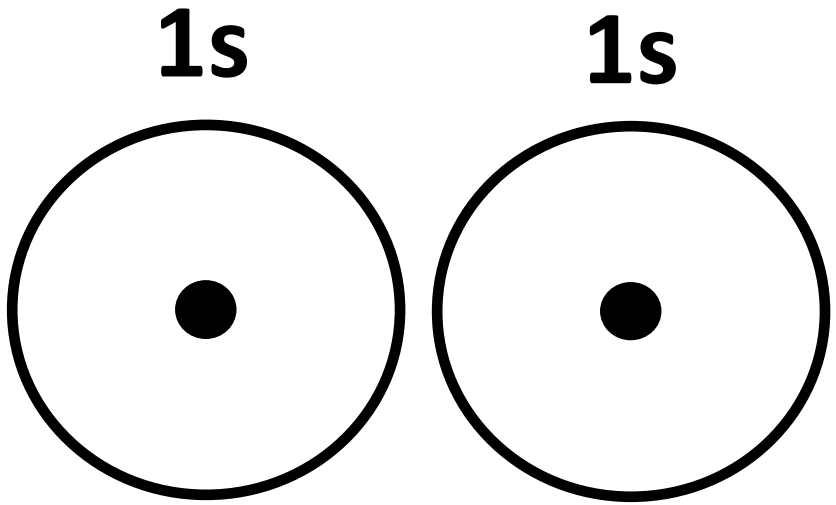
s orbitals are spherical.



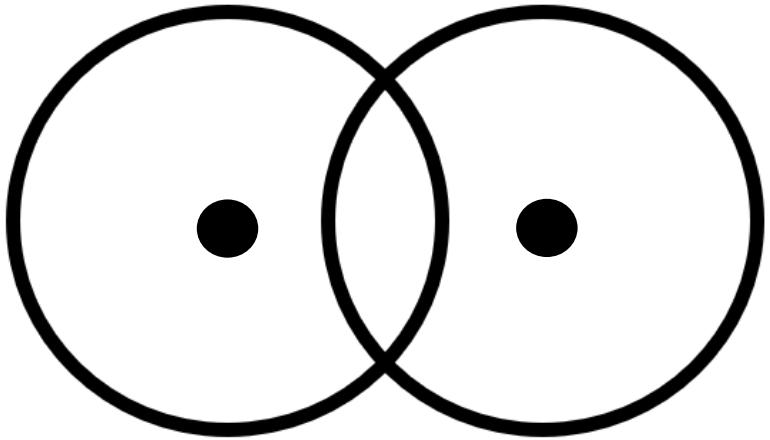
p orbitals are dumbbell shaped.



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.

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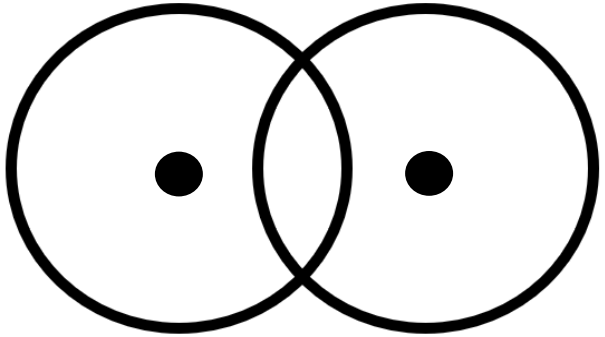
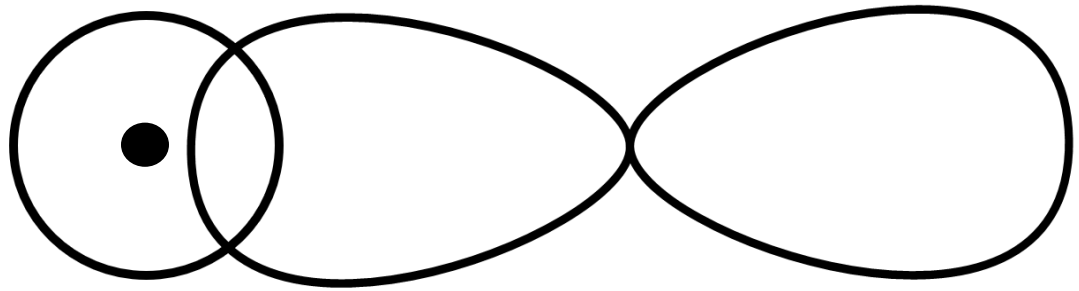
sigma (σ) and pi (π) bonds

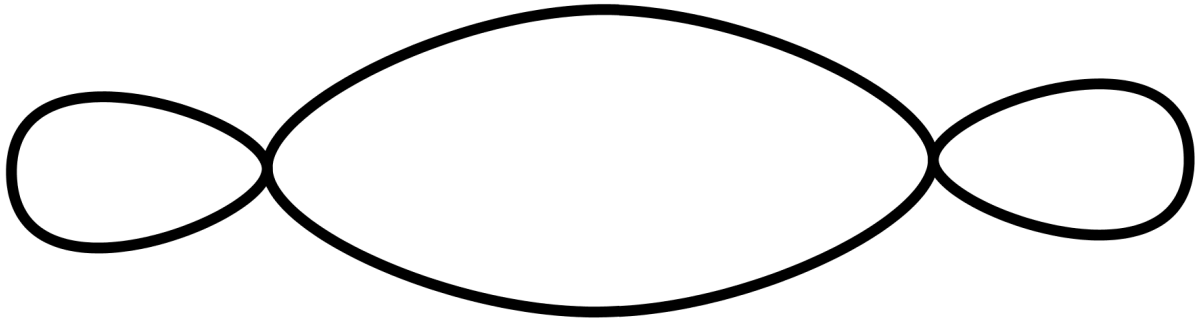
Two s orbitals overlap head-on (s-s)



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

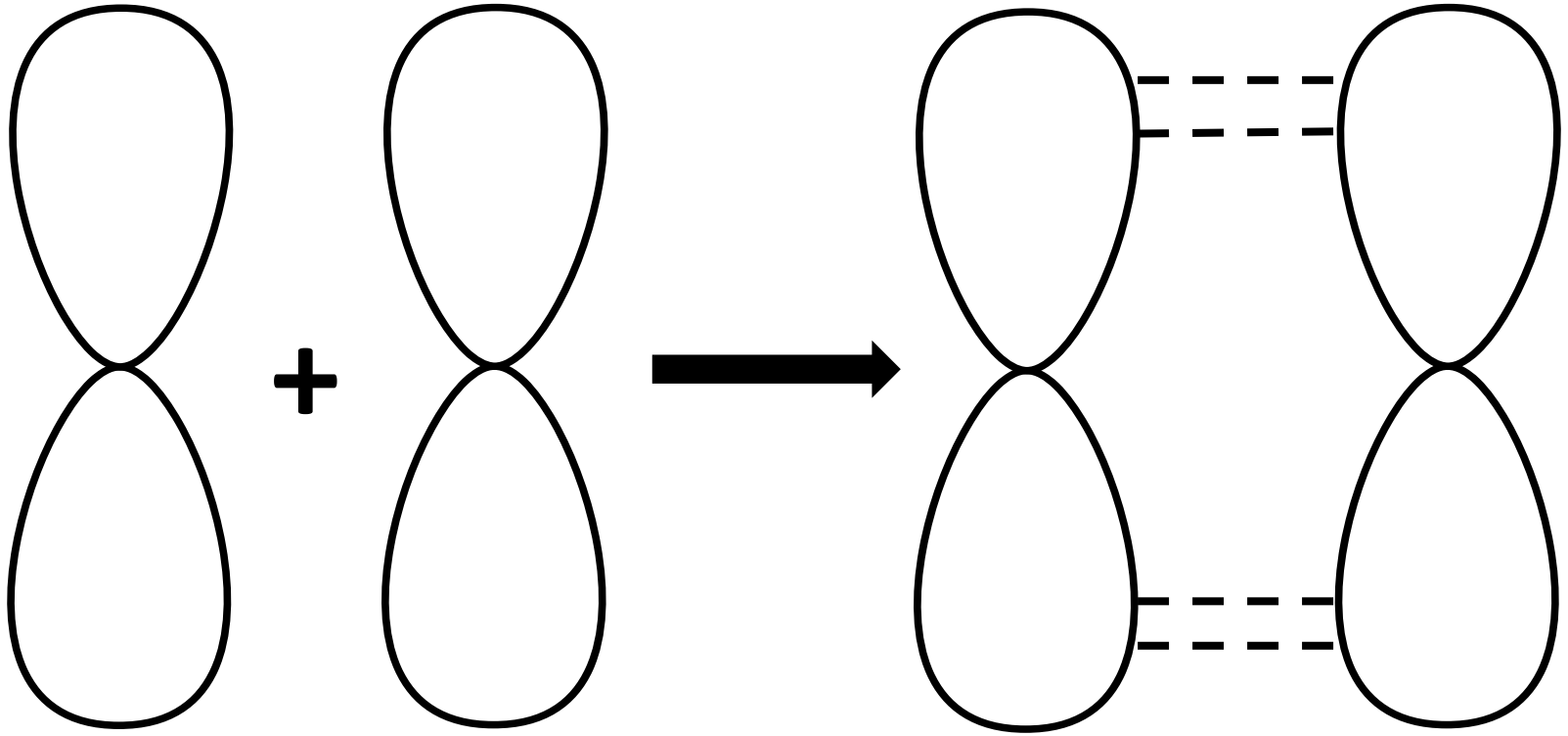


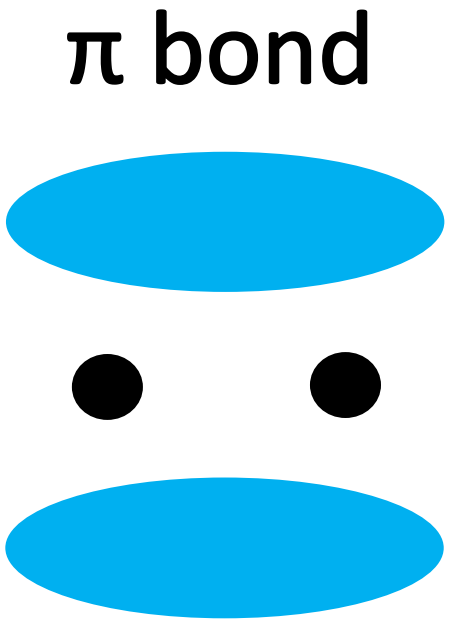
Two p orbitals overlap head-on (p-p)



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.





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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)

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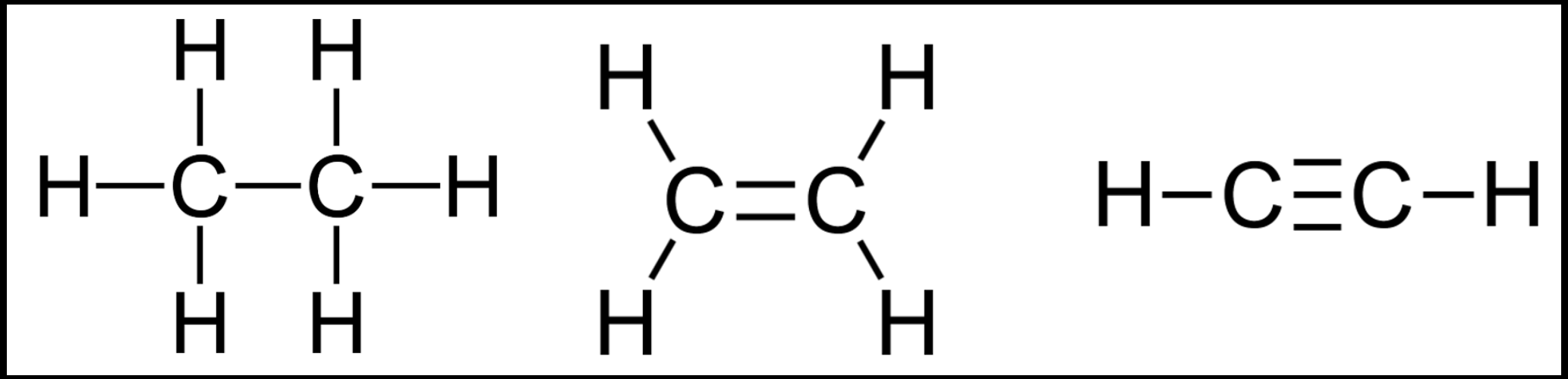
sigma (σ) and pi (π) bonds

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



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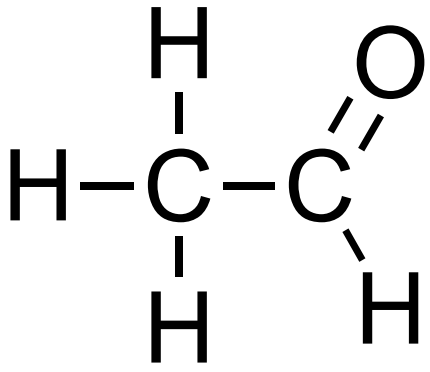
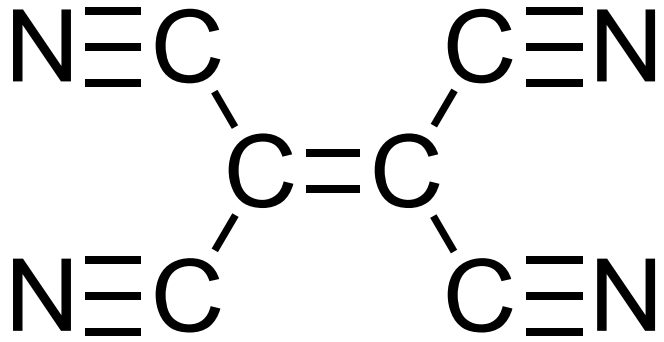
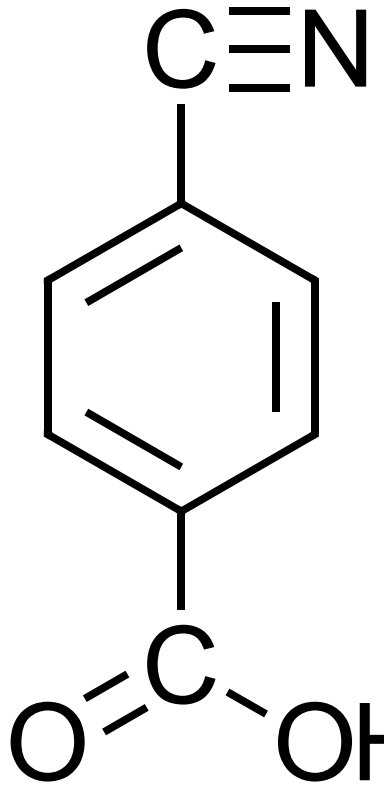
sigma (σ) and pi (π) bonds



6 σ bonds
1 π bond

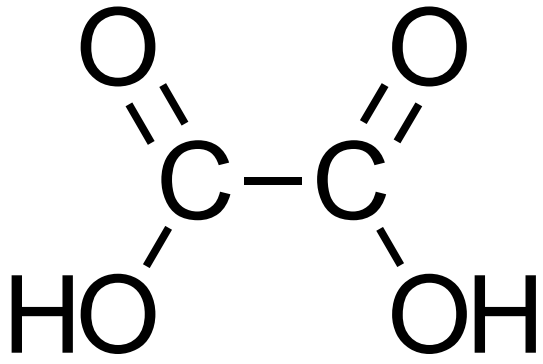


9 σ bonds
9 π bonds



16 σ bonds
6 π bonds

2 σ bonds
2 π bonds



7 σ bonds
2 π bonds

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Hybridisation

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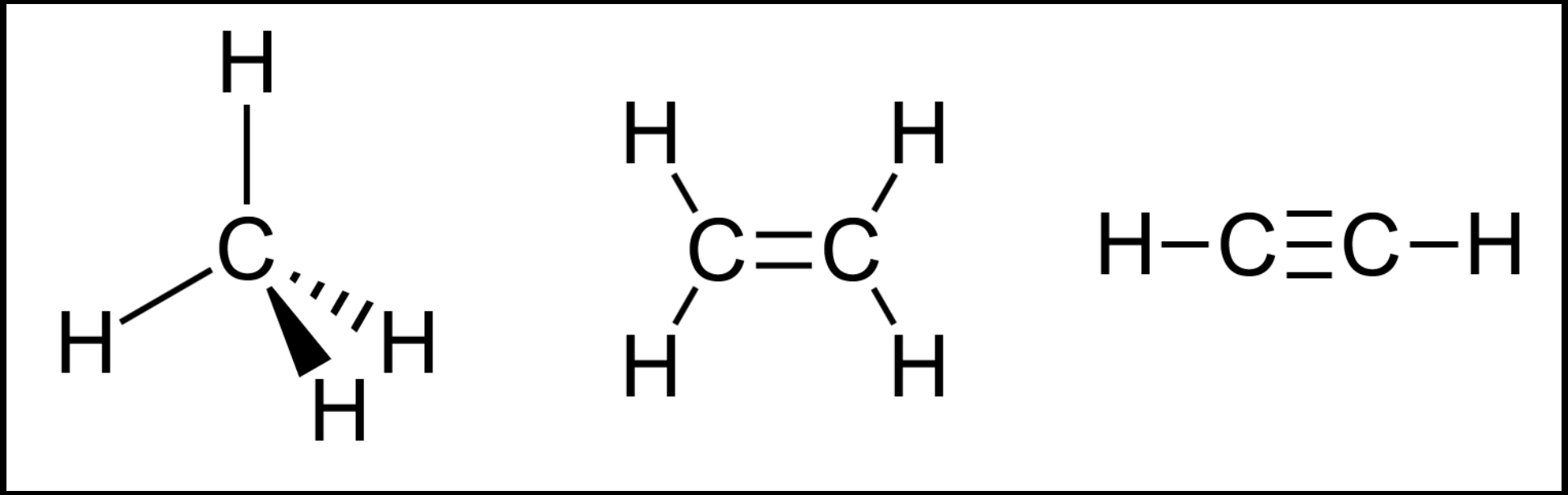
Hybridisation

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



Methane	Ethene	Ethyne
sp^3 hybridisation	sp^2 hybridisation	sp hybridisation

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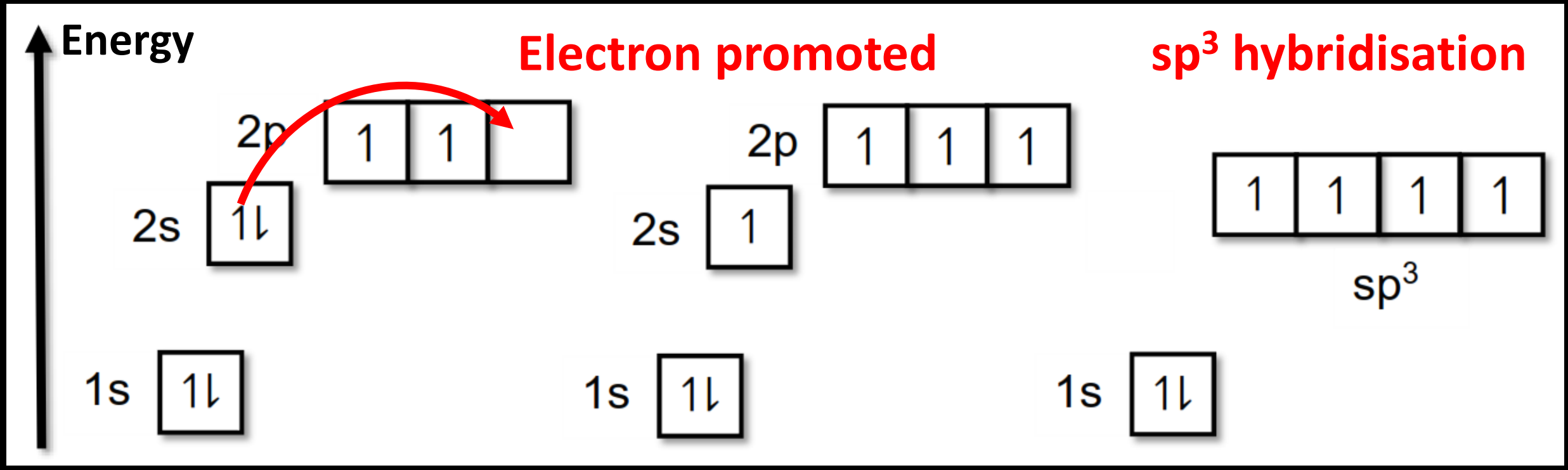
sp^3 hybridisation



Carbon atom in its ground state

Carbon atom in its excited state

Four sp^3 hybrid orbitals

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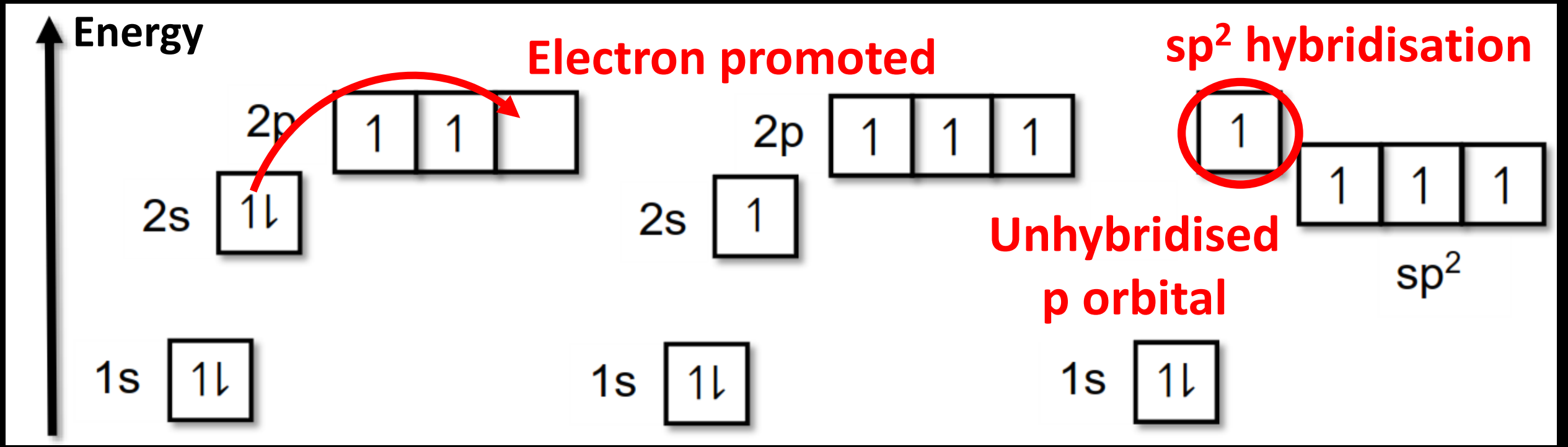
sp^2 hybridisation



Carbon atom in its ground state

Carbon atom in its excited state

Three sp^2 hybrid orbitals

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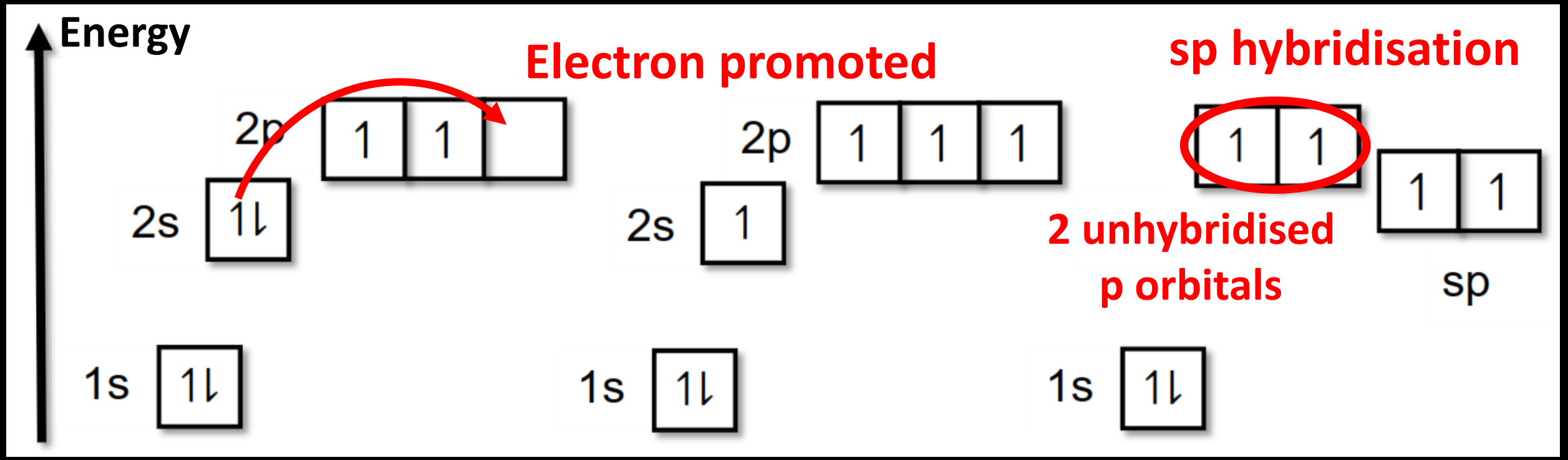
sp hybridisation



Carbon atom in its ground state

Carbon atom in its excited state

Two sp hybrid orbitals

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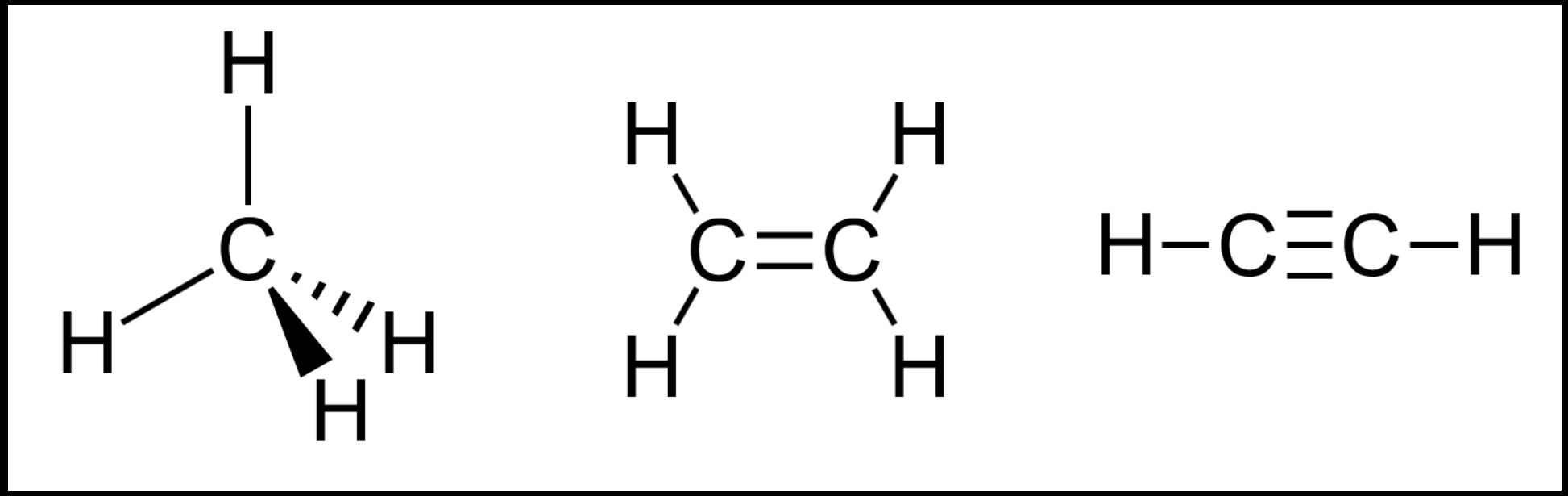
Hybridisation

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



Methane	Ethene	Ethyne
sp^3 hybridisation	sp^2 hybridisation	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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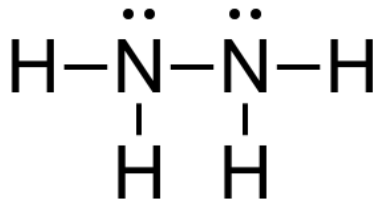
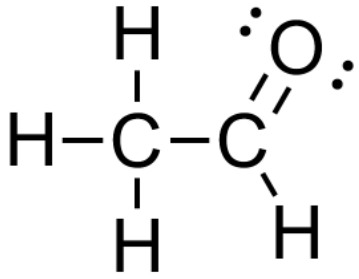
Hybridisation and molecular geometry

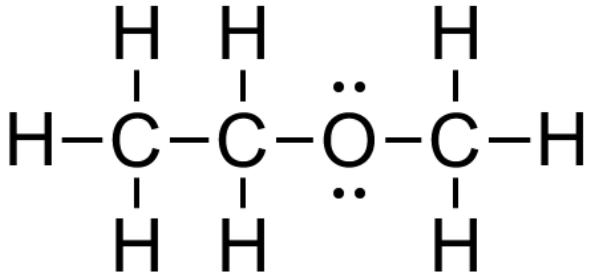
Hydrazine

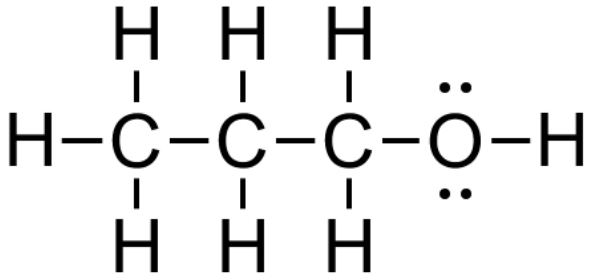


Ethanal

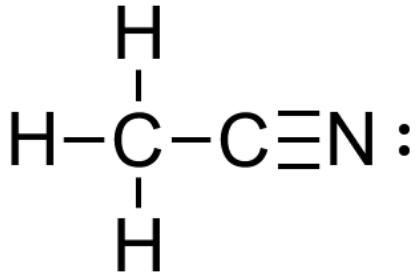


Methoxyethane



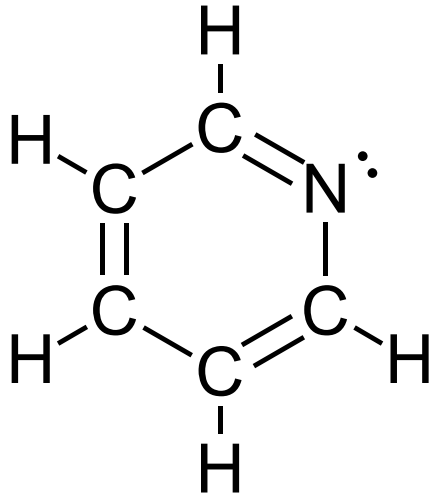


Propan-1-ol



Ethanenitrile

Pyridine



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Molecules with delocalised π electrons

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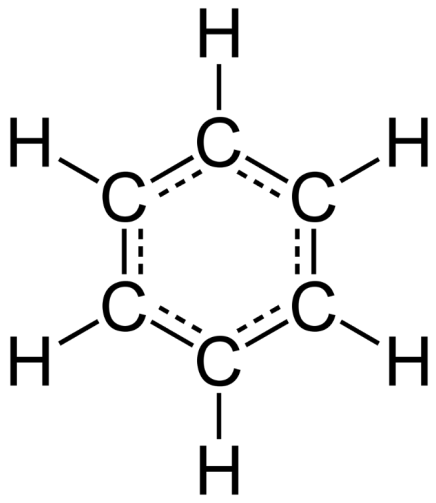
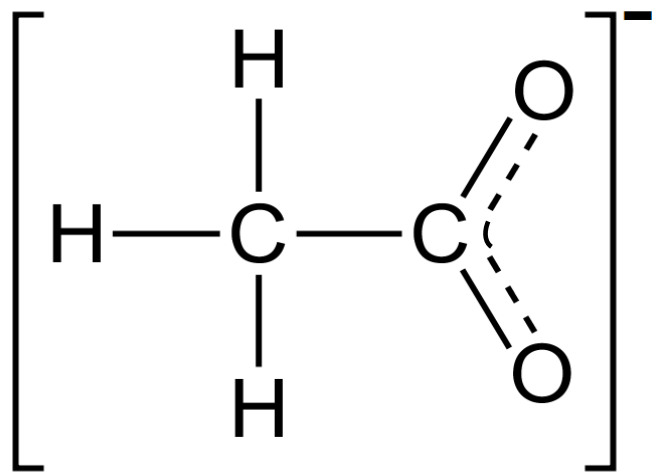
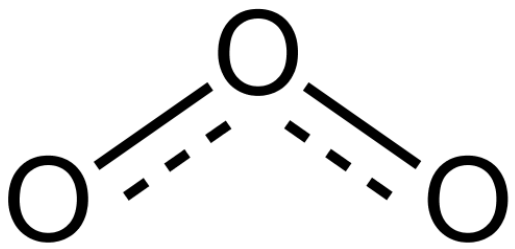
Delocalised π electrons

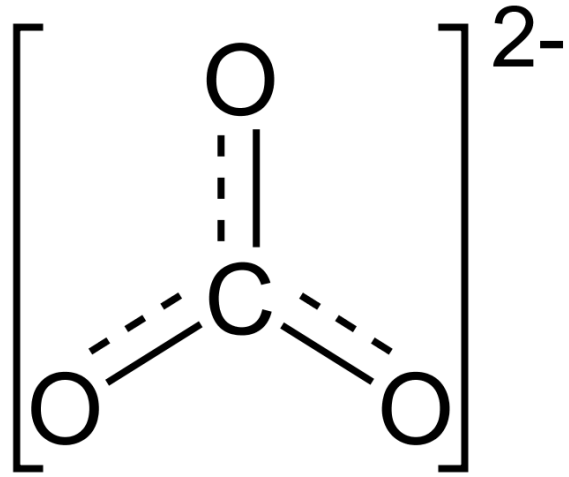
Delocalised π electrons are electrons that are shared between more than two nuclei.

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









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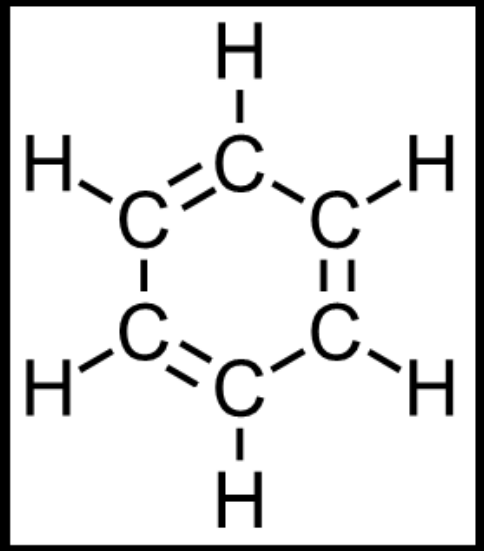
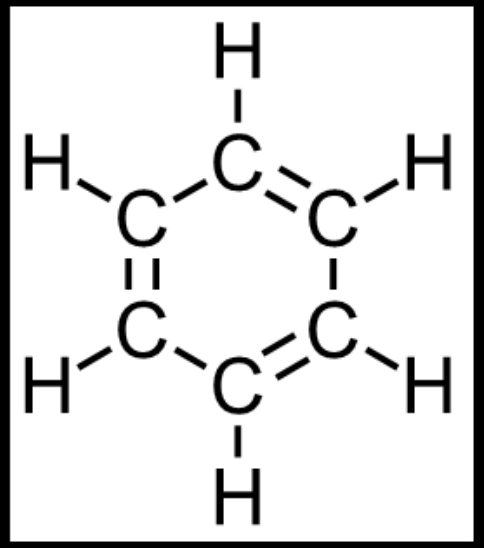
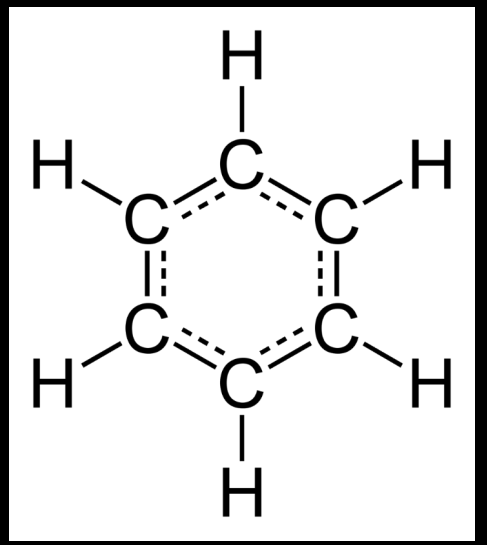
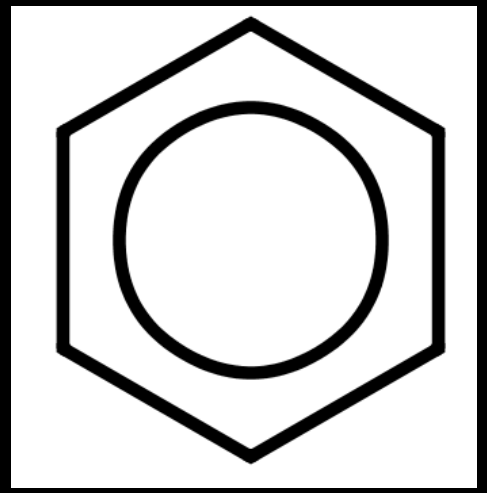
Delocalised π electrons

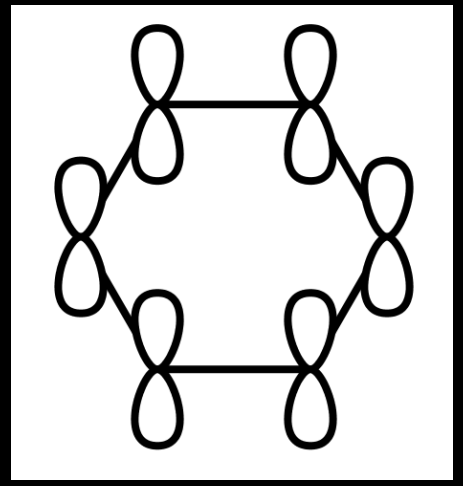
Benzene C_6H_6

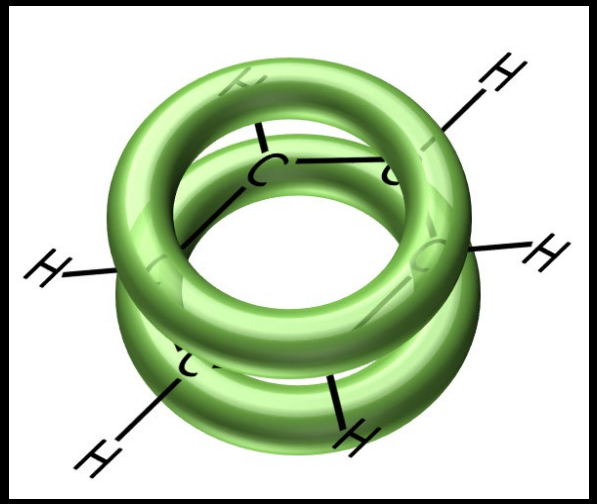












Benzene contains a total of 6 pi electrons - one from each unhybridised p orbital.

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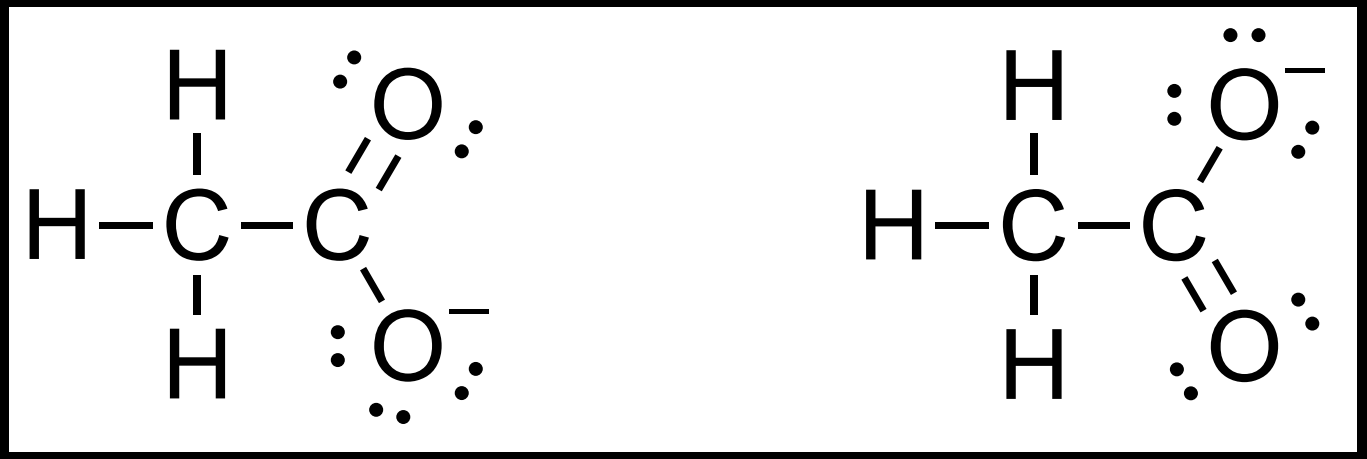
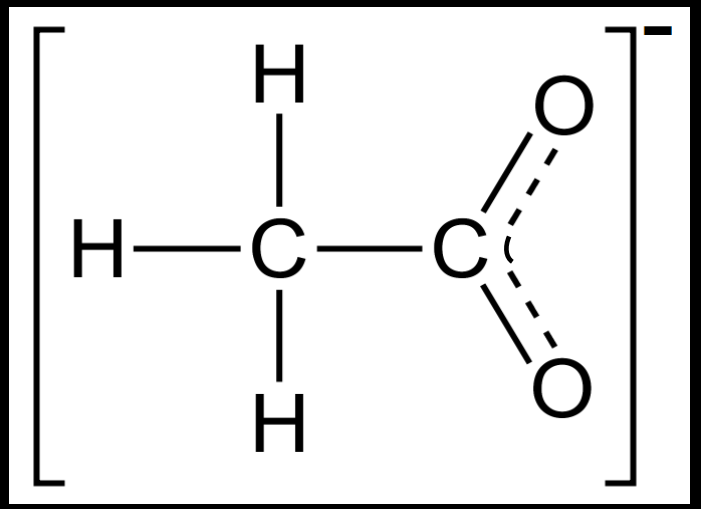
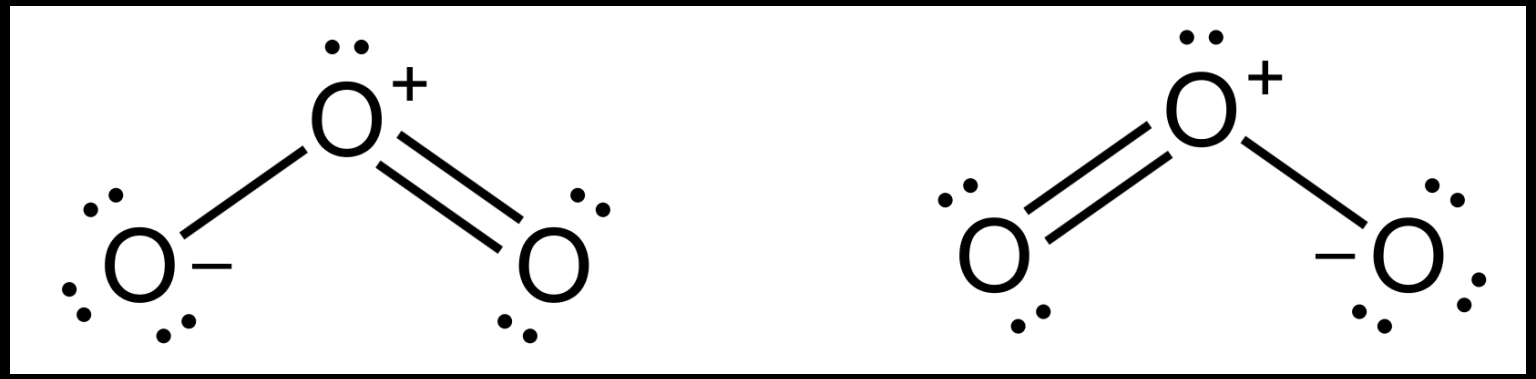
Delocalised π electrons

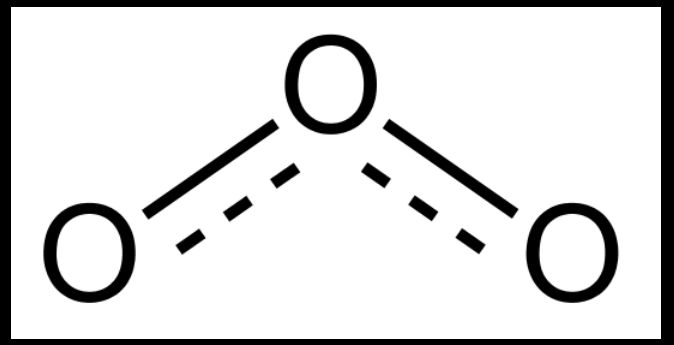
Ethanoate ion CH_3COO^-





Ozone, O_3





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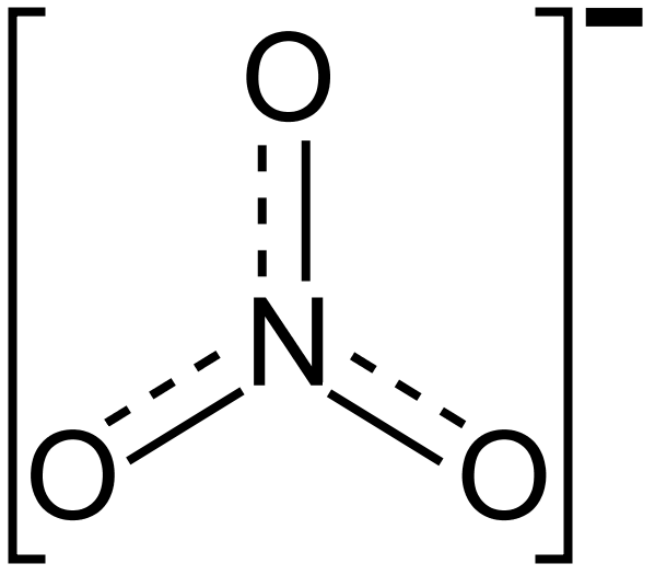
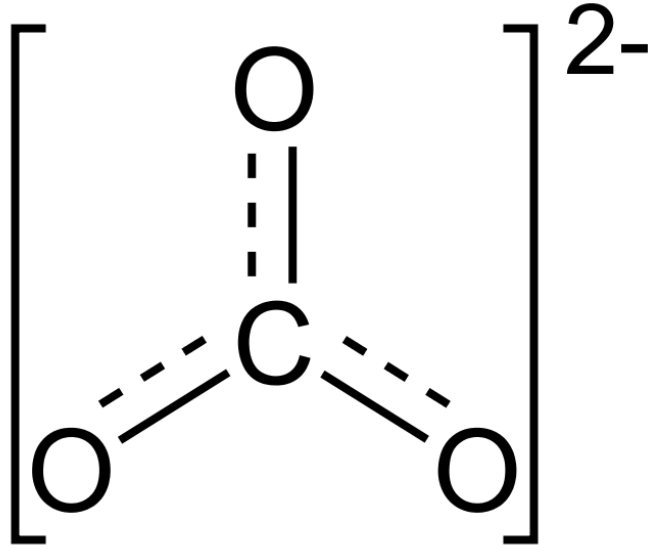
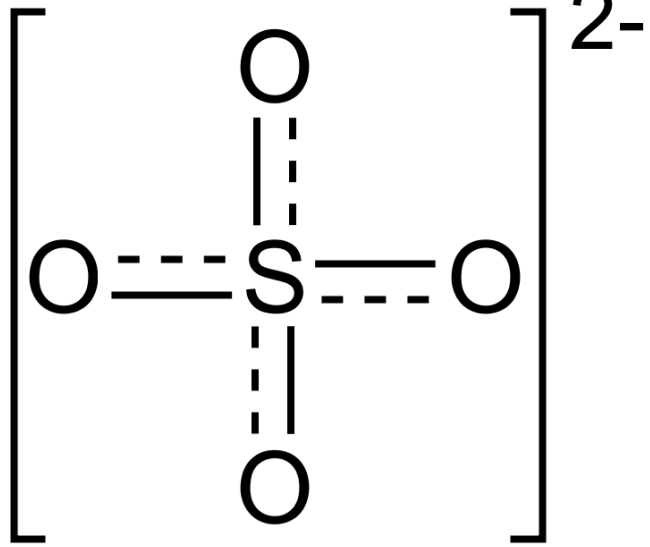
Delocalised π electrons

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.

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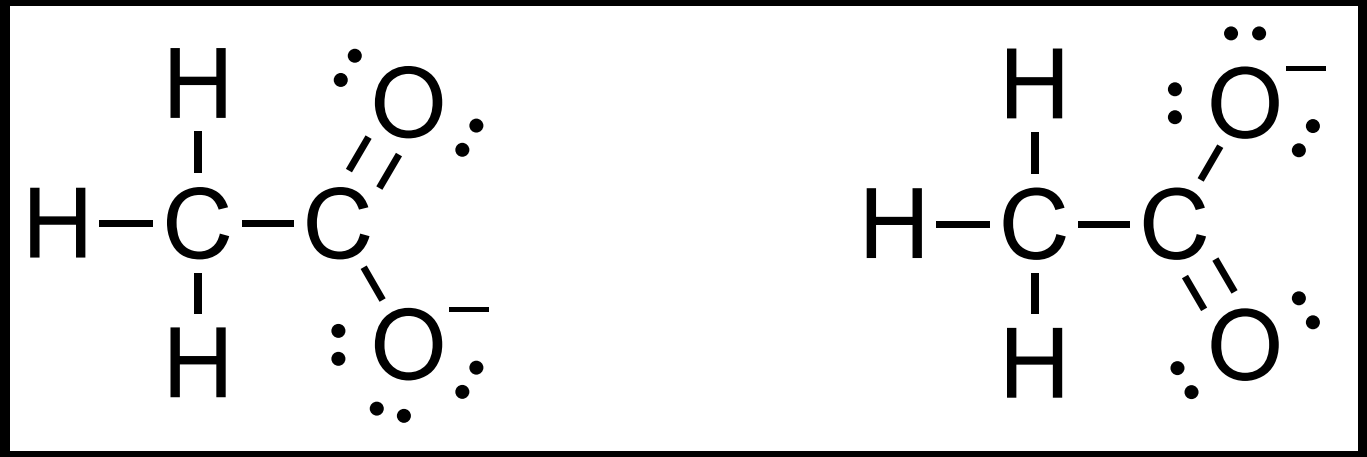
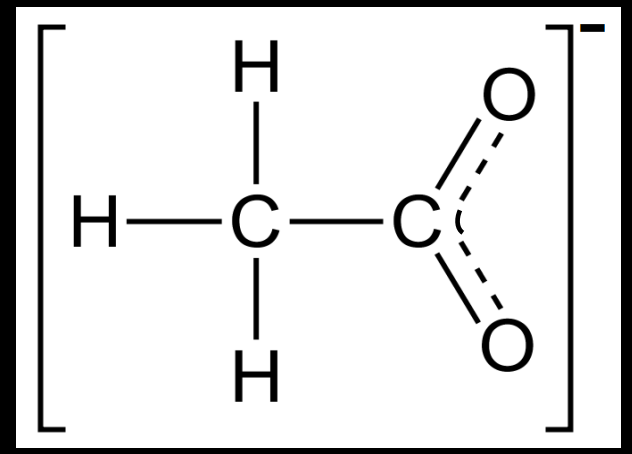
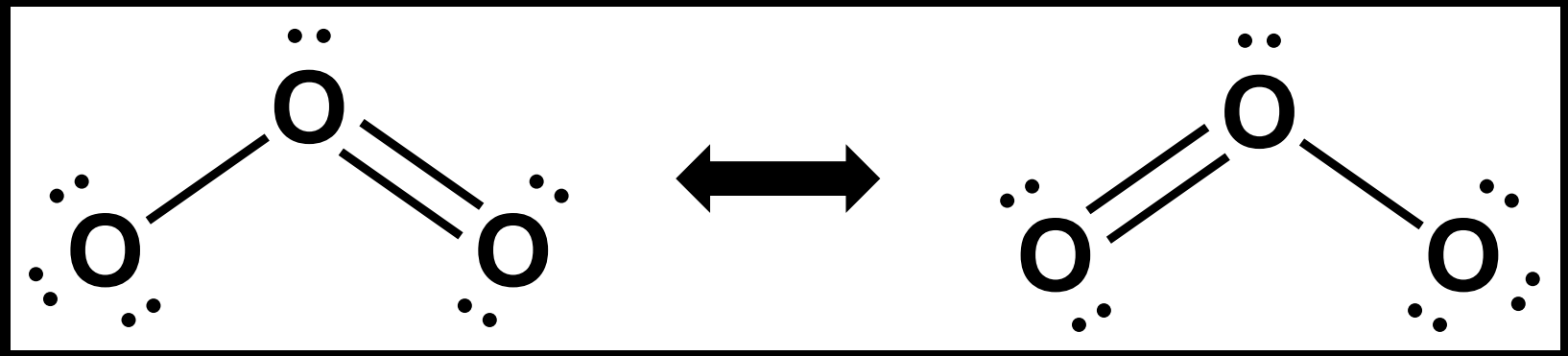
Delocalised π electrons

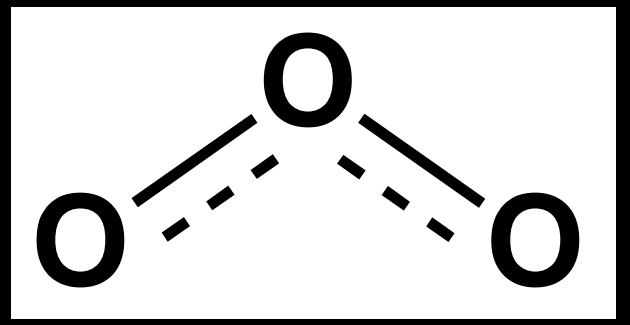
Ethanoate ion CH_3COO^-





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.

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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 ½ bonding electrons

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

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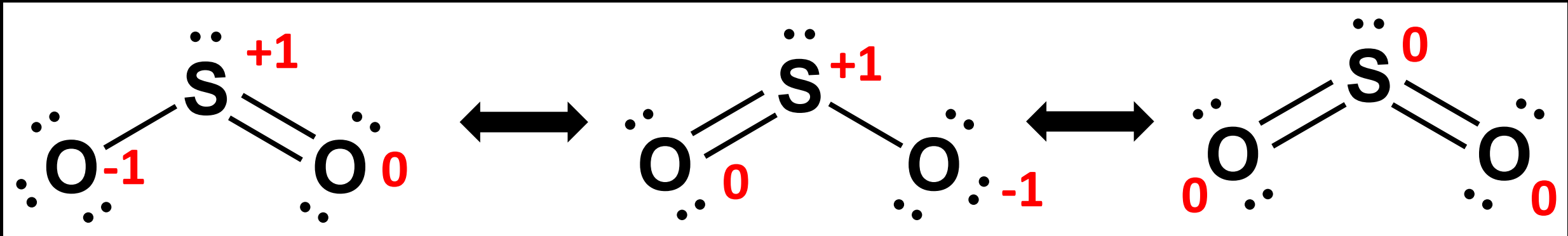
Formal charge

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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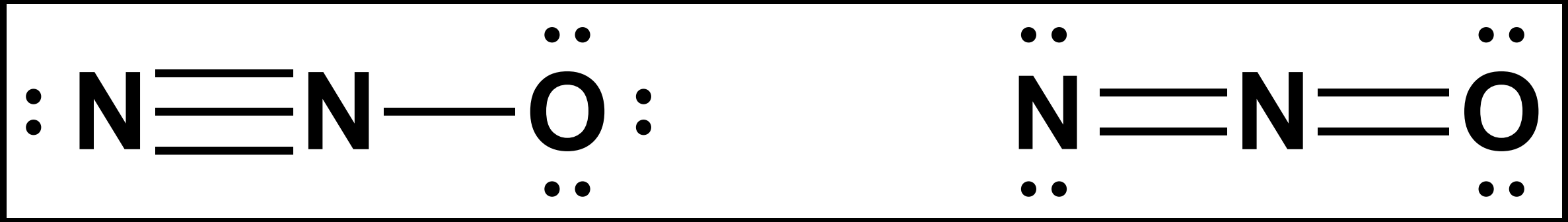
Formal charge

Two possible Lewis structures for N_2O are shown below.



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

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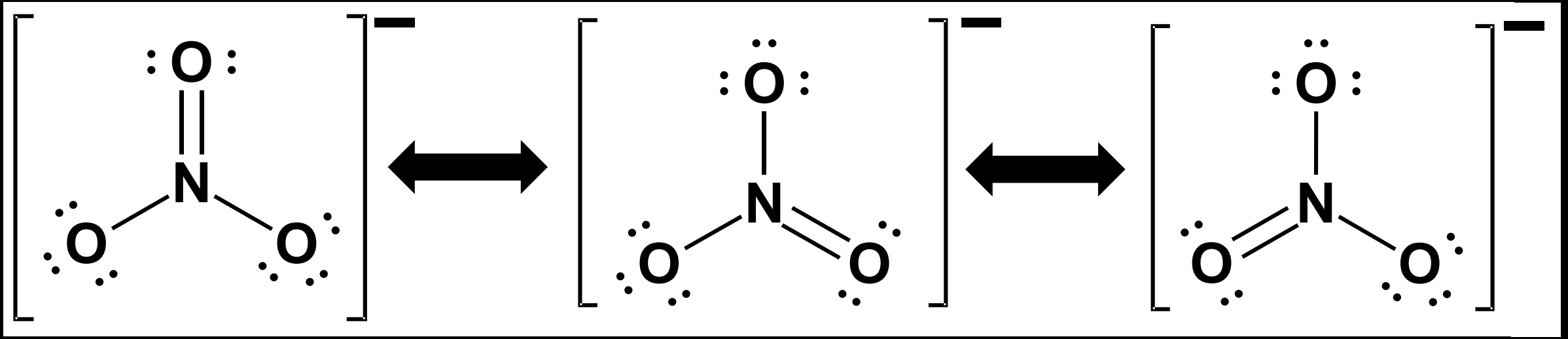
Formal charge

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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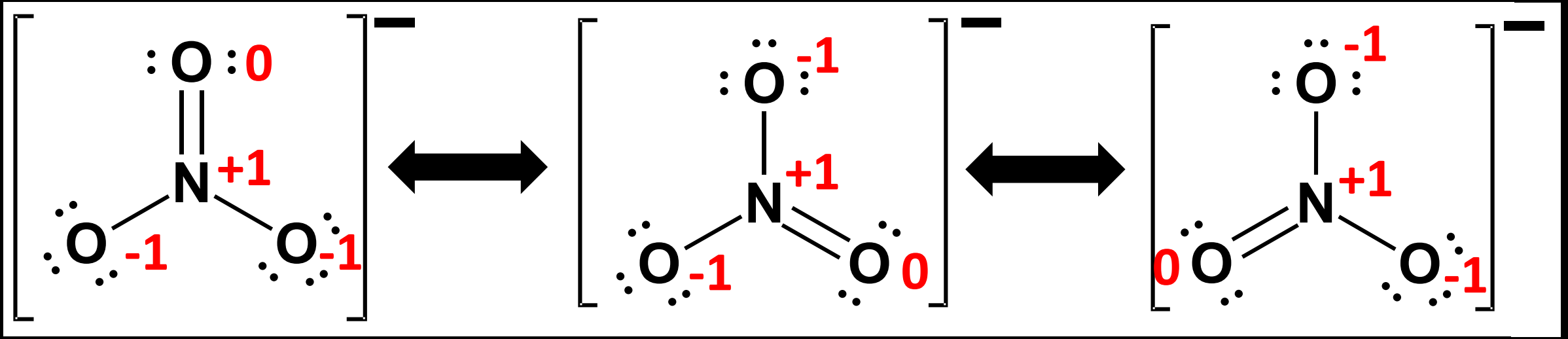
Formal charge

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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Calculating wavelength from bond enthalpy values

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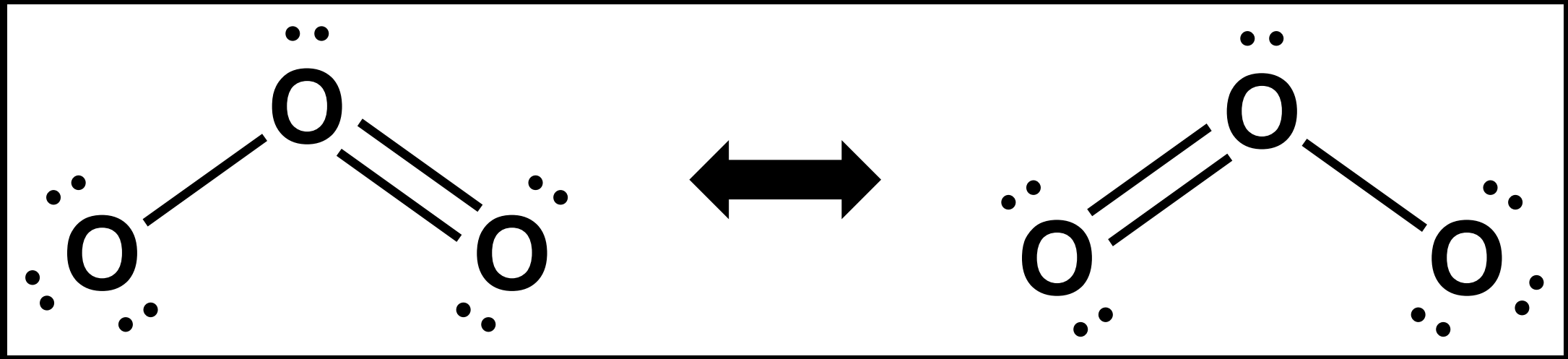
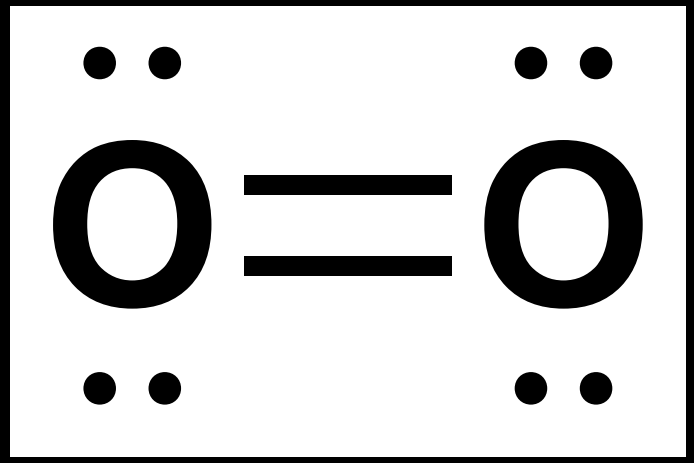
Calculating λ from bond enthalpy

Ozone, O_3, exists as two resonance structures.





Bond	Bond enthalpy (kJ mol^{-1})
O-O in O_3	364
O=O in O_2	498

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Calculating λ from bond enthalpy

$$E = h\nu$$

$$c = \nu\lambda$$

E – energy (J)

h – Planck's constant

6.63×10^{-34} J•s

ν – frequency (s^{-1})

c – speed of light

3.00×10^{8} m s^{-1}

λ – wavelength (m)

ν – frequency (s^{-1})

$$\lambda = \frac{hc}{E}$$

Calculating λ from bond enthalpy

$$\lambda = \frac{(6.63 \times 10^{-34}\ \mathrm{J}\ s)\ (3.00 \times 10^{8}\ m\ s^{-1})}{E}$$

$$E = \frac{498\ \mathrm{kJ\ mol^{-1}} \times 1000}{6.02 \times 10^{23}\ \mathrm{mol^{-1}}}$$

Calculating λ from bond enthalpy

$$\lambda = \frac{(6.63 \times 10^{-34}\ \mathrm{J}\ s)\ (3.00 \times 10^{8}\ m\ s^{-1})}{\frac{498\ \mathrm{kJ\ mol^{-1}} \times 1000}{6.02 \times 10^{23}\ \mathrm{mol^{-1}}}}$$

$$\lambda = 2.40 \times 10^{-7} m$$

$$\lambda = 240\ nm$$

Calculating λ from bond enthalpy

$$\lambda = \frac{(6.63 \times 10^{-34}\ \mathrm{J}\ s)\ (3.00 \times 10^{8}\ m\ s^{-1})}{E}$$

$$E = \frac{364\ \mathrm{kJ\ mol^{-1}} \times\ 1000}{6.02 \times 10^{23}\ \mathrm{mol^{-1}}}$$

Calculating λ from bond enthalpy

$$\lambda = \frac{(6.63 \times 10^{-34}\ \mathrm{J}\ s)\ (3.00 \times 10^{8}\ m\ s^{-1})}{\frac{364\ \mathrm{kJ\ mol^{-1}} \times\ 1000}{6.02 \times 10^{23}\ \mathrm{mol^{-1}}}}$$

$$\lambda = 3.30 \times 10^{-7} m$$

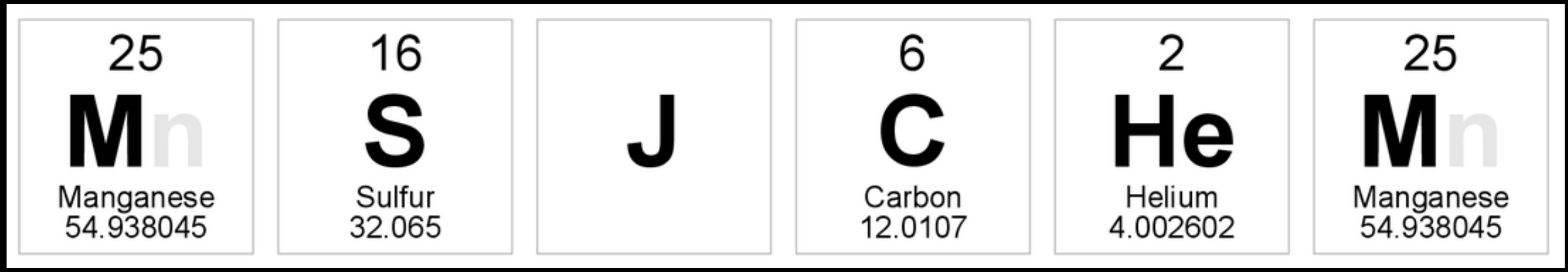
$$\lambda = 330\ nm$$

Calculating λ from bond enthalpy

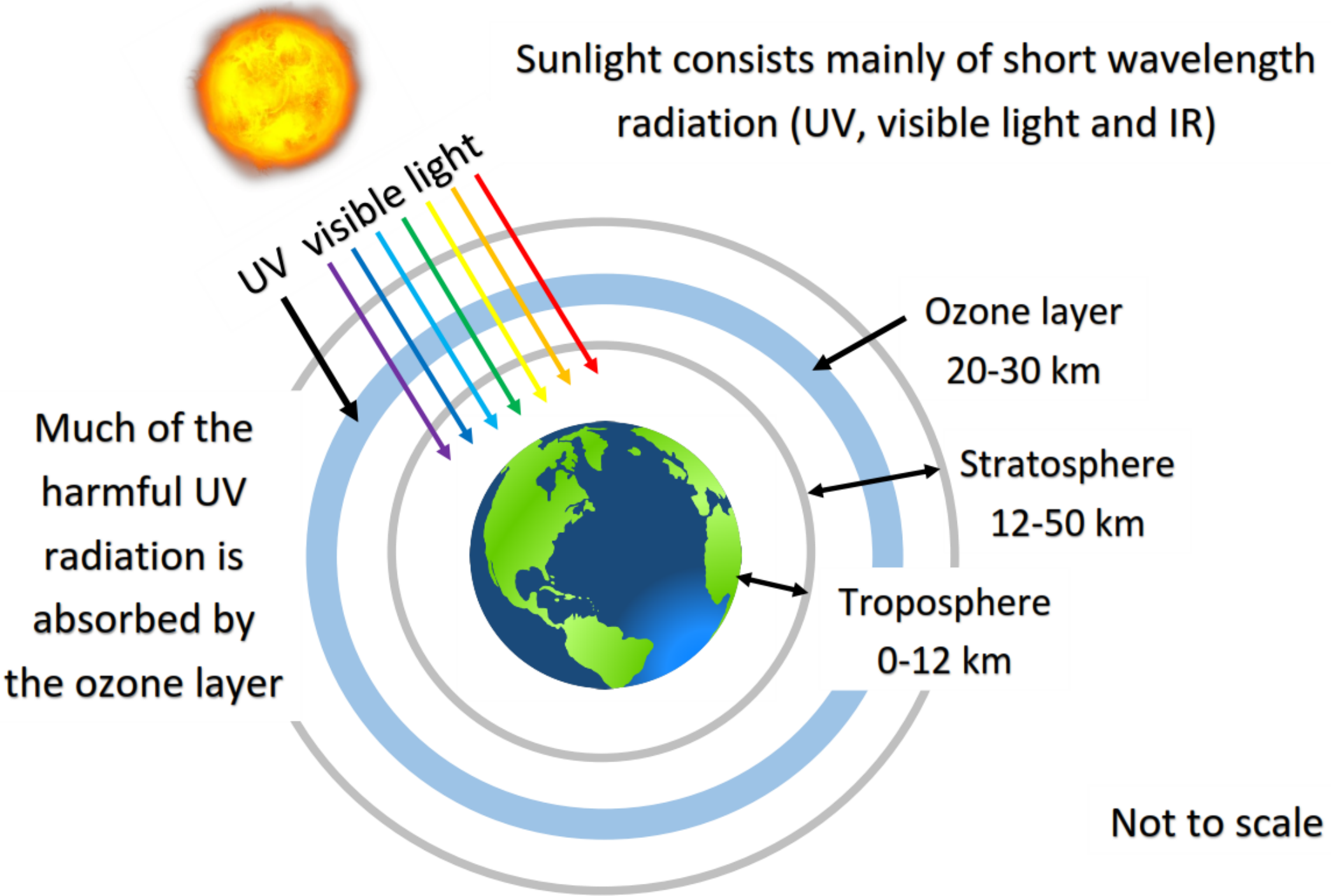
Bond	Bond enthalpy ($kJ\ mol^{-1}$)	λ (m) absorbed by one bond
O-O in O_3	364	3.30×10^{-7}
O=O in O_2	498	2.40×10^{-7}

The stronger double bond in O_2 absorbs shorter wavelength UV radiation.

The weaker bonds in O_3 absorb longer wavelength UV radiation.



Catalytic destruction of ozone (NO and CFCs)


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

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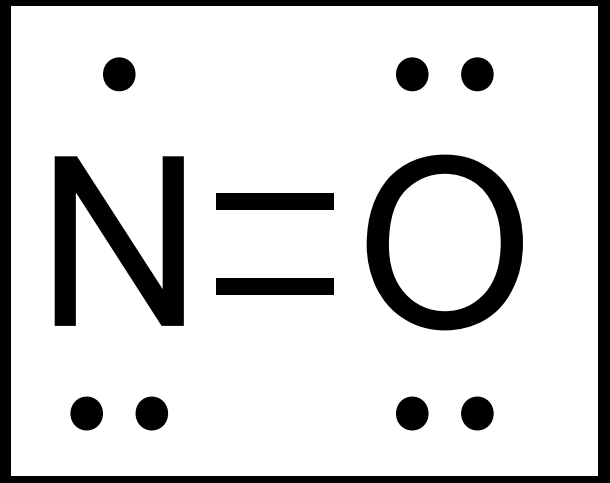
Catalytic destruction of ozone

NO in the stratosphere is produced in jet engines by the reaction of nitrogen and oxygen at high temperatures.

$$N_{2(g)} + O_{2(g)} \rightarrow 2NO_{(g)}$$



Free radicals (radicals) are highly reactive species that have unpaired electrons.

Catalytic destruction of ozone

NO in the stratosphere is produced in jet engines by the reaction of nitrogen and oxygen at high temperatures.

$$N_{2(g)} + O_{2(g)} \rightarrow 2NO_{(g)}$$

$$\cdot NO_{(g)} + O_{3(g)} \rightarrow \cdot NO_{2(g)} + O_{2(g)}$$

$$\cdot NO_{2(g)} + O_{3(g)} \rightarrow \cdot NO_{(g)} + 2O_{2(g)}$$

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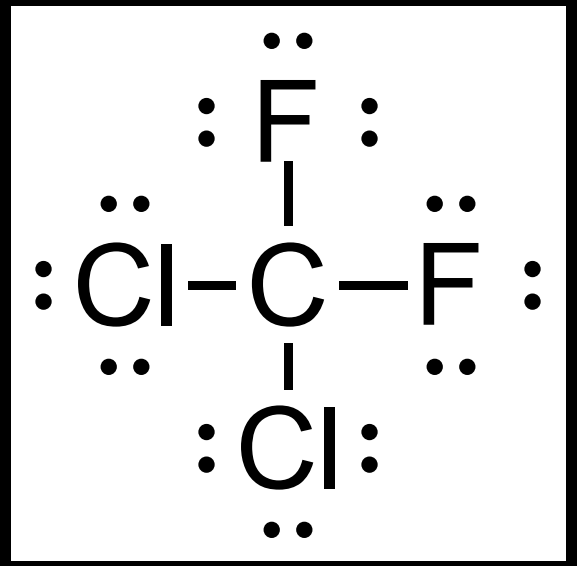
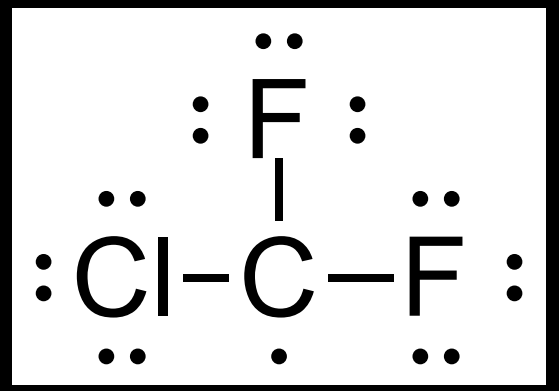
Catalytic destruction of ozone

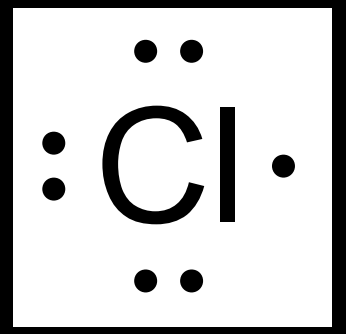
CFCs were widely used in aerosols, refrigerants, solvents and plastics due to their low toxicity, low flammability and lack of reactivity.

Freon-12



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





Catalytic destruction of ozone

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

$$Cl^{\cdot}_{(g)} + O_{3(g)} \rightarrow ClO^{\cdot}_{(g)} + O_{2(g)}$$

$$ClO^{\cdot}_{(g)} + O^{\cdot}_{(g)} \rightarrow O_{2(g)} + Cl^{\cdot}_{(g)}$$

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Molecular geometry (HL)

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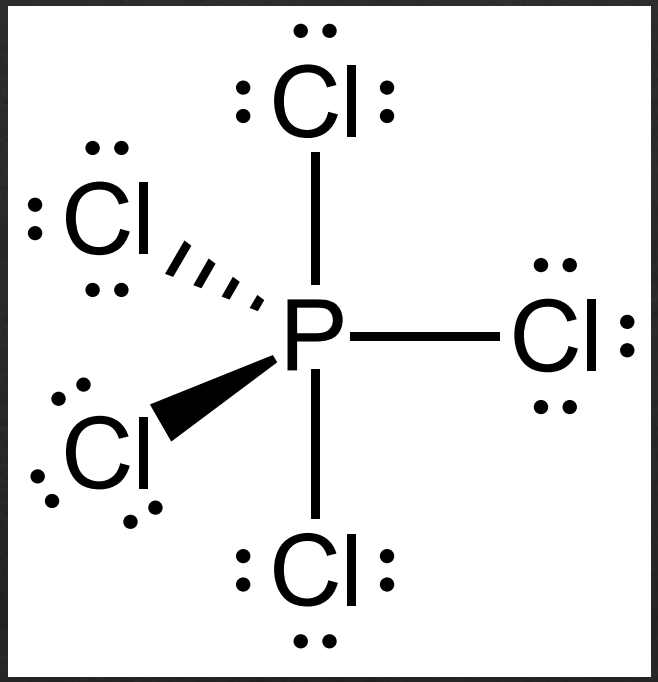
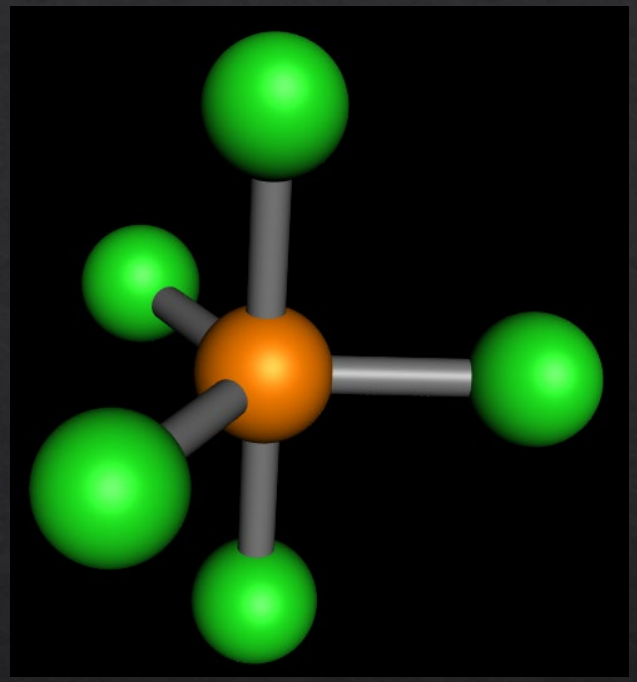
VSEPR HL

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

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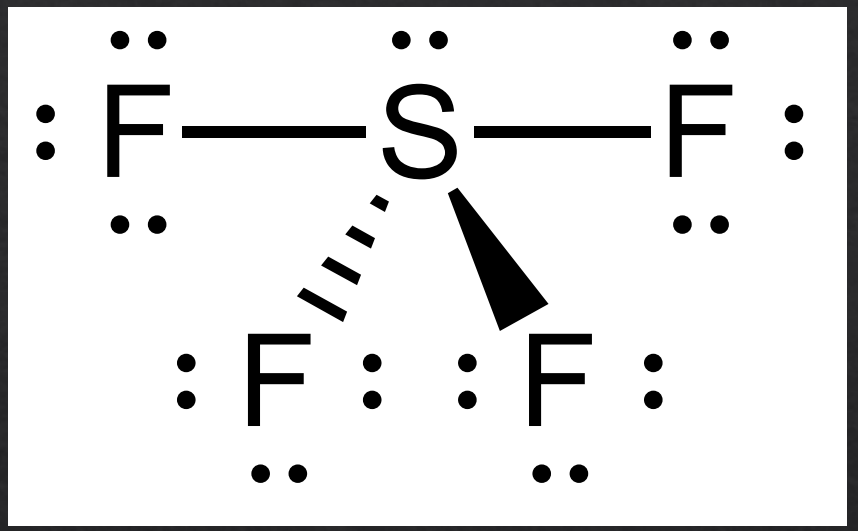
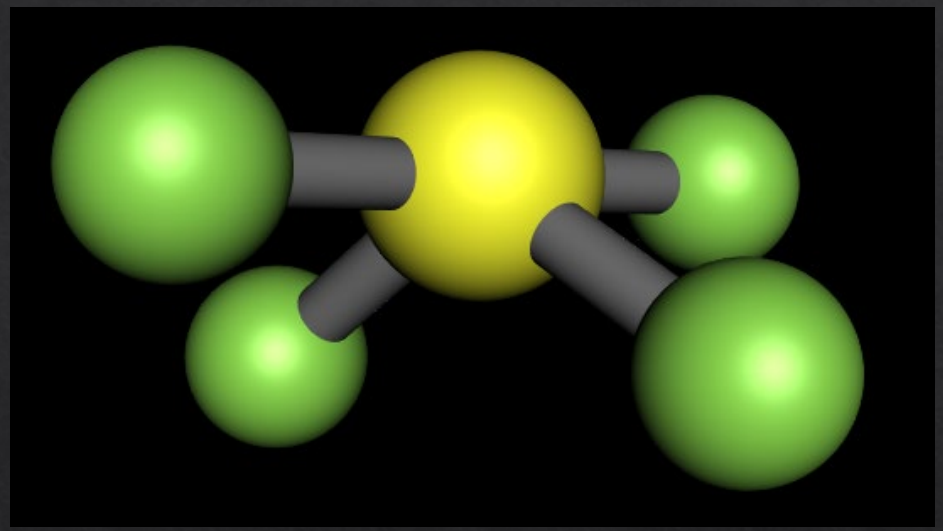
SF_4
sulfur
tetrafluoride





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

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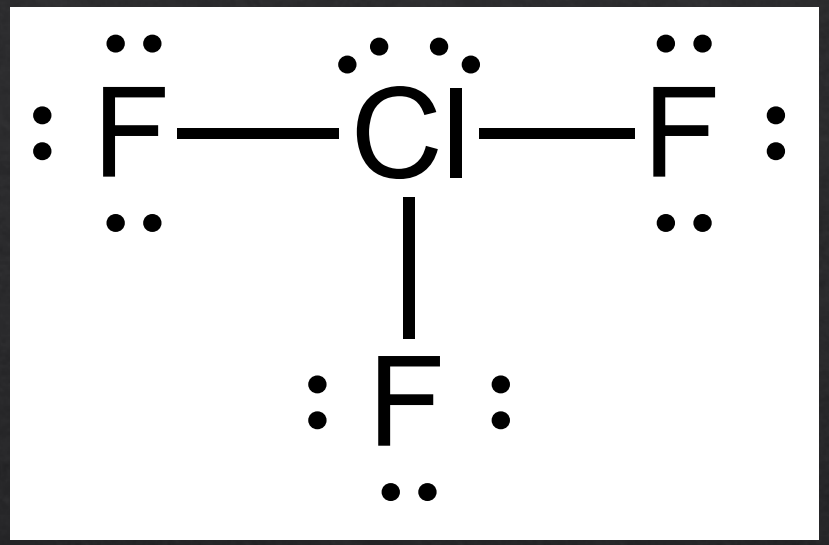
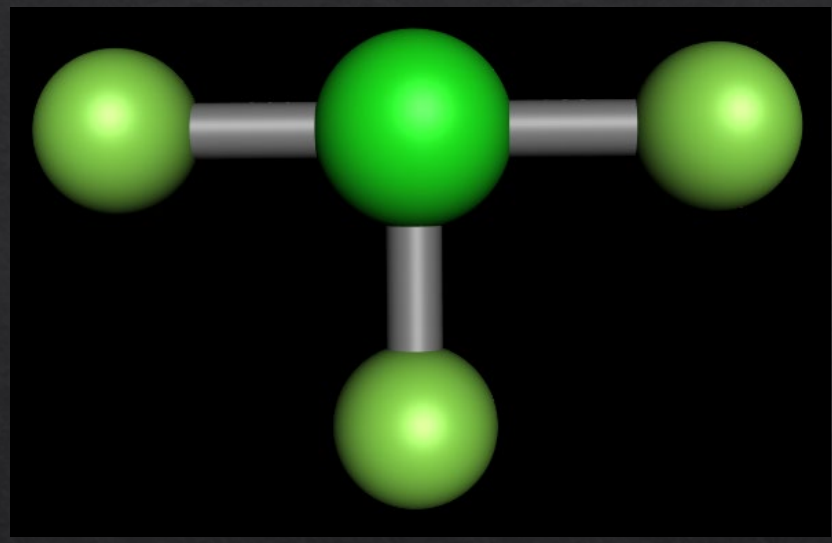
VSEPR HL

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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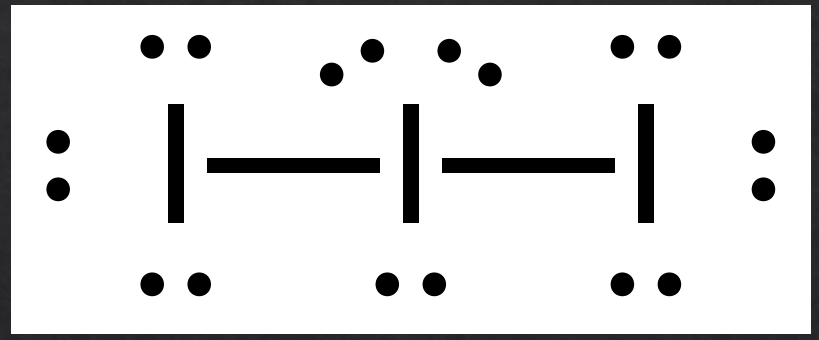
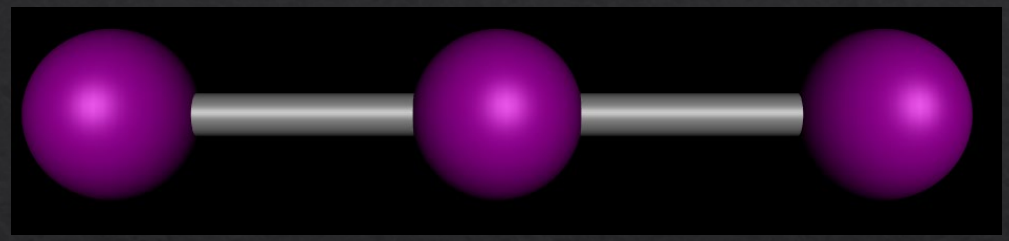
VSEPR HL

I_3^-
triiodide ion





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

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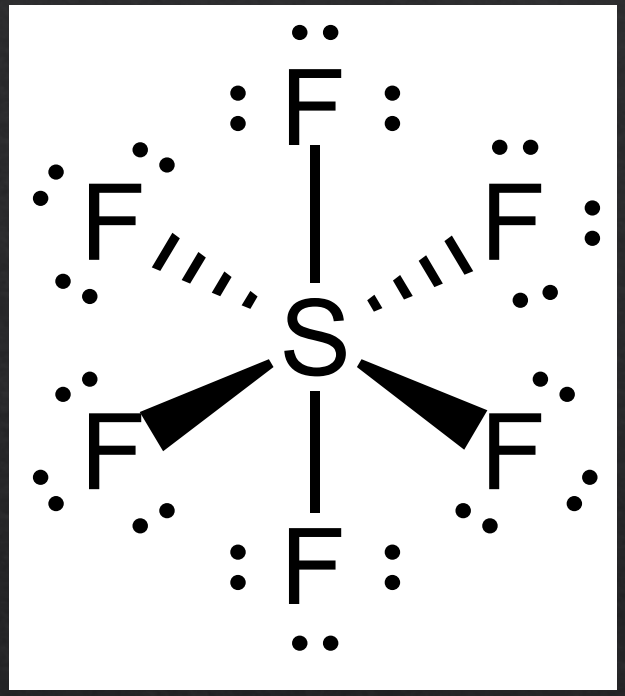
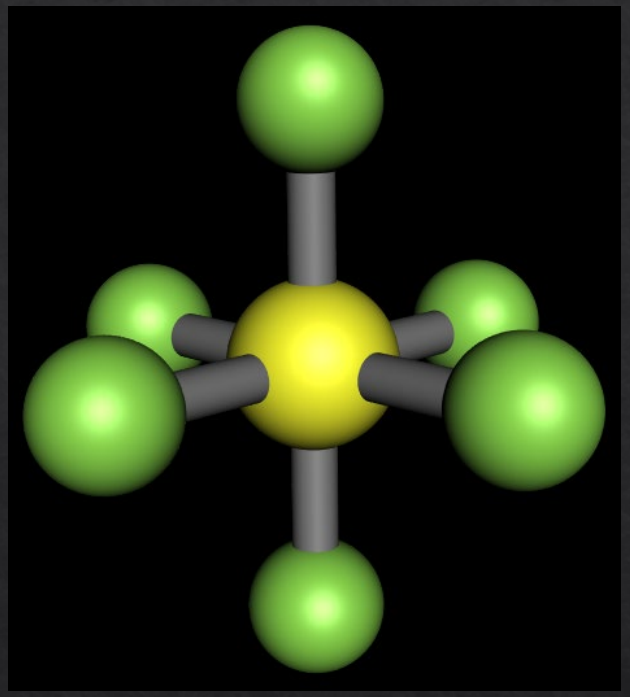
VSEPR HL

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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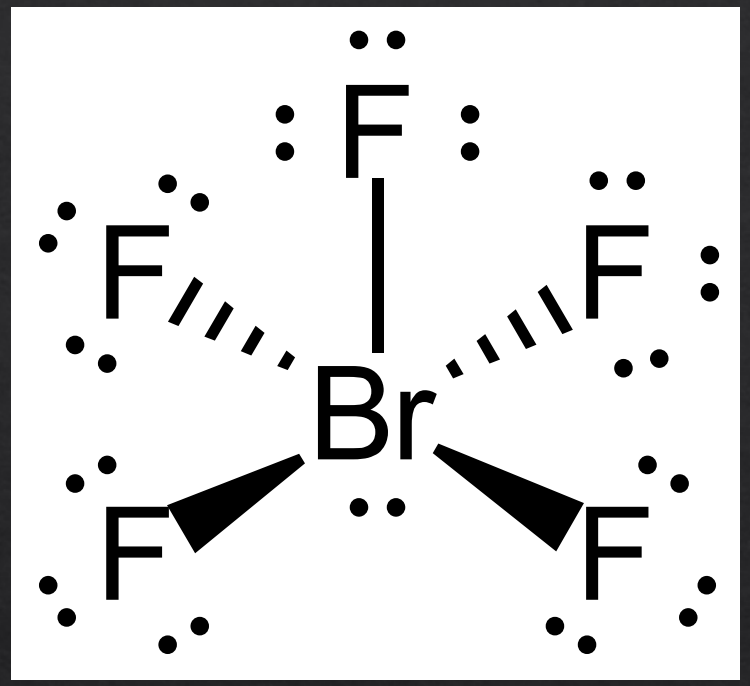
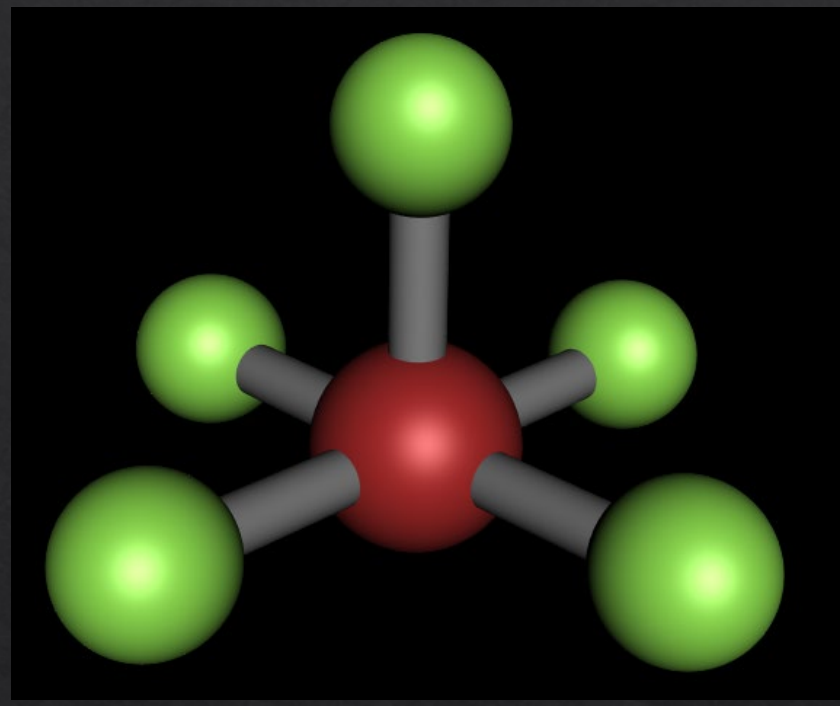
VSEPR HL

BrF_5
bromine
pentafluoride





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

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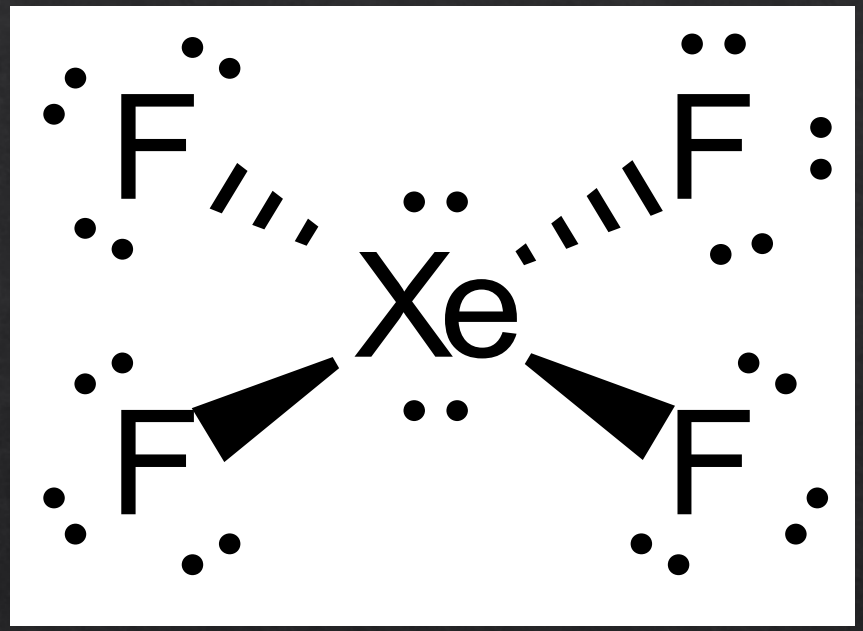
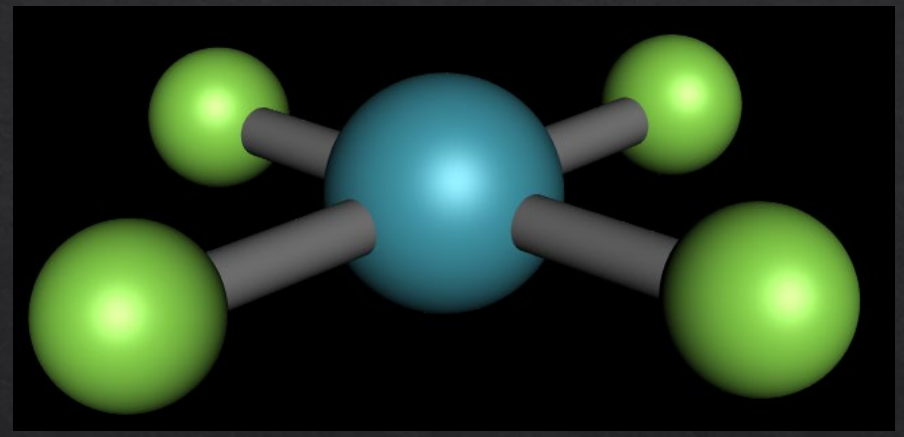
VSEPR HL

XeF_4
xenon
tetrafluoride





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