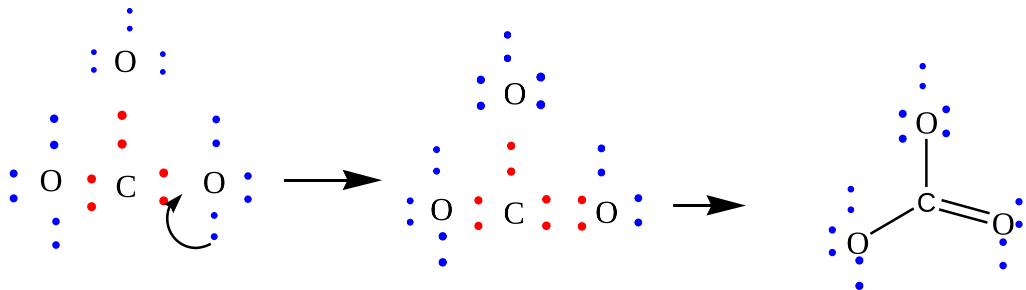
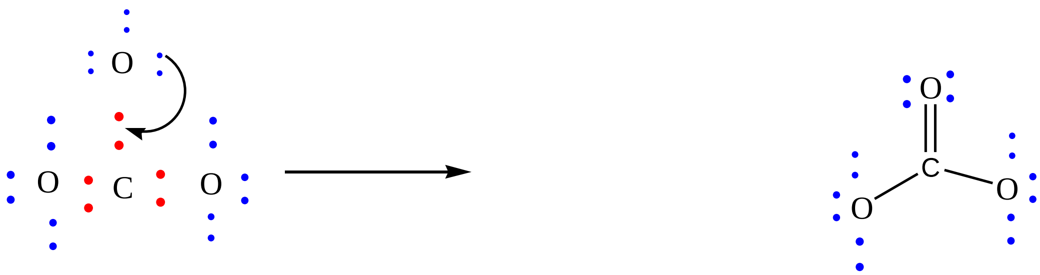
Resonance and curved arrow formalism



I



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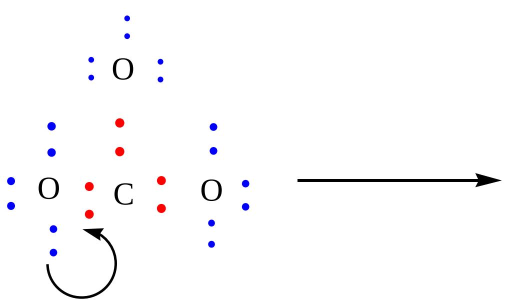

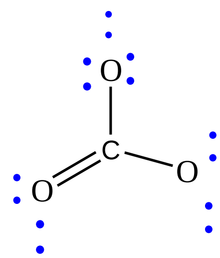

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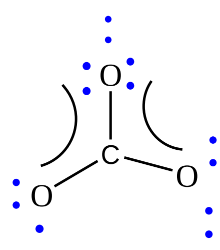
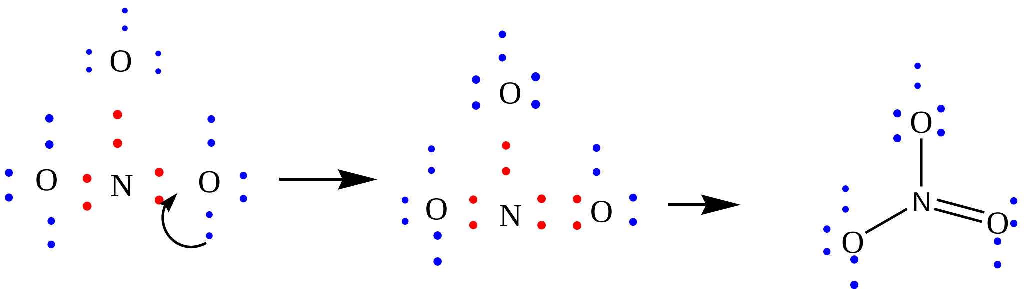


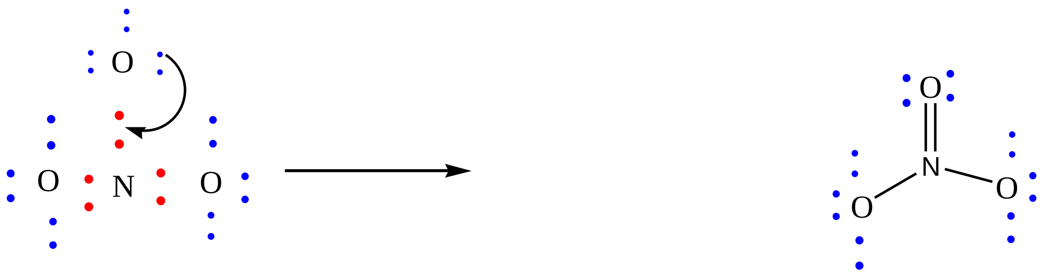
IV

Hybrid structure is mix of I+II+III

NO_3^{-1}



I



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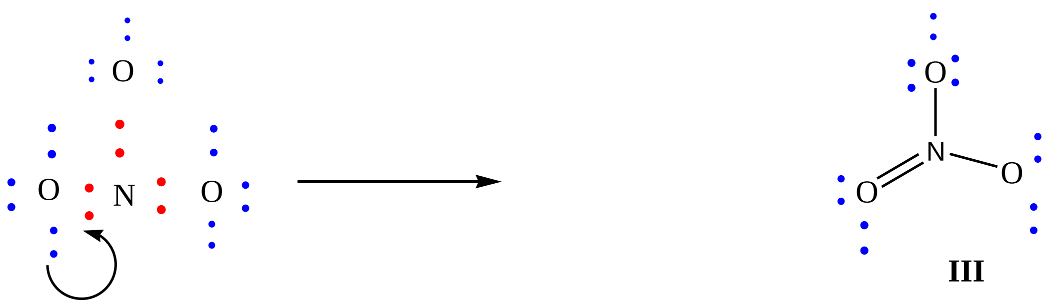
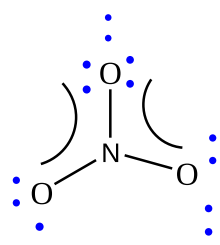


III



IV

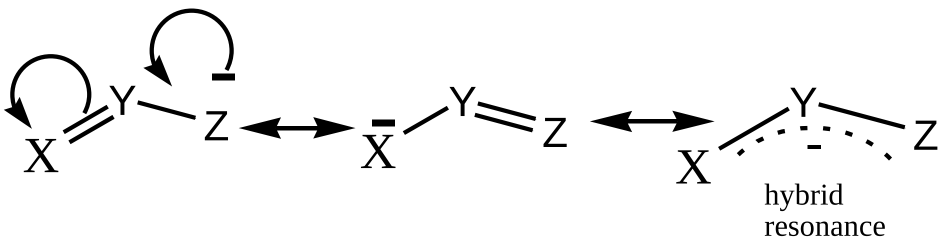
Hybrid structure is mix of I+II+III

In order the resonance to occur it should be:

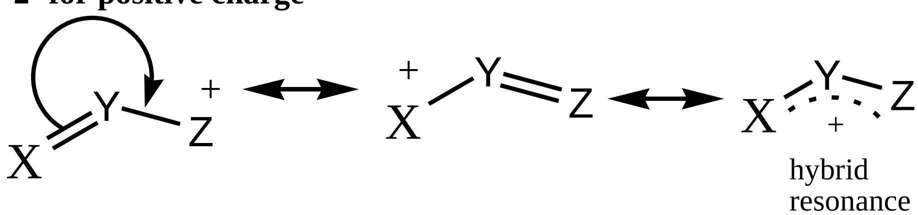
1. **Charged center carrying, negative or positive charge or radical.**
2. **This charged center should be conjucated to double or triple bond(s)**
3. **Double or triple bond conjucated with another**

Curved arrow representations for negative, positive and radical charges

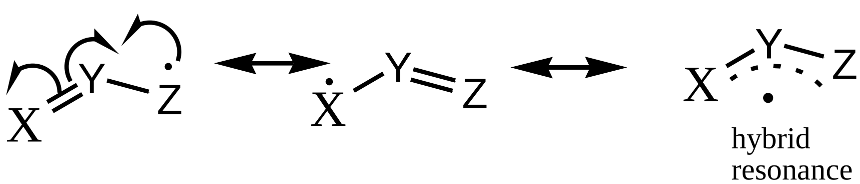
1- for negative charge



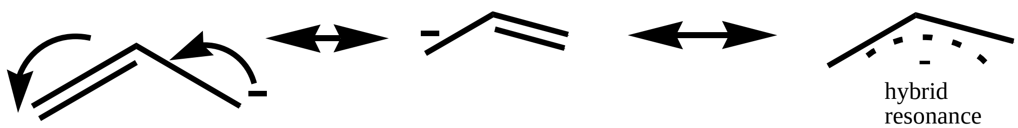
2- for positive charge



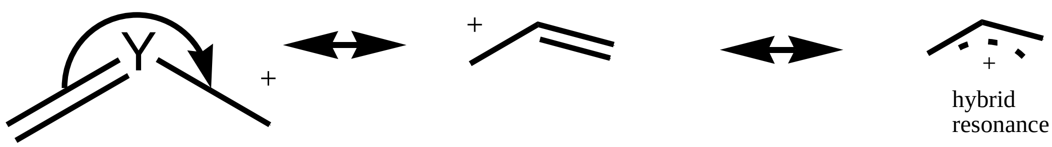
3- for radical



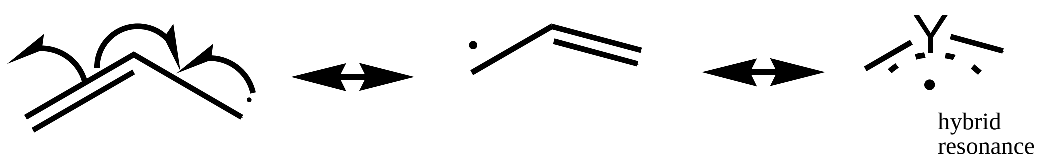
1- for negative charge



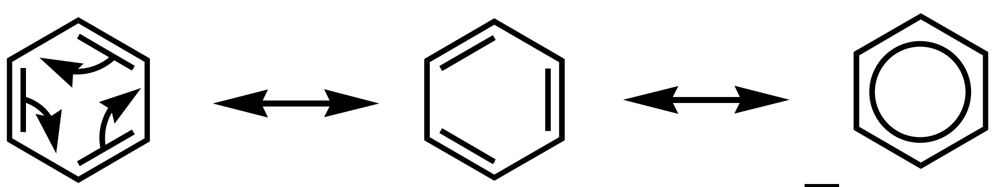
2- for positive charge

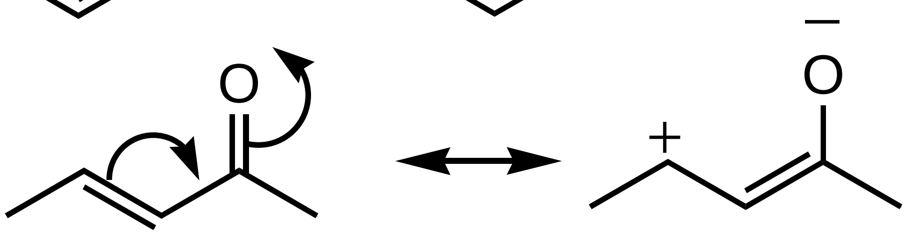


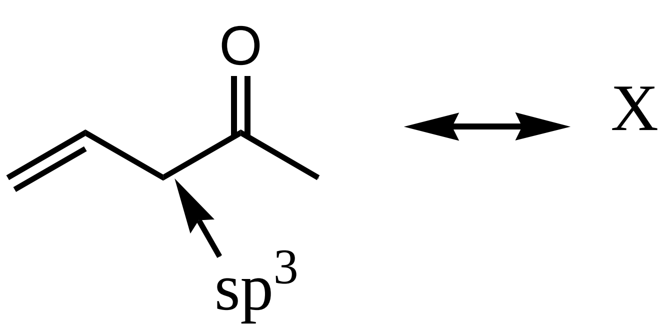
3- for radical



4- for double or triple conjucated







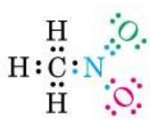
Formal Charges

- Sometimes it is necessary to have structures with *formal charges* on individual atoms
- We compare the bonding of the atom in the molecule to the valence electron structure
- If the atom has one more electron in the molecule, it is shown with a "-" charge
- If the atom has one less electron, it is shown with a "+" charge
- Neutral molecules with both a "+" and a "-" are dipolar
- In order to calculate formal charge, you should be able to draw the Lewis structure first.

$$\textbf{Formal charge} = \left(\begin{array}{c}\text{Number of}\\ \text{valence electrons}\\ \text{in free atom}\end{array}\right) - \left(\begin{array}{c}\text{Number of}\\ \text{valence electrons}\\ \text{in bound atom}\end{array}\right)$$

$$= \left(\begin{array}{c}\text{Number of}\\ \text{valence}\\ \text{electrons}\end{array}\right) - \left(\begin{array}{c}\text{Half of}\\ \text{bonding}\\ \text{electrons}\end{array}\right) - \left(\begin{array}{c}\text{Number of}\\ \text{nonbonding}\\ \text{electrons}\end{array}\right)$$

For the nitromethane nitrogen:

CH_3NO_2 = 

Nitrogen valence electrons	=	5
Nitrogen bonding electrons	=	8
Nitrogen nonbonding electrons	=	0

$$\text{Formal charge} = 5 - \tfrac{8}{2} - 0 \quad = +1$$

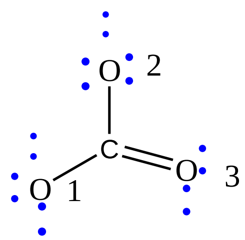
For the singly bonded nitromethane oxygen:

Oxygen valence electrons	=	6
Oxygen bonding electrons	=	2
Oxygen nonbonding electrons	=	6

$$\text{Formal charge} = 6 - \tfrac{2}{2} - 6 \quad = -1$$

Example: calculate the formal charge for each atom in CO_3^{-2}

1. Draw its lewis structure.



2. Then calculate the formal charge for each atom

Formal charge of O1 = 6 – 0.5(2) – 6 = -1

Formal charge of O2 = 6 – 0.5(2) – 6 = -1

Formal charge of O3 = 6 – 0.5(4) – 4 = 0.0

Formal charge of C = 4 – 0.5(8) – 0.0= 0.0

Questions: calculate the formal charge for the following

NO_3^{-1}

$NH4^{+1}$