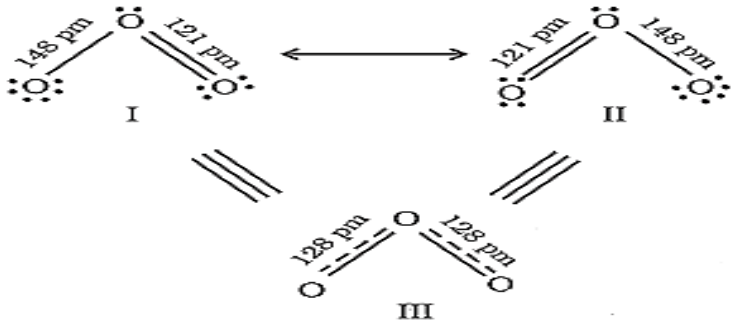
Resonance Structures

It is often observed that a single Lewis structure is inadequate for the representation of a molecule in conformity with its experimentally determined parameters. For example, the ozone, $\mathbf{O_3}$ molecule can be equally represented by the structures **I** and **II** shown below:

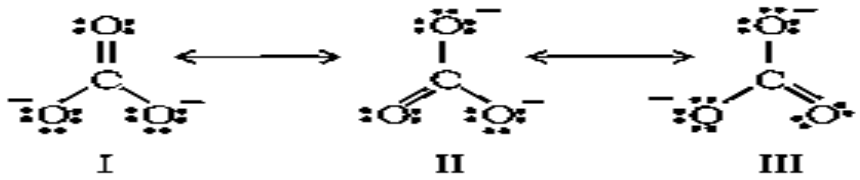


Resonance in the O_3 molecule

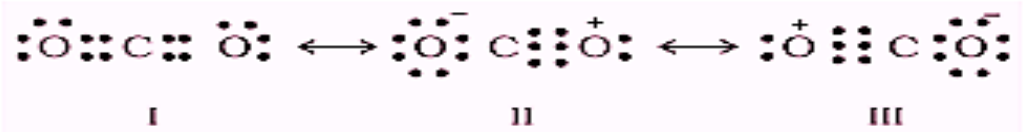
*(structures **I** and **II** represent the two canonical forms while the structure III is the resonance hybrid).

According to the concept of resonance, whenever a single Lewis structure cannot describe a molecule accurately, a number of structures with **similar energy**, **positions of nuclei**, **bonding and non-bonding pairs of electrons** are taken as the ***canonical structures*** of the ***hybrid*** which describes the molecule accurately. Thus for $\mathbf{O_3}$, the two structures shown above constitute the canonical structures or resonance structures and their hybrid, the **III** structure represents the structure of $\mathbf{O_3}$ more accurately. This is also called **resonance hybrid**. Resonance is represented by a double headed arrow.

* Some of the other examples of resonance structures are provided by the **carbonate ion** and the **carbon dioxide** molecule.

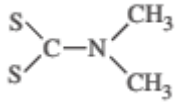


Resonance in CO_3^{2-}, I, II and III represent the three canonical forms.



Resonance in CO_2 molecule, I, II and III represent the three canonical forms

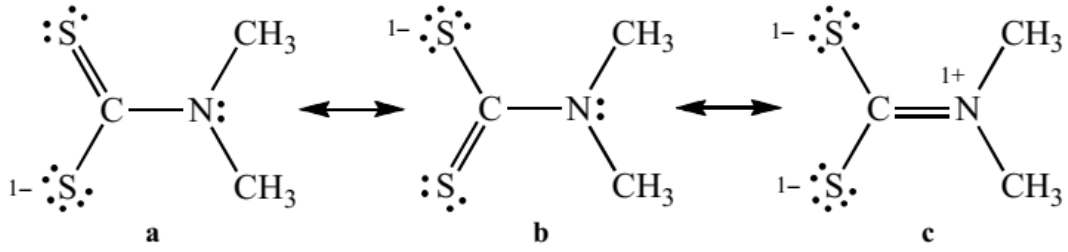
Ex:- The dimethyldithiocarbamate ion, **$[S_2CN(CH_3)_2]^-$**, has the following skeletal structure:



Give the important resonance structures of this ion, including any formal charges where necessary. Select the resonance structure likely to provide the best description of this ion .

Ans.:-

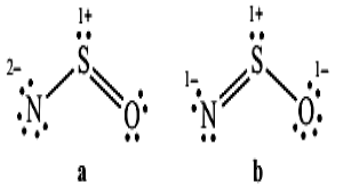
Structures **a** and **b** are **more likely** than **c**, because the negative formal charge is on the electronegative **S**. In structure **c**, the electronegative **N** has a positive charge.



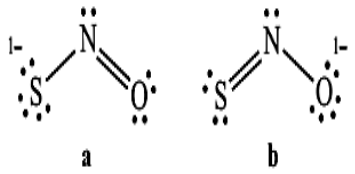
Ex:- Draw the resonance structures for the **isoelectronic** ions **NSO^-** and **SNO^-**, and assign formal charges. Which ion is likely to be more stable?.

Ans.

NSO^-: a has 2– formal charge on N, 1+ on S. Large formal charges, not very likely. b has 1– formal charges on N and O, 1+ on S, and is a better structure.

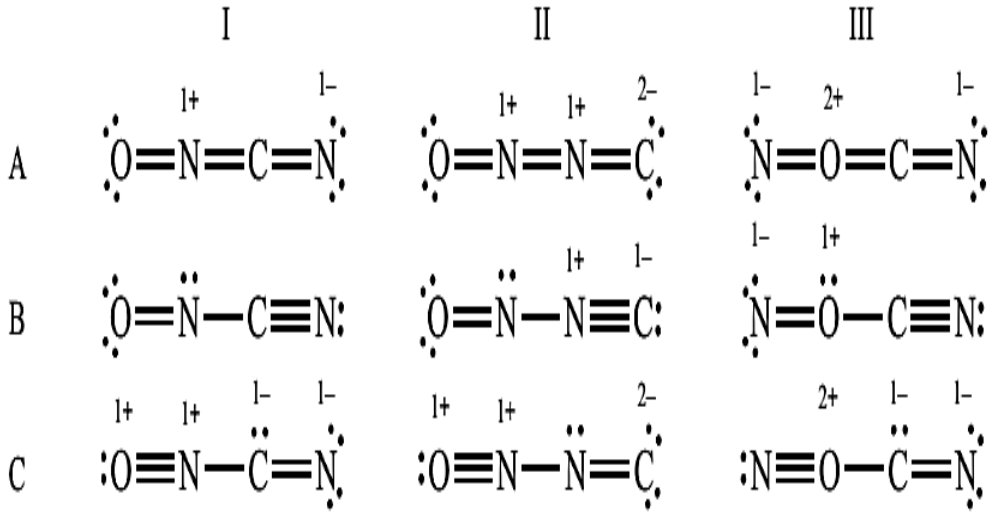


SNO^-: a has a 1– formal charge on S. Not very likely, doesn't match electronegativity (negative formal charge is not on most electronegative atoms). b has 1– formal charge on O, and is a better structure.



Overall, the $S{=}N{-}O^-$ structure is better based on formal charges, since it has only a negative charge on O, the most electronegative atom in the ion.

Ex:- Three isomers having the formula N_2CO are known: ONCN (nitrosyl cyanide), ONNC (nitrosyl isocyanide), and NOCN (isonitrosyl cyanide). Draw the most important resonance structures of these isomers, and determine the formal charges. Which isomer do you predict to be the most stable (lowest energy) form?.



Structure IB is best by the formal charge criterion, with no formal charges, and is expected to be the most stable. None of the structures II or III are as good; they have unlikely charges (by electronegativity arguments) or large charges.