

Formal Charge

Formal Charge: a way to identify the best Lewis dot structure when more than one valid dot structure exists

- Formal charges are hypothetical charges assigned to each element in the dot structure

$$\text{Formal Charge} = \# \text{ of valence electrons} - \# \text{ non-bonding electrons (lone)} - \frac{1}{2} \# \text{ bonding electrons}$$

You do NOT need to show work for formal charge calculations!!! 😊

Formal Charge Rules (Which dot structure is best?)

- Small (or even better, ϕ) formal charges are more stable.
- formal charge on the more electronegative atoms.
- + formal charge on the less electronegative atoms.
- Sum of all formal charges must equal the charge of the molecule.

Hint: Formal charge = ϕ when the atom forms the number of bonds you would predict based on its Lewis structure.

Formal Charge = 0

H	B	C	N	O	F
H-		$\begin{array}{c} \\ -C- \\ \\ -C\equiv \\ =C= \\ \text{etc} \end{array}$	$\begin{array}{c} -\ddot{N}= \\ -\ddot{N}- \\ \\ :N\equiv \end{array}$	$\begin{array}{c} \ddot{O}: \\ \\ \ddot{O}= \end{array}$	$\begin{array}{c} \ddot{F}- \\ \ddot{F} \end{array}$

Let's Practice!

The compound SO_2 can be drawn with multiple valid Lewis dot structures:

	$:\ddot{O}-\ddot{S}-\ddot{O}:$	$\ddot{O}=\ddot{S}-\ddot{O}:$	$:\ddot{O}-\ddot{S}=\ddot{O}:$
# of valence e^-	6 6 6	6 6 6	6 6 6
- # of nonbonding e^-	-6 -2 -6	-4 -2 -6	-6 -2 -4
- $\frac{1}{2}$ (# of bonding e^-)	-1 -2 -1	-2 -3 -1	-1 -3 -2
Formal Charge	-1 +2 -1	ϕ +1 -1	-1 +1 ϕ

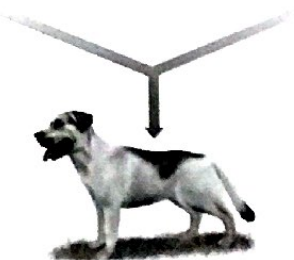
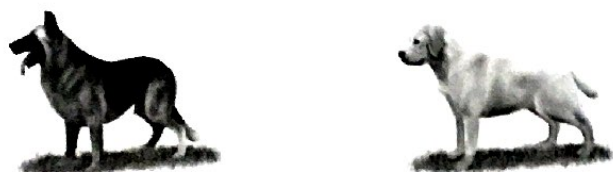
- Which structure(s) best represents a molecule of SO_2 ? Justify your answer in terms of formal charge.

The last two structures both best represent a molecule of SO_2 :
they have the smallest formal charges AND the -1 is found on the most EN atom, and the +1 is on the least EN atom.

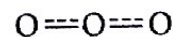
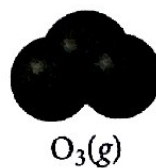
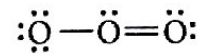
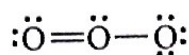
Resonance Structures

Resonance structures: when two or more Lewis structures can validly represent a molecule (or ion)

- Each resonance structure contributes to the real (observed) structure.
- The atoms of the molecule (or ion) stay in the same relative position: only the distribution of electrons is different!
- The actual structure, the resonance hybrid, is intermediate between the two or more resonance structures.
 - All possible dot structures contribute to the real structure, BUT more stable ones (↓ formal charge) contribute more.



Hybrid



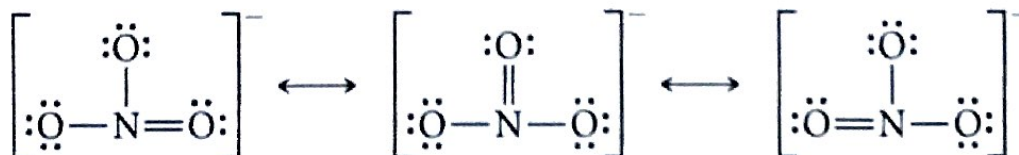
Resonance hybrid structure

Important Notes about Resonance Structures:

- Bonds are more equivalent to a "bond and a half" or a "bond and a third" in terms of length and strength, and are represented by one full line and one dashed line.
- Double edged arrows are used to indicate resonance.
- Resonance structures often occur in compounds with a double or triple bond.

Example: Nitrate (NO_3^-)

Resonance Structures:



Resonance Hybrid (Real, Observed Structure):

