Formal Charges

Definitions

Oxidation Numbers	Assigned by assuming e^- in a bond spend all of their time around the most Electronegative element
Formal Charges	Assume e^- are shared equally Determined by equation: $F.C. = \#\, valence\ e^- - unbonded\ e^- - \frac{1}{2}(bonded\ e^-)$ **Best Structure** • Best structure contains the lowest sum of Formal Charges • Most E.N. element with the lowest F.C. (usually negative)

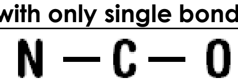
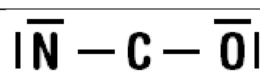
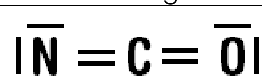
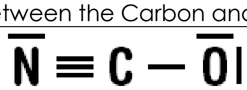
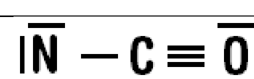
$$F.C. = \#\, valence\ e^- - unbonded\ e^- - \frac{1}{2}(bonded\ e^-)$$

Example 1
NCO^-

1. Find total valence e^-

Element	Charge on element	Valence e^- $= (8e^- + Charge)$	Total e^-
Nitrogen (N)	-3	$8e^- - 3 = 5$	$5 + 4 + 6 + 1 = 16e^-$
Carbon (C)	-4	$8e^- - 4 = 4$	
Oxygen (O)	-2	$8e^- - 2 = 6$	
NCO^-	-1	1	

2. Draw preliminary diagrams

Step	**Total e^- remaining**
To draw the preliminary diagram, start with only single bonds (only 1 line)	$16\ e^- - (2 \cdot 2e^-) = 12e^-$
Ex → 	
Upon that, add the remaining pairs of electrons surrounding the outer elements In this case, surround both Nitrogen and Oxygen with 3 lines, each representing $2e^-$, for a total of $8e^-$	$12\ e^- - (6 \cdot 2e^-) = 0e^-$
Ex → 	
The number of e^- on the central atom must add up to $8e^-$. In this case, Carbon only has $4e^-$, meaning that it still needs $4e^-$. The only way you can add e^- to a central atom is to increase the number of bonds surrounding it.	
Ex → 	
There are usually many ways to draw the diagram. Draw all possibilities (or however many are necessary) Here's where this gets interesting (or confusing). There is more than one way to balance the electrons in this example. For example, you can have a triple bond between the Nitrogen and the Carbon with a single bond between the Carbon and Oxygen. Or you can have a triple bond between the Oxygen and the Carbon with a single bond between the Carbon and the Nitrogen.	
Ex →  	

3. Determine Formal Charges

In this step, you must find the Formal Charges for all elements for all diagrams (yes, it's tedious. Suck it up.)

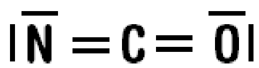
Diagram 1	Element	$F.C._{element}$	$F.C. = \#\ valence\ e^- - unbonded\ e^- - \frac{1}{2}(bonded\ e^-)$	F.C.
	Nitrogen	$F.C._N$	$5e^- - (2 \cdot 2e^-) - \frac{1}{2}(2 \cdot 2e^-)$	-1
	Oxygen	$F.C._C$	$6e^- - (2 \cdot 2e^-) - \frac{1}{2}(2 \cdot 2e^-)$	0
	Carbon	$F.C._O$	$4e^- - (0) - \frac{1}{2}(4 \cdot 2e^-)$	0
			Final Charge	-1

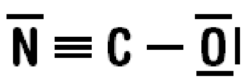
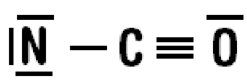
Diagram 2	Element	$F.C._{element}$	$F.C. = \#\ valence\ e^- - unbonded\ e^- - \frac{1}{2}(bonded\ e^-)$	F.C.
	Nitrogen	$F.C._N$	$5e^- - (1 \cdot 2e^-) - \frac{1}{2}(3 \cdot 2e^-)$	0
	Oxygen	$F.C._C$	$6e^- - (3 \cdot 2e^-) - \frac{1}{2}(1 \cdot 2e^-)$	-1
	Carbon	$F.C._O$	$4e^- - (0) - \frac{1}{2}(4 \cdot 2e^-)$	0
			Final Charge	-1

Diagram 3	Element	$F.C._{element}$	$F.C. = \#\ valence\ e^- - unbonded\ e^- - \frac{1}{2}(bonded\ e^-)$	F.C.
	Nitrogen	$F.C._N$	$5e^- - (3 \cdot 2e^-) - \frac{1}{2}(1 \cdot 2e^-)$	-2
	Oxygen	$F.C._C$	$6e^- - (1 \cdot 2e^-) - \frac{1}{2}(3 \cdot 2e^-)$	$+1$
	Carbon	$F.C._O$	$4e^- - (0) - \frac{1}{2}(4 \cdot 2e^-)$	0
			Final Charge	-1

Since the final charge on each of the diagrams is the same (-1), therefore, find the lowest charge on the most E.N element. In this case, the most E.N. element is Oxygen.

Final Charge on Oxygen	
Diagram	Formal Charge
1	0
2	-1
3	$+1$

$$Since\ Diagram\ 2\ has\ the\ lowest\ charge\ on\ its\ most\ E.N. element\ of\ -1, \therefore\ it's\ the\ best\ structure.$$

Best Structure →