Formal Charges

# Definitions

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| --- | --- |
| 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

$$NCO^{-}$$

### 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) | $$-2$$ | $$8e^{-}-2=6$$ |
| $$NCO^{-}$$ | $$-1$$ | $$1$$ |

### Draw preliminary diagrams

|  |  |
| --- | --- |
| **Step** | **Total** $e^{-}$ **remaining** |
| **To draw the preliminary diagram, start with only single bonds (only 1 line)** | $16 e^{-}-\left(2∙2e^{-}\right)=12e^{-}$  |
| **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 2$e^{-}$, for a total of 8$e^{-}$ | $12 e^{-}-\left(6∙2e^{-}\right)=0e^{-}$  |
| **Ex** 🡪 |
| **The number of** $e^{-}$ **on the central atom must add up to 8**$e^{-}$**.** In this case, Carbon only has 4$e^{-}$, meaning that it still needs 4$e^{-}$. 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 🡪** |

### 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.)

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| --- | --- | --- | --- | --- |
| Diagram 1 | Element | $$F.C.\_{element}$$ | $$F.C. =\# valence e^{-}-unbonded e^{-}-\frac{1}{2}(bonded e^{-})$$ | F.C. |
|  | Nitrogen | $$F.C.\_{N}$$ | $$5e^{-}-\left(2∙2e^{-}\right)-\frac{1}{2}\left(2∙2e^{-}\right)$$ | $$-1$$ |
| Oxygen | $$F.C.\_{C}$$ | $$6e^{-}-\left(2∙2e^{-}\right)-\frac{1}{2}\left(2∙2e^{-}\right)$$ | $$0$$ |
| Carbon | $$F.C.\_{O}$$ | $$4e^{-}-\left(0\right)-\frac{1}{2}\left(4∙2e^{-}\right)$$ | $$0$$ |
| Final Charge | $$-1$$ |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Diagram 2 | Element | $$F.C.\_{element}$$ | $$F.C. =\# valence e^{-}-unbonded e^{-}-\frac{1}{2}(bonded e^{-})$$ | F.C. |
|  | Nitrogen | $$F.C.\_{N}$$ | $$5e^{-}-\left(1∙2e^{-}\right)-\frac{1}{2}\left(3∙2e^{-}\right)$$ | $$0$$ |
| Oxygen | $$F.C.\_{C}$$ | $$6e^{-}-\left(3∙2e^{-}\right)-\frac{1}{2}\left(1∙2e^{-}\right)$$ | $$-1$$ |
| Carbon | $$F.C.\_{O}$$ | $$4e^{-}-\left(0\right)-\frac{1}{2}\left(4∙2e^{-}\right)$$ | $$0$$ |
| Final Charge | $$-1$$ |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Diagram 3 | Element | $$F.C.\_{element}$$ | $$F.C. =\# valence e^{-}-unbonded e^{-}-\frac{1}{2}(bonded e^{-})$$ | F.C. |
|  | Nitrogen | $$F.C.\_{N}$$ | $$5e^{-}-\left(3∙2e^{-}\right)-\frac{1}{2}\left(1∙2e^{-}\right)$$ | $$-2$$ |
| Oxygen | $$F.C.\_{C}$$ | $$6e^{-}-\left(1∙2e^{-}\right)-\frac{1}{2}\left(3∙2e^{-}\right)$$ | $$+1$$ |
| Carbon | $$F.C.\_{O}$$ | $$4e^{-}-\left(0\right)-\frac{1}{2}\left(4∙2e^{-}\right)$$ | $$0$$ |
| 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.

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

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



**Best Structure** 🡪