

Formal Charge

Applied to covalent compounds or ions containing covalent bonds

The compound SF_6 has the OS (oxidation state) of S = +6 and that for F = -1. For the covalent bonds in SF_6 these OSs are "fictitious charges" which only serve to identify the more electronegative element in a bond of shared electron pairs and possibly identify reactive atoms. Given the compound NO_2F the OSs are +5, -2, and -1, respectively. These OSs have little to no relationship to the partial charge an atom develops in a shared electron pair bond. Linus Pauling actually stated that atoms in a molecule attempt to share electrons such that each atom's partial charge is close to zero: the electroneutrality principle. Formal charge calculations are an attempt to apply this principle to Lewis structures, including resonance structures. Formal charge can then help to predict reasonable structures with most or all atoms achieving known bonding capacity (C: 4 bonds, N: 3 bonds, O: 2 bonds, F: one bond). As with Lewis structures, oxidation states, and resonance structures, formal charge is yet another human invention that tries to explain chemistry without using quantum mechanics; for many things it works well enough, for others it falls flat on its face.

Calculating Formal Charge

NO_2F 24 valence e^-

- 1) Draw the Lewis Structure and all resonance structures
- 2) For each atom in each structure calculate: $\text{FC} = (\# \text{ of valence } e^-) - (\# \text{ of lone } e^-) - (\# \text{ of bond } e^-/2)$
- 3) Confirm that the sum of all FC equals the overall charge of the molecule or ion.

