

ONF₃, OCF₃⁻, FNO₂ Projects

Oxidation States and Ionic Contributions to Bonding

We have used oxidation state differences between bound atoms and molecular orbital images in an attempt to interpret bonding in the species ONF₃, OCF₃⁻ and FNO₂. The calculated bond lengths in these molecules is not in accord with the Lewis structure models and in every case appears to suggest a valence at the central atom greater than four. We have used series of related molecules, ONF₃ through ONH₃; OCF₃⁻ through OCH₃⁻ and FNO₂ through HNO₂ to study the variation of bond lengths and to relate these to changes in ionic character as described by oxidation state differences. This has been combined with molecular orbital modeling to provide an understanding of the nature of bonding in these molecules.