

# **Anomaly Between Bond Length, Bond Strength and Bond Dissociation Energy Relationship: A Case Study of Donor-Acceptor Complexes**

## **Abstract**

The usual correlation between bond length, bond strength and dissociation energies has been the cornerstone of chemistry. However, this relation has been shown to fail in some examples, if not all. The breakdown of bond length - bond strength correlation in normal covalent bonds is mostly observed on fluorination. In this report, density functional calculations at BP86/TZVP level of theory have been used to study structure and bonding of donor-acceptor complexes of group 13 and group 15 elements. Here also, we obtained such a breakdown of bond length and bond strength relationship on fluorination. The apparent shortening and simultaneous weakening of bonds on fluorination is mainly due to 'hybridization defect'. This hybridization defect is the inherent property of heavier p-block elements which becomes more prominent on fluorination. On the other hand, we also noticed a breakdown of the usual relationship between bond strength and bond dissociation energies. We found that bond dissociation energies do not correlate with bond strengths, rather, the bond dissociation energies of these complexes were found to depend on the pyramidalization angle around the group 13 elements in their donor-acceptor complexes.