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# New insights into the intrinsic cooperativity of intermolecular or intramolecular bonds

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There are some well-known methodologies for evaluating the cooperativity of intermolecular noncovalent bonds [1,2]. However, in this work, we report our methodology for study on the intrinsic cooperativity of both intermolecular noncovalent bonds and intramolecular metal–ligand bonds. Indeed, we improve and extend the methodology proposed in our research group [3] and show that the quantitative evaluation of the impact of chemical bonds on the strength of each other is not restricted to the intermolecular noncovalent bonds. New equations are proved for calculating the total stabilization and interaction energies as well as the cooperative energies of bonds in any system that can be considered as three fragments and two chemical bonds. We report also the calculation of the cooperativity of bonds in some metal complexes of the type LML′, where L and L′ represent a single ligand or a group of ligands. The results show that both the M−L and M−L′ bonds will strengthen or weaken depending on the degree of cooperativity or anticooperativity of bonds. Thus, the rational design of a system with a very weak or a very strong bond is possible, where we know the type and degree of cooperatvity of bonds.

***Keywords:*** Theoretical study, Cooperativity of bonds, Noncovalent bond, Metal−ligand bonds.

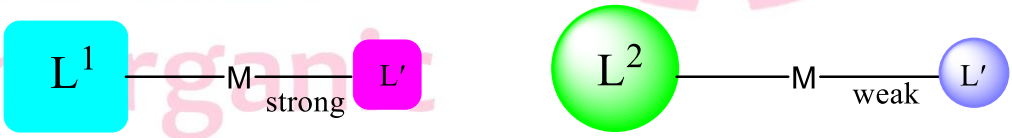



**Figure 1.** Changing the strength of M−L′ bond due to the existence of cooperativity and anticooperativity with M−$L^1$ and M−$L^2$ bonds, respectively.

**References**

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