Molecular descriptors for the "valence shell" of the molecule

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The electronegativity (χ) and the hardness (η) defined for the outermost (valence) shell of an atom describes the easiness of that atom to accept or to donate electron densities or its opposition to those processes.

Since OMO (Occupied Molecular Orbitals) and UMO (Unoccupied Molecular Orbitals) play the role of valence shell for the molecule, by similitude with the atomic χ and η quantities one may define new molecular descriptors expressing the capability of a molecule to accept/donate electron densities or its opposition to such a process.

The following molecular descriptors can be defined for the unoccupied (UMO) and occupied molecular (OMO) molecular orbitals:

$$\chi_{OMO} = \Sigma c^2_{OMO}\chi(\mathbf{Q})_{atom} \quad \text{and} \quad \chi_{UMO} = \Sigma c'^2_{UMO}\chi(\mathbf{Q})_{atom}$$

$$\eta_{OMO} = \Sigma c^2_{OMO}\eta(\mathbf{Q})_{atom} \quad \text{and} \quad \eta_{UMO} = \Sigma c'^2_{UMO}\eta(\mathbf{Q})_{atom}$$

where $\chi(Q) = \chi_0 + \eta(Q)Q$ (electronegativity) and $\eta(Q) = \eta_0 + \frac{3}{2}\frac{b^2 Q}{n^2}$ (hardness) are expression for the electronegativity (χ) and hardness (η) obtained with the Slater Type Orbitals, "n" being the principal quantum number, "b" the shield constant (b=0.3 for n=1 and 0.35 for n ≠ 1) and "Q" the electric charge of the atoms in molecule.

Such descriptors have successfully been used in QSAR/QSPR studies for a series of substances exerting a specific biological activity as well in the proton electron transfer processes.