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Electronic chemical potential and orbital electronegativity of univalent substituents

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Abstract

The relations were analyzed between the electronic chemical potential of a chemical group in the ground state and the orbital chemical potential of its valence state, the latter being equal in absolute value to its orbital electronegativity. These quantities should be equivalent for univalent substituents whose ground electronic state can be described by one-determinant wave function allowing localization of molecular orbitals in a closed shell. In this case, the orbital electronegativity of a chemical group can be calculated in terms of nonempirical quantum-chemical methods. The results of the variation calculation of orbital electronegativities of a series of univalent substituents gave rise to a quantum-chemical scale of group electronegativities which may be used for testing of approximate calculation procedures.

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