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Physical interpretation of the electronegativity

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Abstract

An additivity scheme of electronegativities of univalent substituents has been proposed on the basis on the Van Vleck orbital model of valence states of atoms. The electronegativity of any organic or heteroelement-containing substituent can be calculated from the orbital electronegativities and hardnesses of atoms constituting that substituent. The proposed additivity scheme is the most consistent among those currently available for calculation of orbital electronegativities of univalent substituents. The scheme was substantiated with the aid of quantum-chemical scale of group electronegativities.

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