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"Inductive" electronegativity scale: 2. 'Inductive' analog of chemical hardness

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Abstract

On the basis of a previously suggested approach to the calculation of "inductive" electronegativities of atoms and groups a simple method of theoretical estimation of in situ inductive electronegativities is elaborated. The method also allows the determination of inductive local and global chemical hardness parameters on the basis of geometric characteristics of bonded atoms. This made it possible to provide a new "steric" interpretation for some known chemical rules, such as the principle of maximum hardness. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

1.1. Inductive electronegativity scale

In our previous works [1–3], additive models for calculating of R_S—steric and σ^*—inductive constants of substituent, based on fundamental characteristics of its constituent atoms, have been described

$$\sigma^* = \sum_i^n \frac{\Delta\chi_i R_i^2}{r_i^2}, \quad (1)$$

$$R_S = \sum_i^n \frac{R_i^2}{4r_i^2}, \quad (2)$$

where n is the number of atoms in the substituent, R_i is the covalent radius of the i-th atom, r_i is the distance from it to the atom-reaction center and $\Delta\chi_i$ is the difference in inductive electronegativities of the i-th atom and reaction center.

On the basis of these models the method of calculation of 'inductive' group electronegativity χ_g, reflecting the donor–acceptor properties of substituent, immediately attached to the atom-reaction center, have also been suggested [4]

$$\chi_g = \frac{\sum_i^n \frac{\chi_i R_i^2}{r_i^2}}{\sum_i^n \frac{R_i^2}{r_i^2}}, \quad (3)$$

where χ_i is the inductive electronegativity of the i-th atom.

The scale of the atomic inductive electronegativities reproduces that of Pauling's with the exception of the value of carbon ($\chi(C) = 2.55$ in Pauling's scale

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