The concept of electronegativity. the current state of the problem

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Abstract

A systematic account is given of the current ideas about atomic and group electronegativities and the trends in the development of the concept of electronegativity are analysed. Attention is concentrated on the latest approaches to the definition of electronegativity - the concept of 'orbital' electronegativities and the density functional theory. A procedure is proposed for the determination of 'inductive' electronegativities, which permits a correct theoretical calculation of the electronegativity of a substituent from the electronegativities of individual atoms and the steric structure. It is shown that the approach developed has a series of important advantages - for example, it makes it possible to calculate the group electronegativities of isomeric substituents avoiding the principle of the equalisation of electronegativities. A survey of literature data and generalisation of the method proposed by the authors have made it possible to formulate the concept of electronegativity as an unchanging fundamental immanent characteristic of a chemical element. © 1998 Russian Academy of Sciences and Turpion Ltd.