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On methods of assessment of the components of chemical bond and the need to take into account metallic character in chemical substances

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Abstract

In the present paper a review of methods to describe the chemical bond within classical ideas in terms of covalent, metallic and ionic components was made. Special attention is paid to the bond metallic character; the need to take it into account to characterize correctly chemical bond was shown. It was shown that among chemists there is a strong demand for characterizing chemical bonds in terms of their covalent, metallic and ionic characters. It was also shown that attempts to assess quantitatively the chemical bond components (covalent, metallic and ionic character) made by different authors using various methods are not systematic. They cover limited number of chemical compounds and do not assess comprehensively the effects of chemical composition and the ratio of chemical bonds components on structure of chemical compounds (e.g., molecular or nonmolecular, etc.), which in turn determines properties of a substance.

The authors and their colleagues developed the method to determine two or three components of homo- and heteronuclear chemical bond, respectively, using electronegativity. The effects of chemical bond components' ratio on specific properties of substances and materials was shown. The quantitative assessment of metallic character in homo- and heteronuclear bonds using quantum-mechanical calculations showed certain agreement with the results obtained by using electronegativity. It was also shown that traditional chemical approaches are not only not inferior to the quantum-mechanical methods, but often describe more adequately the magnitude and transformation of a number of bonds' metallic character.

Examples of practical interest to characterizing chemical bonds in terms of their covalent, metallic and ionic character by using various methods, as a rule, are due to the need to quantitatively describe different chemical bonds. This is due to the need to assess the effects of chemical bond type on structure and specific properties of substances and often the impossibility to do this by using quantum-mechanical methods only.

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