

Nature of chemical bonds in MCCH(M=Li, Na, K) based on the topological analysis of electron localisation function (ELF) and electron density.

Autorzy

Krzysztof Mierzwicki

Sławomir Berski

Zdzisław Latajka

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Streszczenie

Topological analysis of the electron localisation function (ELF) and the theory of atoms in molecules are applied to analyse the nature of bonds in MCCH (M=Li, Na, K) molecules. The substitution of hydrogen by alkali metal leads to a transfer of about one electron from M to C₁C₂H and all alkali metal acetylides may be described by the M⁺[C₁C₂H]⁻ formula. This means that the bonding between carbon and metal is mainly of ionic nature. One can explain the observed difference in properties of organosodium compounds by rather high electronegativity of sodium according to the Allred–Rochow scale.

Adres publiczny

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