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A fundamental approach to compute atomic electrophilicity index

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Abstract

Electrophilicity index (ω) is an important theoretical construct of atoms and molecules and is widely used to understand various chemical phenomena and determine physico-chemical properties. Accordingly, it becomes useful to find an accurate expression for it which is free from any inconsistencies. In view of this, a simple yet rigorous expression is proposed to compute Electrophilicity Index. Since our model is based on ionization potential and electron affinity, it provides a more reliable measure for any electronic changes taking place in a species. Our suggested definition is free from any operational and dimensional discrepancies. We have reported atomic electrophilicity indices for 74 elements of the periodic table invoking our proposed ansatz. The proposed model follows all the sine qua non of existing scale of electrophilicity index. Electrophilicity Equalization Principle is also validated through our computed values. In general, the new expression appears to be powerful and suitable for application in diverse realms.

Keywords:

Density functional theory (DFT), Electron affirnity, Electrophilicity equalization principle (EEP), Ionization energy, Periodicity

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