Paper No: PU-SOE - Chemistry - 06

A scale of absolute radii derived from electrophilicity index

Hiteshi Tandon¹, Tanmoy Chakraborty², Vandana Suhag³

- 1. Department of Chemistry, Manipal University Jaipur, Jaipur, 303007, India
- 2. Department of Chemistry, School of Engineering, Presidency University, Bengaluru, 560064, India
- 3. Department of Applied Sciences, BML Munjal University, Gurugram, 122413, India

Abstract

Atomic radius plays a key role in the realm of science to understand atomic/molecular physico-chemical properties. Looking at the enormous potential this descriptor has, a model is proposed for absolute radius (r) in terms of electrophilicity index (ω). Atomic radii for 103 elements of the periodic table are reported. Considering the periodic relationship between absolute radius and atomic electrophilicity, this empirical model is proposed invoking regression analysis. The computed radii obey sine qua non of periodic properties. Relativistic effects are also distinct in the newly computed radii. On comparison, the computed data is noted to be in close conformity with the reported radii. Further, some size-dependent properties are calculated by employing the computed absolute radius. These present a substantial periodic behaviour and association with absolute radii.

Keywords:

Atomic radii, electrophilicity Index, periodic descriptor, hardness, polarizability

Publication Details:

Journal Name	Vol.	Month & Year	Page No.	Publisher	Scimago Ranking
Molecular Physics	119 (4)	Sept, 2020	1820594	Taylor & Francis	Q2