Chapter 3
Commonality in the Origin and the Manifestation in the Real World of Electronegativity and Hardness

Nazmul Islam
University of Kalyani, India & Techno Global-Balurghat, India

Dulal C. Ghosh
University of Kalyani, India

ABSTRACT

The electronegativity and the hardness are two different fundamental descriptors of atoms and molecules, and this chapter describes how the authors have logistically discovered the commonality between the heuristic and basic philosophical structures of their origin and also the manifestation in the real world. Also, the chapter demonstrates that the physical hardness and the chemical hardness with evolution of time have converged to one and the same general principle— the hardness. The authors also try to expose the physical basis and operational significance of another very important descriptor—the electronegativity. The chapter also explores whether the hardness equalization principle can be conceived analogous to the well established electronegativity equalization principle. The authors hypothesize that the electronegativity and the absolute hardness are two different appearances of the one and the same fundamental property of atoms, and the Hardness Equalization Principle can be equally conceived like the electronegativity equalization principle. To test this hypothesis, the authors have made several comparative studies by evaluating some well known chemico-physical descriptors of the real world, such as hetero nuclear bond distances, dipole charges, and dipole moments of molecules. The detailed comparative study suggests that the paradigm of the hardness equalization principle may be another law of nature like the established electronegativity equalization principle.

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INTRODUCTION

Our history says that the periodic table was written in Russian, the explanation in quantum mechanics was written in German, and our understandings were spoken in English. The periodicity is in the central plenum and the periodic table is the central icon of nature. The powerful chemical and physical organizing power of the periodic table is highly manifest in chemistry and physics. The grand unification of the periodic properties, like the atomic size, ionization energies of atoms, electronegativity, and chemical hardness, is done by periodic table by connecting the seemingly different properties in one string. Mathematical algorithm can be developed for the evaluation of one in terms of the other. The present status shows that the periodic table does not follow from the Schrödinger equation but the chemical periodicity is correlated in terms of the shell structure and Pauli Exclusion Principle.

The Electronegativity

Electronegativity has been one of the most useful theoretical constructs in chemistry from the early days of the history of science. Though fundamentally a conundrum, the electronegativity concept is widely used by chemists, physicists, biologists and geologists. The electron distribution is fundamental in determining the physico-chemical properties of molecules in both ground and excited states (Pritchard & Skinner, 1955, Ghosh, 2003). The electronegativity is an important tool in sketching the static distribution and dynamic rearrangement of electronic charge in molecules (Coulson, 1951, Fukui, 1982).

The bond energies, bond polarities and the dipole moments, force constants and the inductive effects are some very fundamental descriptors of organic, inorganic and physical chemistry. Such descriptors can only be conceived, rationalized and modeled for evaluation in terms of the concept of electronegativity. Although the idea of electronegativity is very old, it was only in 1932 when Pauling (Pauling, 1932, 1960) offered scientific meaning of the word “electronegativity” and suggested a scale of its measurement. Pauling identified electronegativity with “the power of an atom in a molecule to attract electrons to it”. This definition of electronegativity has been heuristically important and is deeply implanted in minds of chemists even today.

The Global Hardness

The hardness is a very old and one of the most useful conceptual constructs of chemistry and physics. The notion of hardness was first introduced by Mulliken (1952) who pointed out that the ‘Hard’ and ‘Soft’ behavior of various atoms, molecules and ions can be conceived during acid-base chemical interaction. Soon after Mulliken’s classification, the terms hardness and softness were in the glossary of conceptual chemistry and implicitly signified the deformability of atoms, molecules and ions under small perturbation. Thereafter, Pearson (1963) and Klopman (1964) tried to systematize and rationalize this intrinsic property of atoms and molecules. Pearson classified molecules, atoms and ions in three classes, hard, soft and borderline- known as the HSAB principle. But the classification was qualitative in nature and its basis was empirical. It was very difficult to ascertain the relative hardness of the molecules and atoms in terms of Pearson’s classification.

It is apparent that the hardness as conceived in chemistry fundamentally signifies the resistance towards the deformation or polarization of the electron cloud of the atoms, ions or molecules under small perturbation generated during the process of chemical reaction. Thus, the general operational significance of the hard-soft chemical species may be understood in the following statement– If the electron cloud is strongly held
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