

Isoelectronic Series: A Novel Tool

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ABSTRACT

In this communication, we propose a potential use of isoelectronic series and develop a methodology for relationship exploration through them.

Keywords: Isoelectronic series; Methodology; Relationship exploration.

INTRODUCTION

Isoelectronic species are the species having equal number of electrons. Surprisingly, these are some of the periodic trends which are often overlooked and forgotten. They are useful in predicting reactions or existence of compounds.

The isoelectronic concept foundation was laid by Irving Langmuir¹. He applied it to molecular species and ions. Recently, Geoff² has extended its predictive ability and has given a good account of molecular isoelectronic species. However, not much has been spoken about the atomic isoelectronic species. In this communication, we propose their potential use and develop a methodology for relationship exploration *via* isoelectronic series.

THEORETICAL BACKGROUND

Isoelectronic Species

The prefix *-iso* means the same, therefore, the literal meaning of isoelectronic is “same electron” or “equal electric”. For isoelectronic species two definitions are most common i.e. the species having the same total number of electrons and the species having the same number of valence electrons. Recently, a logical definition of isoelectronic species has been suggested as “Species (atoms, molecules, ions) are isoelectronic with each other if they have the same total number of atoms and electrons and of valence electrons”².

In an atom, electrons surround the nucleus. In neutral atoms, number of surrounding electrons equals the atomic number of the element. Atomic isoelectronic species i.e species having same total number of electrons will be formed due to addition and removal of electrons. The anionic and cationic species resulting from addition and removal of electrons can be multivalent as well. These atomic (neutral or ionic) isoelectronic species will have the

same total number of electrons, but different atomic numbers.

An isoelectronic series is a group consisting of neutral, cationic and anionic isoelectronic species.

Slater's Rules

The distribution of electrons around the nucleus is not random, but well organised, determined by certain rules and quantum numbers. Each of the electrons is repelled by the inner orbital and same orbital electrons.

Slater has suggested set of rules to calculate electronic repulsion by the same orbital and inner orbital electrons, in the form of screening constants. The screening constants and Slater orbitals have enabled a whole generation of chemists and physicists to calculate approximate values of many of the physical properties of atoms. The use of screening constants implies that an atomic orbital corresponding to a given set of electronic quantum numbers is the same, except for a uniform scaling of the coordinates, quite irrespective of which atom or ion is under consideration. This concept of interchangeability of orbitals has greatly simplified the mental picture of atomic structure. However, detail description of Slater's rules is not required for the present work.

THE METHODOLOGY TO EXPLORE RELATIONSHIP

Our methodology is very simple yet novel. It is based on the fact that in isoelectronic species the number of electrons is same and hence the electronic configuration as well as the mutual screening of the electrons or the screening constants. This is in accordance with the underlined philosophy of Slater's rule also. The change in any atomic property or properties will mainly depend on the atomic number. Therefore, if we plot two

sets of isoelectronic data with each other, then, from the kind of variation(s), we can predict the mutual relationship of two data for neutral atomic species, provided, a smooth variation or trend with high degree of correlation is there. *The neutral atomic species is a part of the isoelectronic series and its data would usually be an extrapolated value.*

Recently, we have used this methodology to explore relationship between an important theoretical descriptor, the electronegativity and fundamental atomic property, the atomic number⁴. Our inference has justified the previously suggested relationship⁴. We have used this methodology to explore relationship between hardness and atomic number, electronegativity and hardness, and several other properties also; these will be discussed in coming publications.

CONCLUSION

The usefulness of atomic isoelectronic species and series is often overlooked. A potential use of isoelectronic series can be for relationship exploration and we have developed a novel methodology for that. Recently, by using this methodology, we have explored relationship between electronegativity and atomic number, and justified the previously suggested relationship.

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