Randic and Schultz molecular topological indices and their correlation with some X-ray absorption parameters

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Abstract. The properties of a molecular system are affected by the topology of molecule. Therefore many studies have been made where the various physic-chemical properties are correlated with the topological indices. These studies have shown a very good correlation demonstrating the utility of the graph theoretical approach. It is, therefore, very natural to expect that the various physical properties obtained by the X-ray absorption spectra may also show correlation with the topological indices. Some complexes were used to establish correlation between topological indices and some X-ray absorption parameters like chemical shift. The result obtained in these studies shows that the topological indices of organic molecule acting as a legands can be used for estimating edge shift theoretically.

1. Introduction

Earlier, we have established a correlation between topological Index (Winer and Randic) and X-ray parameters.¹, ², ³ In present work we have now established a correlation between X-ray absorption parameter like chemical shift with Randic and Schultz index respectively.

2. Generation of Randic and Schultz Index

The Randic index⁴ makes use of vertices present in the chemical graph and therefore, it is sensitive to the shape also. Hence this index is also known as molecular connectivity index χ. It is equal to the sum of the values of all molecular edges.

\[ \chi = \sum_{\text{all bonds}} \left( \frac{1}{m \cdot n} \right)^{1/2} \]

The variables m and n are the valencies of the bond end points of each edge. Multiple bonds and hetro atoms have been included in the Randic index by assigning valencies value (v) to the concerned atoms using the expression:

\[ v = z^v - h_i \]

and/or the expression
Where $z$ is the total number of electrons. $z^i$ is the number of valence electrons of atom $i$ and $h_i$ is the number of hydrogen atom attached to it.

The Schultz molecular topological index of $G$ denoted by MTI, is defined as

$$MTI = \sum_{i=1}^{n} e_i$$

where $e_i$'s (1, 2, 3, ….. n) represents the elements of the following row matrix of order n.

$$V(G) [A(G) + D(G)] = [e_1, e_2, e_3 ........ e_n]$$

where $V(G)$ is the valence row matrix, $A(G)$ and $D(G)$ are adjacency and distance matrix respectively.

### 3. Results and Discussion

Table 1 contains name of complexes and their molecular graph. Table 2 contains chemical shift, Randic and Schultz Index.

Table 1 Name of the complexes and their molecular graphs

| No. | Name of complexes                                                                 | Molecular graph |
|-----|-----------------------------------------------------------------------------------|-----------------|
| 1.  | N-Phenyl-3-methyl-4- [{4'- (2” – (5, 6-dimethyl oxazolyl) Sulphonamoyl]} Phenylazo-Pyrazolin-5-one Cobalt (II) (CoPzS) | ![Molecular Graph](image1) |
| 2.  | N-Phenyl-3-Methyl-4- [{4’ – (2” – Pyrimidimyl sulphamoly)] Phenylazo-Pyrazolin-5-one cobalt (II) (CoPZ) | ![Molecular Graph](image2) |
| 3.  | Co-P Complex using Sulphadiazine (CoP5)                                             | ![Molecular Graph](image3) |
| 4.  | N-Phenyl-3-Methyl-4- (4’ – nitro) Phenylhydrozone Pyrozolone-5-one (CoPN)           | ![Molecular Graph](image4) |
| 5.  | Co complex of P-toluidine [CoPT]                                                   | ![Molecular Graph](image5) |
Table 2 Chemical Shift ($\Delta E$), Randic and Schultz Index for Co-substituted Pyrazolm-5-one complex

| No. | Complex | Chemical Shift $\Delta E \pm 0.3$ ev | Randic Index | Schultz Index |
|-----|---------|-------------------------------------|--------------|--------------|
| 1.  | CoPZ5   | 10.0                                | 10.60        | 26433        |
| 2.  | CoPZ    | 11.3                                | 9.82         | 26240        |
| 3.  | CoPS    | 8.5                                 | 5.34         | 4569         |
| 4.  | CoPN    | 12.1                                | 7.48         | 14000        |
| 5.  | CoPT    | 10.7                                | 7.39         | 9246         |

The position of X-ray absorption edge depends upon the valence of the absorbing ion the effective charge on the central atom and also upon the geometry of the complex. In the present work the K-absorption edge for all Co(TI) complexes is found to be on the higher energy side. The order of chemical shifts for complexes as indicated by their values has been found to be as follows:

CoPN > CoPZ > CoPT > CoPZ5 > CoP5

The order is due to fact that –NH and –C = 0 stretching frequencies are observed at 3380 and 1750 cm$^{-1}$ respectively. However, upon complexation the bond due to the –NH stretching is again retained at 3380 cm$^{-1}$ because of the presence of another –NH group.

In sulphonomoyl moiety large values of chemical shift in all the complexes show that the complexes are more ionic in character. As the shift is taken to be proportional to ionic character, the role of various bonds attached to the central metal ion is prominent in determining the overall chemical shift in a metal complex. Further not only ligation of a particular type, e.g. Co–O, Co–N is responsible in imparting ionic character to the complex, but their position in the planar ring / axial position also contributes to the ionic character.

![Randic Index](image1)

Randic Index
Figure 1 Correlation of Randic Index with chemical shift for Co (II) complexes

![Schultz Index](image2)

Schultz Index
Figure 2 Correlation of Schultz Index with chemical shift for Co (II) complexes

Figure 1 and 2 shows correlation between chemical shift with Randic Index and Schultz Index respectively.
The correlation assumes the general form

$$(\text{TI})^2 = -4a (\Delta E)$$

Where TI stands for a particular topological index and $a$ is constant.

The Figure 1 represents the correlation for chemical shift and Randic Index.

While Figure 2 demonstrates the correlation for Schultz indices and chemical shift. Both the plots yield excellent parabola (second order polynomial)

It is gratifying that the correlations with the Schultz index are better than that with Randic Index. As the chemical shift not only depends on ligation of particular type e.g. Co–O–Co–N is responsible in imparting ionic character to the complex, but their position in the planar ring / axial position also contributes to the ionic character. Thus result obtained in this study show that the correlation with Schultz indices is very effective.

4. Conclusion
Randic and Schultz molecular topological indices contain important structural information. One can say that the X-ray absorption parameter, thus estimated, indicate that topological indices of the organic molecules acting as legands can be used for estimating X-ray absorption parameter theoretically. Thus the topological understanding of molecular properties can lead to the development of new area of the present and future interest i.e. tracking the effect of pollutants in the environment, designing of drugs and prediction of carcinogenicity of molecule.

5. References
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