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CORRELATION OF EFFECTIVE CHARGE WITH BALABAN INDEX

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ABSTRACT

Many studies have been made where the various physico-chemical properties are correlated with the topological indices. In present work the Balaban Index is the average distance sum of connectivity are use to correlating with X-ray absorption parameter like effective charge. Some hydroxy substituted pyridine copper (II) complexes are used to establish this type of correlation. The results have indicated that the effective chargeis sensitive to the topological structure of coordinating ligand moieties. Thus the topological understanding of molecular properties can lead to development of new area of the present and future interest i.e. tracking the effects of pollutants in the environment, designing of drugs and the prediction of carcinogenicity of molecule.

I. 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 effective chargewith Balaban index.[4]

II. GENERATION OF BALABAN INDEX

The Balaban index[4] is the average distance sum of connectivity and is defined as:

$$J = \frac{M}{\mu + 1} \sum_{\substack{\text{All Edges} \\ i \neq j}} \frac{1}{(D_i D_j)^{\frac{1}{2}}}$$

Where M is the number of edges in the graph (G). μ is the cyclomatic number of graph (G) and is equal to zero for a 'tree' and one for 'mono-cycles'. Di is the distance sum and is equal to the sum of all entries in the corresponding row of the distance matrix.

III. RESULT AND DISCUSSION

Table contains name of complexes, their molecular graph, Balaban Index and effective charge

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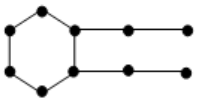
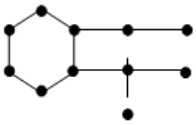
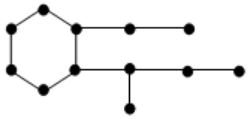
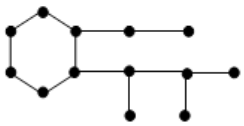
Table:- Name of the Ligand, Molecular Graphs, Balaban Index and effective charge

Sr. No.	Name of Ligand	Molecular Graphs	Balaban Index J	effective charge Z_{eff} (electron/atom)
1	Cu (II) 2, 3 – dihydroxypyridine (DHP)		2.35	1.21
2	Cu (II) 2 – Amino, 3-hydroxy-phyridine (AHP)		2.42	1.10
3	Cu (II) 3 – Hydroxypyridine 2 – Carboxylic acid (HPC)		2.46	1.05
4	Cu (II) 3 – Hydroxy 2 – Picolinamide (HPA)		2.54	0.96

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 complexes[5, 6]. In the present work the K-absorption edge for all Cu(II) complexes is found to be higher energy side. The order of effective charge for complexes as indicated by their values has been found to be as follows:

Cu(DHP) > Cu (AHP) > Cu (HPC) > Cu (HPA)

The larger values of effective charge in all Cu (11) complexes show that the complexes are more ionic in character. As the shift is taken to be proportional to the ionic character.[7]

According to Suchet[8] the effective charge is a result of two factor –

1. Electronegativity difference between the constituent atoms which tends to bring them to complete ionic electronic configuration and
2. Polarisation due to the inter penetrations of the electron clouds.

Not only ligation of a particular type e.g. Cu – O or Cu – N is responsible in imparting ionic character to the complex, but their position in the planer ring / axial position also contributes to the ionic character. We have used Gianturco and Coulson method [9] for calculating effective charge.

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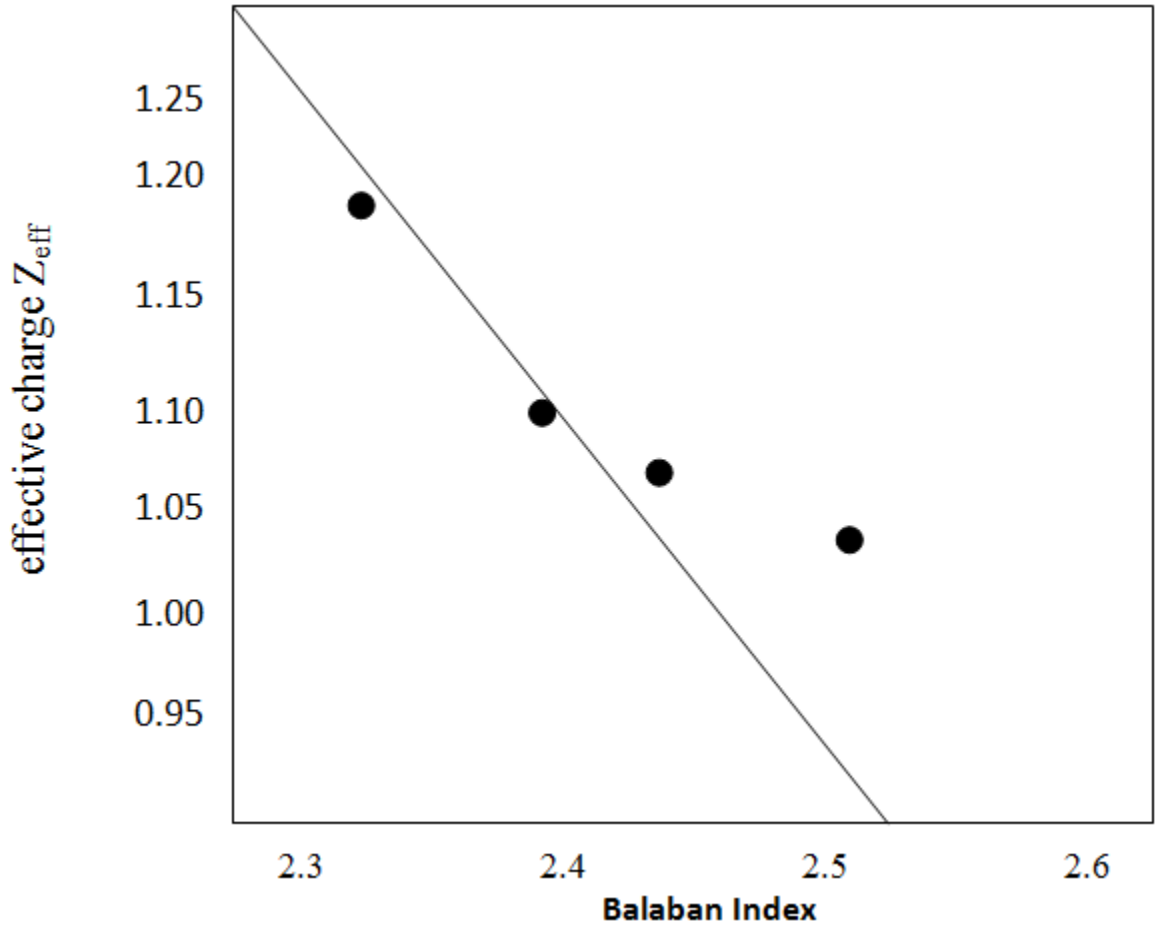

Figure 1: Correlation of Balaban Index with effective charge for Cu (II) Complexes

Figure shows correlation between Balaban Index of substituted hydroxypyridine ligands and corresponding effective charge. The correlation assumes the general form

$$Zeff = -m(J) + C$$

where J stands for Balaban Index

The plots yield excellent straight lines. The results obtained in this study demonstrate the correlation of Z_{eff} with Balaban Index is very effective. We can say that the effective charge thus estimated indicates that topological indices of the organic molecules acting as ligands can be used for estimating effective charge theoretically.

IV. CONCLUSION

Topological indices contain valuable information about molecular structure and molecular properties. the prediction of the properties of molecules before their synthesis should be made by topological indices.

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