Journal of Chemistry and Chemical Sciences, *Vol.8(5), 838-843, May 2018* *ISSN 2229-760X (Print)*
(An International Research Journal), *www.chemistry-journal.org* *ISSN 2319-7625 (Online)*

Determination of Topological Bond Orders of Phenanthrene Molecule Using Its Cardinality

Piyali Ghosh

Department of Chemistry,
M.U.C. Women's College, Burdwan, Burdwan-713104, INDIA.
email:dr.piyalighosh@gmail.com.

(Received on: April 29, 2018)

ABSTRACT

In this paper cardinality of phenanthrene molecule is determined. A method for the determination of topological bond orders of phenanthrene molecule has been developed. In this method cardinality of the phenanthrene molecule itself and its subgraphs are utilized. Correlation between topological bond orders and Hückel bond orders for the corresponding phenanthrene molecular graph is studied. Fairly good correlation with these two bond orders are obtained.

Keywords: cardinality; topological bond order; Hückel bond order; phenanthrene molecule.

1. INTRODUCTION

A number of topological indices have been proposed and analyzed by many researchers for studying various physico-chemical properties[3,5,6,11,14]. Topological index or indices are very important regarding physico-chemical property interpretations for QSAR as well as QSPR study. In this paper cardinality, a topological index is determined for phenanthrene molecule and then it is utilized for the determination of all topological bond orders of this molecule. Topological bond orders are very interesting graph-theoretical properties.

Delocalization in conjugated π-electron systems is shown to be closely related to the topological concept of connectivity. A topological bond order is defined as a quantitative measure of the extent to which the subspace of a pair of adjacent atoms approximates a disconnected component of the molecular topological space. The agreement between this measure and molecular-orbital bond orders in the ordering of bond strengths within molecules is near perfect. Bond order is a well-known structural parameter as defined by Coulson[15]. Bond

orders determined by Hückel molecular theory (HMO) are known as Hückel bond orders. In contrast, the topological (graph theoretical) nature of HMO is well established[4,9]. Very preliminary concept of graph theory is discussed here. Graph theory deals with graph which is a diagram consists of two sets of objects called edges and vertices. Graph *'G'* have the edges $E = (e_1, e_2, e_3, ...)$ and vertices $V = (v_1, v_2, v_3, ...)$ as shown in Figure-1. Graph theory is also successfully applied to explore different problems in the field of chemistry (chemical graph theory). Here molecules are represented by their molecular graphs. In that case bonds and atoms are equivalent to edges and vertices respectively. Topological bond order (TBO) in terms of graph cardinality is defined by Merrifield and Simmons[8,10].

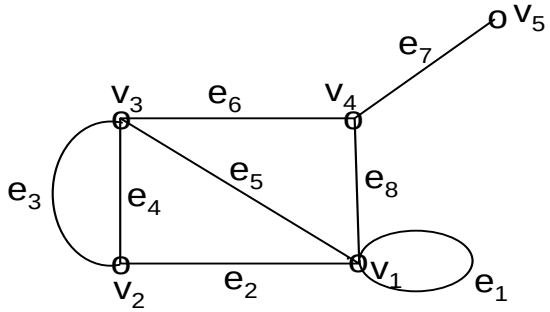

Figure-1: Diagram of a graph

A. Cardinality

Topological indices are uniquely determined numerical quantities that are used to correlate the molecular properties with the structure of the molecule. During its determination connectivity of graph is important not the shape of the graph. Cardinality is an important topological index and it specifies the structural descriptor in the field of graph theory. Two vertices are said to be '*independent'* if they are not connected by an edge and number of sets of such *independent* vertices (including null set, null graph means graph without any edges) are called *'cardinality'* [8,10]. It is calculated mathematically but can be correlated with the physical as well as physico-chemical properties of the molecule. Cardinalities have significant applications such as search for molecular databases, selection of compounds for drug designing, drug modeling etc.

B. Determination of cardinality for a graph

Cardinalities of linear graphs, (graph without any cycle) are related with Fibonacci numbers, given below[2]. Different types of linear graphs are shown in Figure-2.

$$\sigma[L_n] = F_{n+1}$$

Here $\sigma[L_n]$ represents ***'cardinality'*** of linear graph with *'n'* number of vertices (L_n) and F_{n+1} is *(n+1) th* Fibonacci number ($F_0 = 1, F_1 = 1, F_n = F_{n-1} + F_{n-2}$). It is given in the Table-1. For any graph cardinality is given in equation (1).

$$\sigma(G) = \sigma(G - v) + \sigma(G - v - A_v) \quad (1)$$

Where v is any vertex of G and A_v is the set of vertices connected to v. Here $\sigma(G-v)$ is the cardinality of the subgraph resulting from the graph $'G'$ after deletion of vertex v. Similarly $\sigma(G-v-A_v)$ is that of a subgraph obtained from $'G'$ after deletion of the vertex v and all other vertices adjacent to v.

If G contains a number of disconnected components (subgraphs) $G_1, G_2, G_3, G_4 \ldots$ then cardinality of graph $'G'$ i.e. $\sigma(G)$ will be expressed by a relation as given in equation (2)

$$\sigma(G) = \sigma(G_1)\sigma(G_2)\sigma(G_3)\sigma(G_4)\ldots \quad (2)$$

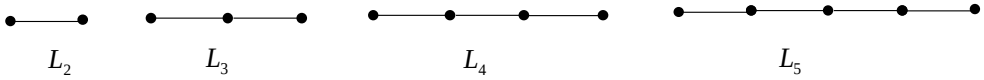

Figure-2: Different types of linear graphs

C. Cardinality and topological bond order (TBO)

The general formula for topological bond order (π_{ij}) of the bond between the *i*th and *j*th atoms of a conjugated molecule is given below[2,7,12,13]

$$\pi_{ij} = \{[\frac{\sigma(G)}{\sigma(G-i-j)}] - 1\}/2 \quad (3)$$

Here $\sigma(G)$ specifies the cardinality of graph *G* and $\sigma(G-i-j)$ is the cardinality of sub graph of *G* resulting from deletion of bond connecting *i*th and *j*th atoms.

Table-1: Fibonacci numbers and cardinality of linear graphs.

n	L_n	F_{n+1}	$\sigma[L_n]$
$n=1$	L_1	F_2 =2	2
$n=2$	L_2	F_3 =3	3
$n=3$	L_3	F_4 =5	5
$n=4$	L_4	F_5 =8	8
$n=5$	L_5	F_6 =13	13
$n=6$	L_6	F_7 =21	21
$n=7$	L_7	F_8 =34	34
$n=8$	L_8	F_9 =55	55
$n=9$	L_9	F_{10} =89	89
$n=10$	L_{10}	F_{11} =144	144
$n=11$	L_{11}	F_{12} =233	233
$n=12$	L_{12}	F_{13} =377	377

2. DETERMINATION OF CARDINALITY OF PHENENTHRENE MOLECULE

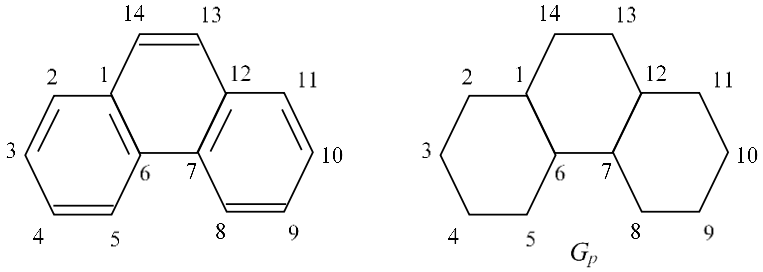

Figure-3: Phenanthrene molecule along with its graph

Equation (1) and (2) are utilized to calculate the cardinality of phenanthrene molecule, $\sigma[G_P]$. The procedure is illustrated below:

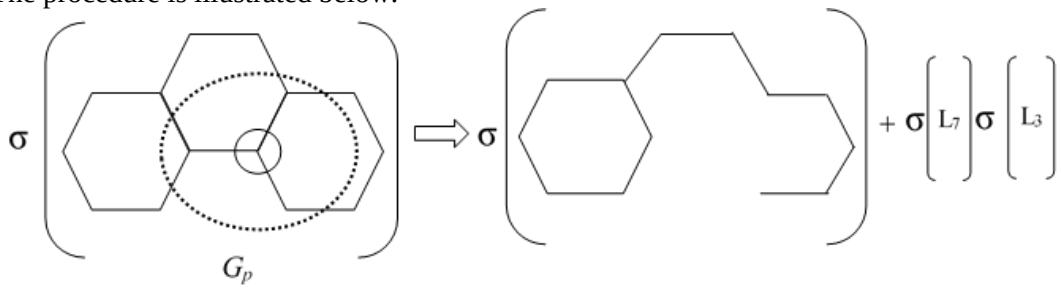

Figure-4: Illustration for the derivation of cardinality of phenanthrene molecule

$$\sigma[G_P] = \sigma[L_{12}] + \sigma[L_3]\sigma[L_7] + \sigma[L_3]\sigma[L_7]$$

$$= 377 + 2(5 \times 34)$$

$$= 717$$

Therefore cardinality of phenanthrene molecule is 717.

3. DETERMINATION OF DIFFERENT BOND ORDERS OF PHENANTHRENE MOLECULE

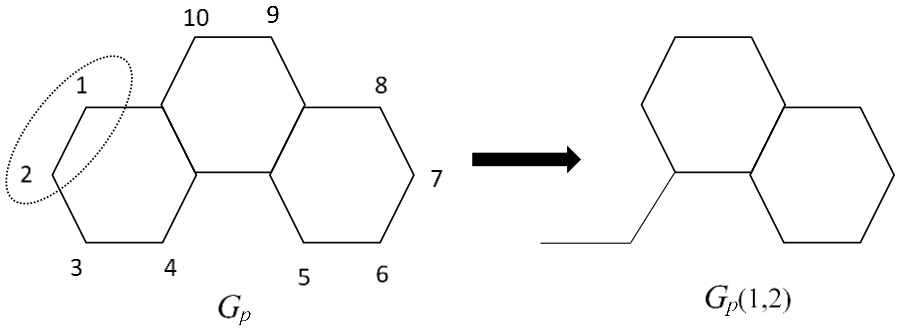

Figure-5: Illustration for the determination of bond order of phenanthrene molecule

Using the formula given in equation (3) we have:

$$\pi_{1,2}(G_p) = \{\frac{\sigma[G_p]}{\sigma[G_p(1,2)]} - 1\}/2 = (\frac{717}{308} - 1)/2 = 0.663$$

$\sigma[G_p(1,2)]$ can be determined using Fibonacci numbers after its fragmentations into subgraphs.

Similarly the other π bond orders (TOB) can be determined and these are given as follows:

$\pi_{1,2} = \pi_{7,8} = 0.663$

$\pi_{2,3} = \pi_{6,7} = 0.599$

$\pi_{3,4} = \pi_{5,6} = 0.652$

$\pi_{9,10} = 0.698$

Double bond characters, as per Hückel Theory (HMO) are also known as

$\pi_{1,2} = \pi_{7,8} = 0.6$

$\pi_{2,3} = \pi_{6,7} = 0.4$

$\pi_{3,5} = \pi_{5,6} = 0.6$

$\pi_{9,10} = 0.8$

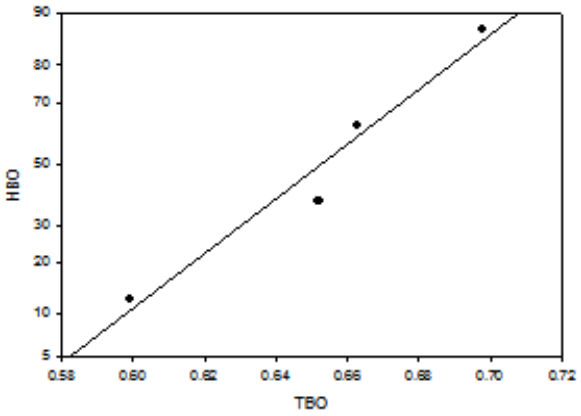

Figure-6: Correlation between Huckel Bond Order (HBO) & Topological Bond Order (TBO)

CONCLUSION

We must conclude that the approach for obtaining bond orders from cardinalities of conjugated hydrocarbon graph is quite general, it was first proposed by Merrifield and Simmons. Topological bond orders and bond orders obtained from HMO have good correlation. Cardinality is an important topological index, thus can be correlated with some physical properties such as density and bulk modulus for few poly(*p*-phenylene) molecules[1].

REFERENCES

1. Ghosh, P., Karmakar, S., and Mandal, B., Cardinalities of poly(p-phenylene) graphs, *Mol. Phys*., 112: 2646-2653 (2014).
2. Mandal, B., Banerjee, M., and Mukherjee, A. K., Cardinalities of reciprocal graphs, *Int. J. Quantum Chem*., 99: 119-126 (2004).
3. Balaban, A. T., (Eds.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach Science Publishers, The Netherlands (1999).
4. Dias, J. R., Molecular Orbital Calculations Using Chemical Graph Theory, Springer-Verlag, New York (1993).
5. Trinajstić, N., Chemical Graph Theory, CRC Press, Boca Raton, FL (1992).
6. Klein, D. J., and Randić, M., (Eds.), Mathematical Chemistry, VCH, Weinheim (1990).
7. Randić, M., Plavšić, D., and Trinajstić, N., "On the Difference in Bond Orders Between HMO and PPP Methods, *Int. J. Quantum Chem*., 37: 437-448 (1990).
8. Merrifield, R. E., and Simmons, H. E., Topological Methods in Chemistry, Wiley, New York (1989).
9. Gutman, I., and Polansky, O. E., Mathematical Concepts in Organic Chemistry, Springer-Verlag, New York (1986).
10. Merrifield, R. E., and Simmons, H. E., Topology of bonding in π-electron systems, *Proc. Natl. Acad. Sci*., USA., 82: 1-3 (1985).
11. Hosoya, H., A topological index for the totalπ-electron energy, *Bull. Chem. Soc. Japan*., 44: 2332-2339 (1971).
12. Pariser, R., and Parr R. G., A semi-empirical theory of the electronic spectra and electronic structure of complex unsaturated molecules, *J. Chem. Phys*., 21: 466, 767 (1953).
13. Pople, J. A., Electron interaction in unsaturated hydrocarbons, *Trans. Faraday Soc*., 49:1375-1385 (1953).
14. Wiener, H., Structural Determination of Paraffin Boiling Points, *J. Am. Chem. Soc*., 69: 17-20 (1947).
15. Coulson, C. A., Chemical Applications of Group Theory, *Proc. R. Soc. Lond*., A169: 413 (1939).