Review Article

Graph Theory in Chemistry: A Brief Review

Somnath Karmakar*

Department of Chemistry, Raghunathpur College, Raghunathpur 723 133, Purulia,W.B.

Abstract

Although graph theory is a branch of pure mathematics particularly in topology but it pervades all branches of human knowledge. In this context historical background of the development of graph theory and definition of several types of graph are mentioned in short. Some chemical or physical situations, where graph theory can be applied, have been pointed out. Some fields in chemistry especially enumeration of isomers & Kekulé structures, determination of degree of unsaturations, investigation of structures and properties of fullerenes and other carbon cages, calculation of Hückel molecular orbitals (HMO) and related quantities, solution for coupled kinetic rate equations etc., where graph theory have been employed, are discussed briefly.

Key words: graph theory, edge, vertices, Kekulé structures, Hückel molecular orbitals

1. Introduction

Graph theory is one of the few fields of mathematics with a definite date of birth [1-4]. In the year 1736, Euler wrote the first known paper on graph theory [5] where he resolved the then long standing Königsberg bridge problem. G. R. Kirchhoff [6] discovered graphs while solving problems involving the analysis and design of electrical networks with the use of 'spanning trees'. Organic Chemistry played an important role for the discovery and subsequent improvement of graph theory. Aurthur Cayley [7,8] put forward the graphical concept of trees in the year 1857 and applied [9,10] this concept for the purpose of enumerating isomers of alkanes, C_nH_{2n+2}. J. J. Sylvester [11] in 1878 introduced the terminology of 'graph' in mathematics and revealed the possible applications in chemistry as the term 'graphical representation' had been being frequently used to describe the molecular structural formulas. At the time of Kirchhoff and Cayley, two other milestones in graph theory were laid. One was the *four colour conjecture*, which states that four colours are sufficient for colouring any atlas (a map on a plane) such that countries with common boundaries have different colours. The other milestone was the invention of a puzzle with a wooden regular dodecahedron in 1859 by Sir W. R. Hamilton; the objective of the puzzle was to find a route that passes through each of the vertices of dodecahedron

exactly once. This route is called 'Hamiltonian circuit' (or 'Hamilton circuit'). It is important to note that till date no one has found a necessary and sufficient condition for the existence of such a route in an arbitrary graph. D. König [12] collected the works of other mathematicians and compiled his own works to write the first book on graph theory, which was published in 1936. By now this field has become almost a separate discipline in mathematics and a large number of books on mathematical graph theory have appeared, those by Oystein Ore [1], Robin J. Wilson [4] and Frank Harary [2] deserve special mention as text books.

2. Definitions

2.1. A graph

A number of ways a graph may be defined. One of such definitions is: 'A graph G = (V, E) consists of a set of object $V = (v_1, v_2, v_3,...)$, called vertices and another set $E = (e_1, e_2, e_3,...)$, called edges so that each edge e_k is identified by an unordered pair (v_i, v_j) of vertices'. This definition permits an edge to be associated with a vertex pair (v_i, v_i). Commonly a graph is a diagram where vertices are represented by points and the edges by lines as shown in figure 1.
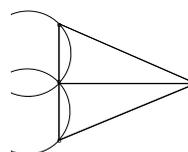

Figure 1: A finite graph

A graph with a finite number of vertices as well as a finite number of edges is said to be a finite graph; otherwise, it is an infinite graph.

2.2. Subgraphs

A graph *g* is said to be a subgraph of graph *G* if all the vertices and all the edges of *g* are in *G*. A subgraph is obtained by deleting some vertices and/or edges from the original graph. In Figure 1.1, $G_{1.1.1}$ and $G_{1.1.2}$ are the subgraphs of the graph $G_{1.1}$. Two special types of subgraphs that play significant

DOI: https://doi.org/10.54280/jse.222103

roles in the chemical applications of graph theory are: Sachs graphs and the matching subgraphs.

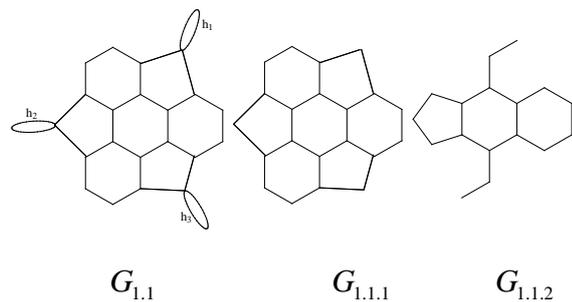$G_{1.1}$ $\quad\quad$ $G_{1.1.1}$ $\quad\quad$ $G_{1.1.2}$

Figure 1.1: Subgraphs $G_{1.1.1}$ and $G_{1.1.2}$ of the graph $G_{1.1}$

2.3. Null graphs

A vertex having no incident edge is called an isolated vertex i.e., isolated vertices are of zero degree. A graph that contains isolated vertices is called a null graph. A null graph has no edges. Null graph of n vertices are denoted by N_n and some null graphs of $n=1, 2, 3, 4, 5$ are shown in Figure 2.
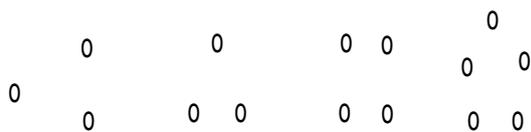
Figure 2: Null graphs of n =1, 2, 3, 4 and 5.

2.4. Complete graphs

A graph in which each pair of vertices is connected by an edge is called complete graph. A complete graph of n vertices is usually denoted by K_n; K_1, K_2, K_3, K_4, K_5 being shown in Figure 3.
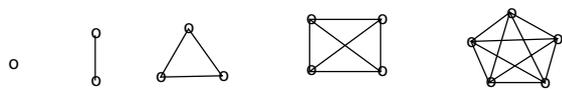
Figure 3: Complete graphs: K_1, K_2, K_3, K_4, K_5

2.5. Regular graphs

A graph in which all vertices are of equal degree is called a regular graph; if every vertex has degree d, the graph is called regular of degree d. Some regular graphs such as polygons of degree 2 and cube of degree 3 are shown in Figure 4.
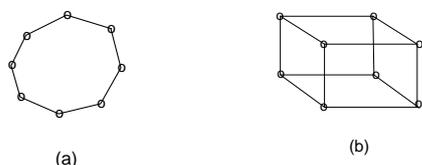
(a) $\quad\quad\quad$ (b)

Figure 4: An octagon (a) and a cube (b).

2.6. Isomorphic graphs

Two graphs are isomorphic if there is a one-one correspondence between the vertices of one graph and those of other with the property that the number of edges joining any two vertices of one graph is equal to number of edges joining the corresponding vertices of the other. Two graphs, $G_{1.1}$ and $G_{1.2}$, shown in Figure 5 are isomorphic to each other under correspondence $u \to l$, $v \to m$, $w \to n$, $x \to r$, $y \to p$, $z \to q$.

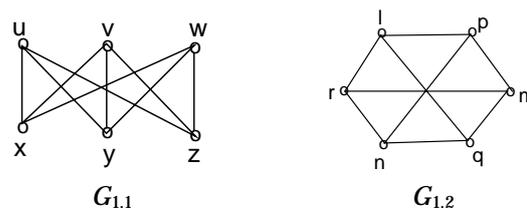$G_{1.1}$ $\quad\quad\quad\quad$ $G_{1.2}$

Figure 5: Two isomorphic graphs, $G_{1.1}$ and $G_{1.2}$.

2.7. Sachs graphs

A Sachs graph is a graph whose components are either cycles and/or complete graphs with two vertices, K_2. For example $G_{1.3.1}$, $G_{1.3.2}$ and $G_{1.3.3}$ are Sachs graphs of $G_{1.3}$ shown in Figure 6.

$G_{1.3}$ $\quad\quad$ $G_{1.3.1}$ $\quad\quad$ $G_{1.3.2}$ $\quad\quad$ $G_{1.3.3}$

Figure 6: Some Sachs graphs of graph $G_{1.3}$.

2.8. Matchings

A k-matching of a graph G is the selection of k mutually independent edges (that are not incident on a common vertex).

So it is evident that every k-matching, containing k copies of K_2, corresponds to a subgraph of G. The number of k-matchings of a graph is denoted by $m(G, k)$. For $G_{1.3}$ (in Figure 1.6.1), $m(G_{1.3}, 3) = 8$ and $m(G_{1.3}, 4) = 1$ as shown in Figure 7.
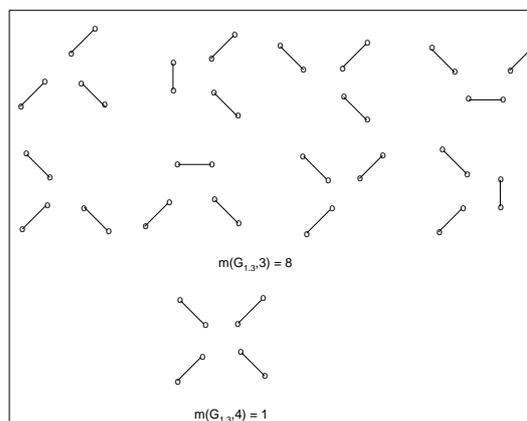
$m(G_{1.3},3) = 8$

$m(G_{1.3},4) = 1$

Figure 7: 3- and 4-matching graphs of $G_{1.3}$.

2.9. Trees and forest

A tree is a connected graph that has no circuits. This means in particular that there are no multiple edges. It also implies that in a tree there is a unique arc connecting any pairs of vertices. A tree can be constructed by selecting any particular vertex v_0 and from this vertex edges are drawn to neighbouring vertices v_1, v_2, v_3, ...; again from each of these vertices (say v_1) edges can also be drawn to its neighbouring vertices v_{11}, v_{12}, v_{13}, ... and so on as shown in Figure 8(a).
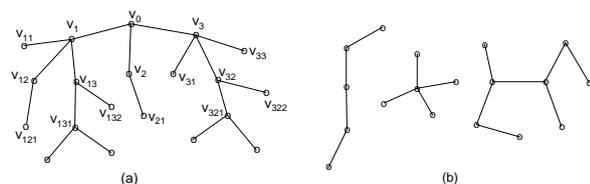

Figure 8: A tree (a) and forest (b).

Therefore, a tree with v vertices has $(v-1)$ edges. A graph that contains more than one tree is called a forest. A graph of three isolated trees shown in Figure 8(b) is an example of a forest. A forest of v vertices and m component has $(v-m)$ edges.

A tree $G(T)$ is said to be a spanning tree of a connected graph G if it is a subgraph of G and it contains all vertices of G. For instance, subgraph (b) of the graph (a) shown in Figure 9 containing edges $b_1 b_2 b_3 b_4 b_5 b_6$ is one of the spanning trees of the said graph. The spanning trees are the largest trees among all the trees in G. So it is quite appropriate to call a spanning tree a maximal tree subgraph or maximal tree of G.
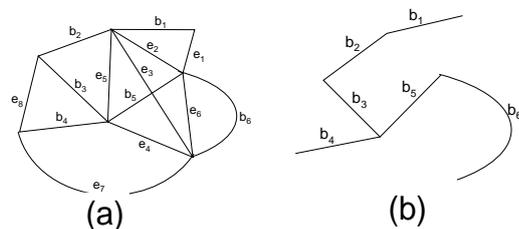

Figure 9: A graph (a) and one of its spanning tree (b).

2.10. Planar graphs

A graph that can be drawn on a plane in some manner so that edges have no intersection except at the vertices is called a planar graph. All polyhedra can be drawn on plane and are represented by planar graphs. A dodecahedron along with its corresponding planar representations is shown in Figure 10.
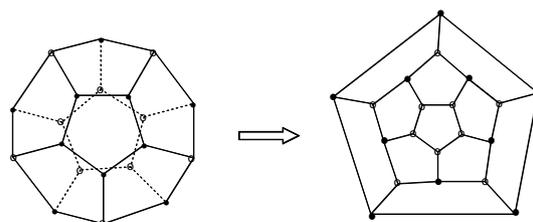

Figure 10: A dodecahedron and its planar representation.

2.11. Weighted graphs

A weighted graph is a graph in which at least one edge or a vertex is weighted i.e., at least one edge weight is other than unity or at least on vertex weight is other than zero. Graphs corresponding to all hydrocarbons (H-deleted graphs) are usual or unweighted graphs, whiles graphs containing heteroatoms are generally weighted graphs. Sometimes weighted graphs appear as subgraph(s) of a parent unweighted graph in graph factorization procedure.

2.12. Adjacency matrix of a graph

Adjacency matrix ($\mathbf{A}$) of a graph G is a square matrix whose ith row and jth column element is

$$[A]_{ij} = A_{ij} = 0 \text{ for } i = j$$

$$= 1 \text{ for } i, j \text{ adjacent}$$

$$= 0 \text{ otherwise.}$$

A six membered cyclic graph and its corresponding adjacency matrix ($\mathbf{A}$) are shown Figure 11 below.

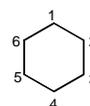**Figure 11:** A graph of 6-membered cycle with labelled vertices

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

2.13. Laplacian Matrix of a graph

Laplacian matrix (L) of a graph G is a square matrix whose ith row and jth column element is

$$[L]_{ij} = L_{ij} = d_j \quad \text{for} \quad j = i$$

$$= -1 \text{ for } i, j \text{ adjacent}$$

$$= 0 \text{ otherwise}$$

where d_j is the degree of the j th vertex.

A six membered cyclic graph shown in Figure 11 and its corresponding Laplacian matrix (L) are shown below.

$$\mathbf{L} = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

3. Where to apply graph theory

For a chemist or a physicist, geometric realization of a problem by a graph (namely collection of 'points' and of 'lines' joining some of these points) is more appealing. For this reason graph theory is becoming more and more acceptable tool for dealing with physico-chemical problems. The following correspondences between graphs and physical/chemical categories have found numerous applications in physics and chemistry:

A graph may correspond to a molecule i.e., points symbolise atoms and lines symbolise chemical bonds

A graph may correspond to a reaction mixture i.e., points symbolise chemical species and lines symbolise chemical conversion among the species

A graph may correspond to a system of interacting particles i.e., points symbolise particle and lines symbolise interaction among the particles.

Thus, a graph can be associated to any chemical or physical situation that has the above correspondence and the properties, which depend on the adjacency or connectivity, may be obtained from graphical operation.

4. Graph theory in some fields of chemistry

Although graph theory seemed to be insignificant at that time of its beginning due to its dealing with entertaining puzzles, its development during past few decades and subsequent applications in numerous fields have given strong impetus for its further enrichment. Due to its inherent simplicity, this theory has been used in a number of fields of

human thought and enriched several fields such as engineering, chemical, physical, social, biological, computer science, linguistics and many others. For instance, the connection between graph theory and chemistry, from the time of birth of the former, has enriched one another and now these two disciplines are so interrelated that very soon graph theory will be included in the chemistry curriculum. There are a large number of fields in chemistry where graph theory has been applied successfully; few such activities may be mentioned as follows.

Enumeration of isomers:

Enumeration of isomers i.e., to find out the number of isomers arising, either by addition to or substituting in, a parent molecule is a fundamental topics in Chemistry. During 1935-1937, G. Pólya [13] developed his powerful theorem for isomer enumeration problems in a direct and elegant manner. Now-a-days there are a large number of methods [7-10,13-19] to handle this problem, some of them are based on Pólya's theorem, while the others are based on double coset representation theory [20,21], the table of marks [22-25], and so on.

Enumeration of Kekulé structures

The study on the Kekulé valence structures [27-29] has been the focus of long time attractions for many researchers. Kekulé valence structures are important parameter to characteristic polycyclic conjugated hydrocarbon, to calculate molecular resonance energy, to predict aromaticity, to guess the reactivity, to assess the stability etc. of polycyclic aromatic hydrocarbons [26-28]. Graph theory can be applied for the enumeration of Kekulé structures in benzenoid hydrocarbons and their applications [30-44]

Some formulae of physicochemical importance

Some important formulae such as Euler's polyhedron formula, degree of unsaturations and nitrogen rule along with some of their consequences have been found to be derived graph theoretically using the concept of tree and can be found in several literatures [1-4, 45-49]

Investigation of structures and properties of fullerenes and other carbon cages

The discovery [50] of fullerenes in laser vapour of graphite has resulted in a surge of activity among theoeretical chemists to analyse the stability and structure of carbon clusters [46, 49, 50-70]. A

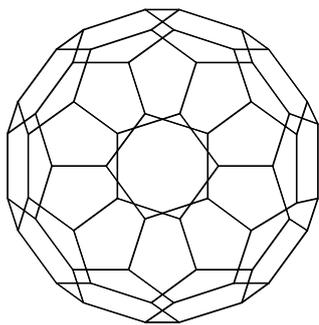Buckminster Fullerene (C$_{60}$) has been shown in the Figure 12 below.

Figure 12: Buckminster Fullerene (C$_{60}$)

Graphene is an allotrope of carbon and is basically monolayer of graphite, i.e., graphene sheets stack to form graphite. Hückel band structure of such graphene sheet has analytically been investigated by several authors..

Carbon nanotube, particularly single walled (SWNT) ones can be imagined to be formed by rolling a single layer graphite (i.e., graphene) sheet into a seamless cylinder and depending on mode of rolling up it can be armchair, zigzag, and chiral. The wrapping of graphene sheet can be represented by a pair of indices (n,m). Cnostruction of a nanotube by rolling up of a graphene sheet is shown in Figure 13. The integers, n and m, are the number of unit vectors along the two directions on the graphene sheet. If m = 0, the nanotube is zigzag (n,0), if n = m, it is armchair (n,n) and if n and m are different it is chiral (n,m).

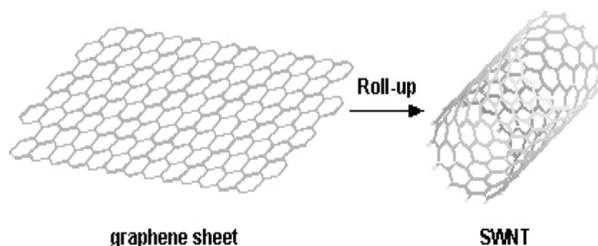**Figure 13:** Construction of nanotube by rolling up of a graphene sheet

Let us consider a nanotube graph which has length l (i.e., number of polyacene belt along the tube length) and circumference r (i.e., number of phenyl rings in each polyacene belt) as shown in the above Figure.

Carbon nanotubes bent into rings are latest nanostructure with surprising properties. Two ends of a nanotube can be glued to make a nanotorous. The amount of twist before two ends are glued result different kinds of nanotori. Here, we are considering only the simple one having zero twist before it gets glued.

Calculations of Hückel molecular orbitals (HMO) and related quantities

This includes characteristic polynomial (CP) coefficients, eigenvalues, eigenvectors, total π-electron energy, charge densities, bond orders etc. [71-78, 14, 30, 31, 79-97].

Search for topological indices and their applications

Topological indices of molecules are some numerical quantities that contain molecular information about the molecular graphs. In this area of theoretical chemistry, significant contributors are: H. Wiener, M. Randić, H. Hosoya, N. Trinajstić, R. E. Merrifield and H. E. Simmons. There are several topological indices e.g. Wiener index, Hosoya Index, Randić branching index, molecular identification number etc. that can be used to predict several molecular properties [30,14,98-114].

Solutions for coupled kinetic rate equations

Solution for multistep coupled kinetic rate equations to obtain the concentration of the species involved has also been carried out in the light of graph theory [115]. This concept has also been extended to the reactions involving linear chains and cycles [116].

Conclusion

As mentioned in this study, graph theory is an important tool to study several properties of molecules, since any molecular structure represents a graph. Although nowadays people are not relying on Hückel molecular orbital theory but in case of large molecules particularly, polycyclic hydrocarbons, fullerenes, nanotubes, nanotori etc., it is difficult to use other more accurate methods which are very satisfactory for small molecule, in that case HMO is convenient to use. Again to gain a first-hand insight still HMO is valuable tool for experimental chemists particularly, organic chemists. So there are many more things to do with HMO theory for polymers and other large polycyclic hydrocarbons.

Although a large number of topological indices were proposed and have been used to study quantitative structure activity relationship (QSAR) and quantitative structure property relationship (QSPR) but there are ample scope to develop algorithms to calculate such indices of some novel chemical compounds with biological importance and also to investigate interrelationship among the proposed indices.

References:

[1] O.Ore, *Graphs and their uses*, The L. W. Singer Company, New York (1963).

[2] F.Harary, *Graph Theory*, Addison- Wesley, Reading, Mass (1969)

[3] N. Deo, *Graph Theory With Applications to Engineering and Computer Science*, Prentice-Hall of India Private Limited, New Delhi (1997).

[4] R. J. Wilson, *Introduction to graph theory*, Longman Group Ltd., London (1978)

[5] L.Euler, *Comment. Acad. Sci. I. Petropolitanae*, **8**, 128 (1736); Translated in *Sci. Amer.*, **189**, 66 (1953).

[6] G. Kirchhoff, *Ann. Phys. Chem.*, **72**, 497 (1842).

[7] A. Cayley, *Philos. Mag.*, **13**, 19 (1857).

[8] A. Cayley, *Philos. Mag.*, **67**, 444 (1874).

[9] A. Cayley, *Ber. dtsch. Chem. Ges.*, **8**, 1056 (1875).

[10] A. Cayley, *Amer. J. Math.*, **4**, 266 (1881).

[11] J. J. Sylvester, *Amer. J. Math.*, **1**, 64 (1878).

[12] D. König, *Theorie Der Endlichen und Unenddlichen Graphen*, Leipzig (1936); Chelsea, New York (1951).

[13] G. Pólya, *Acta Math.*, **68**, 145 (1937).

[14] A. T. Balaban, (Eds.), *Chemical Applications of Graph Theory*, Academic Press, London (1976).

[15] A.T. Balaban, and Z. Simon, *Tertahedron*, **12**, 1511 (1967).

[16] D. H. Rouvray, *Chem. Soc. Revs.*, **3**, 355 (1974).

[17] J. V. Knop, W. R. Müller, K. Szymanski, and N. Trinajstić, *J. Comput. Chem.*, **7**, (1986).

[18] L. Bytautas, and D. J. Klein, *Theor. Chem. Acc.*, **101**, 371 (1999); *Croat. Chem. Acta*, **73**, 331 (2000).

[19] J. R. Dias, *J. Math. Chem.*, **9**, 253 (1992).

[20] E. Ruch, W. Hasselbarth and B. Ritcher, *Theoret. Chim Acta*, **19**, 288 (1970).

[21] J. Brocas, *J. Am. Chem. Soc.*, **108**, 1135 (1986).

[22] W. Hasselbarth, *Theoret. Chim Acta*, **67**, 339 (1985).

[23] S. Fujita, *Theoret. Chim Acta*, **76**, 247 (1989).

[24] S. Fujita, *Bull. Chem. Soc. Jpn.*, **63**, 2759 (1990).

[25] S. Fujita, *Bull. Chem. Soc. Jpn.*, **64**, 3255 (1991).

[26] T. C. Bhadra, *Indian J. Phys.*, **49,** 746 (1975).

[27] S. J. Cyvin, I. Gutman, Kekulé *Structures in Benzenoid Hydrocarbons*, Springer-Verlag, Berlin, 1988.

[28] W. C. Herndon, *J. Chem. Educ.*, **51,** 10 (1974).

[29] M. Randić, *Chem. Rev.*, **103,** 3449 (2003).

[30] I. Gutman, and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, New York (1986).

[31] J. R. Dias, *Molecular Orbital Calculations Using Chemical Graph Theory*, Springer-Verlag, New York (1993).

[32] D. J. Klein, Rep. *Molec. Theor.*, **1**, 91 (1990).

[33] D. J. Klein, *Chem. Phys. Lett.*, **217**, 261 (1994).

[34] H. Hosoya, H. Kumazaki, K. Chida, M. Ohuchi, and Y. D. Gao, *Pure & Appl. Chem.*, **62**, 445 (1990).

[35] D. J. Klein, M. J. Cravey, and G. E. Hite, *Polycyclic Aromatic Compounds*, **2**, 163 (1991).

[36] J. R. Dias, *J. Chem. Inf. Comput. Sci.*, **36**, 361 (1996); *J. Phys. Org. Chem.*, **15**, 94 (2002).

[37] I. Gutman, *Rep. Molec. Theor.*, **1**, 115 (1990).

[38] I. Gutman, *Z. Naturforsch.*, **41a**, 1089 (1986).

[39] I. Gutman, and Ž Tomović, *Indian J. Chem.*, **40A**, 678 (2001).

[40] S. Klavžar, P. Žigert, and I. Gutman, *J. Mol. Struct. (Theochem)*, **586**, 235 (2002).

[41] N. Ohkami, and H. Hosoya, *Theoret. Chim. Acta (Berl.)*, **64**, 153 (1983).

[42] S. El-Basil, and A. N. Osman, *Int. J. Quantum Chem.*, **24**, 571 (1983).

[43] E. C. Kirby, *J. Chem. Soc. Faraday Trans.*, **86**, 447 (1990).

[44] P. Ghosh and B. Mandal, *J. Math. Chem.*, **48**, 1069 (2010).

[45] J. K.Senior, *J. Chem. Phys.*, **19**, 865 (1951).

[46] D. E. Manolopoulos, and P. W. Fowler, *An Atlas of Fullerenes*, Clarendon Press, Oxford (1992).

[47] L. Euler, Elementa doctrinae solidorum, *Novi. Comment. Acad. Sci. I. Petropolitanae*, **4**, 109 (1758).

[48] V. Pellegrin, *J. Chem. Educ.*, **60**, 626 (1983).

[49] B. Mandal, *Chem. Phys. Lett.*, **417**, 395-400 (2006).

[50] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl and R. E. Smalley, Nature, 318 (1985) 162.

[51] B. Mandal, M. Banerjee and A. K. Mukherjee, *Phys. Chem. Chem. Phys.*, **6**, 2040 (2004).

[52] B. Mandal, M. Banerjee and A. K. Mukherjee, *Int. J. Quantum Chem.*, **101**, 119 (2005).

[53] H. W. Kroto, J.R. Heath, S. C. O'Brien, R.F. Curl, and R. E. Smalley, *Nature*, **318**, 162, (1985).

[54] W. Krätschmer, L. D. Lamb, K. Fostiropoulos, and D.R. Huffman, *Nature*, **347**, 354 (1990).

[55] H. W. Kroto, *Nature*, **329**, 529 (1987).

[56] R. E. Smalley, *Acc. Chem. Res.*, **25**, 98 (1992).

[57] D. J. Klein, W. A. Seitz, and T. G. Schmalz,, *Nature*, **323,** 703 (1986); *J. Phys. Chem.*, **97**, 1231 (1993).

[58] D. J. Klein, W.A. Seitz, and T. G. Schmalz, *J. Phys. Chem.*, **97**, 1231 (1993).

[59] P. W. Fowler, *Chem Phys Lett.*, **131**, 444 (1986); *J. Chem. Soc. Faraday Trans.*, **86**, 2073 (1990).

[60] P. W. Fowler and J. I. Steer, *J. Chem. Soc. Chem. Commun.*, 1403 (1987).

[61] D. E. Manolopoulos, J. C. May, and S. E. Down, *Chem. Phys. Lett.*, **181**, 105 (1991).

[62] R. Friedberg, T. D. Lee, and H. C. Ren, *Phys. Rev.*, **B46**, 14150 (1992).

[63] Y. L. Lin, and F. Nori, *Phys. Lett. A*, **183**, 214 (1993); *Phys. Rev.*, **B49**, 5020 (1994).

[64] A. Ceulemans, and P.W. Fowler, *J. Chem. Soc. Faraday Trans.*, **91**, 3089 (1995).

[65] J. Cioslowski, *Electronic Structure Calculations on Fullerenes and Their Derivatives*, Oxford University Press, New York, 1995.

[66] R. C. Haddon, L. E. Brus, and L. Raghavachari, *Chem. Phys. Lett.*, **125**, 459 (1986).

[67] D. B. Redmond, C. M. Quinn, and P. W. Fowler, *J. Math. Chem.*, **23**, 263 (1998).

[68] P. W. Fowler, and K. M. Rogers, *J. Chem. Soc. Faraday Trans.*, **94**, 1019 (1998).

[69] J. R. Dias, *J. Chem. Educ.*, **66**, 1012 (1989).

[70] T. G. Schmalz, W.A. Seitz, D. J. Klein, and G. E. Hite, *J. Am. Chem. Soc.*, **110**, 1113 (1988)

[71] E. Hückel, *Z. Physik,* **70**, 204 (1931); **76**, 628 (1932).

[72] C. A. Coulson, and G. S. Rushbrooke, *Proc. Camb.. Philos. Soc.*, **36**, 193 (1940).

[73] D. E. Rutherford, *Proc. R.. Soc. Edinb.*, **A62,** 229, (1946).

[74] C. A. Coulson, *Proc. Camb. Philos. Soc.*, **46**, 202 (1950).

[75] C. A. Coulson, and A. Jr. Streitwieser, *Dictionary of π-electron calculations*, Pergamon Press, Oxford (1965).

[76] H. Sachs, *Publ. Math. (Debrecen)*, **11**, 119 (1963).

[77] H. H. Gunthard, and H. Primas, *Helv. Chim. Acta*, **39**, 1645 (1956).

[78] H. H. Schmidtke, *J. Chem. Phys.*, **45**, 3920 (1966).

[79] D. M. Cvetković, M. Doob, and H. Sachs, *Spectra of Graphs: Theory and Application*, Academic Press, San Diego, CA (1979).

[80] A. Jr. Streitwieser, *Molecular Orbital Theory for Organic Chemists*, John Wiley & Sons, Inc., New York (1961).

[81] A. Graovac, I. Gutman, and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer, New York (1977).

[82] A. J. Kassam, *Theoret. Chim. Acta*, **67**, 255 (1985).

[83] (a) A. K. Mukherjee, and K. K. Datta, *Proc. Indian Acad. Sci. (Chem. Sci.)*, **101**, 499 (1989); (b) A. K. Mukherjee, and D. K. Das, *Proc. Indian Acad. Sci. (Chem. Sci.)*, **105**, 111 (1993).

[84] (a)R. K. Mishra, B. K. Mishra, and S. Singh, *Indian J. Chem.*, **27A**, 377 (1988); (b) S.

Singh, R. K. Mishra, and B. K. Mishra, *Indian J. Chem.*, **27A**, 653 (1988).

[85] B. Mandal, K. Datta, A. K. Mukherjee and M. Banerjee, *Molec. Phys.*, **96**, 1609 (1999).

[86] B. Mandal, *Int. J. Quantum Chem.*, **103**, 140-148 (2005).

[87] B. Mandal, K. Datta, M. Banerjee and A. K. Mukherjee, *Int. J. Quantum Chem.*, **105**, 201 (2005).

[88] B. Mandal, *Bull. Chem. Soc. Jpn.*, **81**, 956 (2008).

[89] A. S. Tiwary, B. Mandal and A. K. Mukherjee, *Mol. Phys.*, **106**, 1813 (2008).

[90] P. Ghosh, T. Ghosh and B. Mandal, *Mol. Phys.*, **109,** 267 (2011).

[91] D. D. Keeports, *Theoret. Chim. Acta.*, **67**, 491 (1985).

[92] T. Lu, A. Tachinaba and T. Yamabe, *Int. J. Quantum. Chem.*, **38**, 559 (1990).

[93] R. Blankenbecler, D. J. Scalapino and R. L. Sugar, *Phys. Rev.* D, **24**, 2278 (1984).

[94] S. E. Koonin, D. J. Dean and K. Langanke, *Phys. Rep.*, **278**, 1 (1997).

[95] O. Hod, E. Rabani and R. Baer, *Acc. Chem. Res.*, **39**, 109 (2006).

[96] D. Roy, *J. Phys. Cond. Mat.*, **20**, 025206 (2008).

[97] C. Joachim and A. Ratner, *Proc. Natl. Acad. Sci.*, **102**, 8801 (2005).

[98] D. J. Klein and M. Randić, (Eds.), *Mathematical Chemistry*, VCH, Weinheim (1990).

[99] N. Trinajstić, Chemical *Graph Theory*, CRC Press, Boca Raton, FL (1992).

[100] A. T. Balaban, (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach Science Publishers, The Netherlands, 1999.

[101] R. E. Merrifield, and H. E. Simmons, Topological *Methods in Chemistry*, Wiley, New York (1989).

[102] M. A. Johnson, and G. M. Maggiora, *Concepts and Applications of Molecular Similarity*, Wiley Interscience Publication, 1990.

[103] H. Wiener, *J. Am. Chem. Soc.*, **69**, 17 (1947); *J. Phys. Chem.*, **52**, 1082 (1948).

[104] M. Randić, *J. Am. Chem. Soc.*, **97**, 6609 (1975).

[105] H. Hosoya, *Bull. Chem. Soc. Japan*, **44**, 2332 (1971).

[106] H. Hosoya, *J. Chem. Docum.*, **12**, 181 (1972).

[107] H. Hosoya, K. Kawasaki, and K. Mizutani, *Bull. Chem. Soc. Japan*, **45**, 3415 (1972).

[108] H. Narumi, and H. Hosoya, *Bull. Chem. Soc. Japan*, **53**, 1228 (1980).

[109] R. E. Merrifield and H.E. Simmons, *Proc. Natl. Acad. Sci., USA*, **82**, 1 (1985).

[110] Randić, M., *J.Chem.Inf. Comput. Sci.*, **19**, 31 (1980).

[111] P. J. Hansen and P. C. Jurs, *J. Chem. Educ.*, **65**,574 (1988).

[112] B. Mandal, M. Banerjee and A. K. Mukherjee, *Int. J. Quantum Chem.*, **99**, 119 (2004).

[113] B. Mandal, M. Banerjee and A. K. Mukherjee, *Molec. Phys.*, **103**, 2665 (2005).

[114] S. Basu, P. Ghosh and B. Mandal, *Mol. Phys.*, **106**, 2507 (2008).

[115] S. Karmakar, and B. Mandal, *J. Phys.Chem. A*, **118**, 1155 (2014)

[116] S. Karmakar, and B. Mandal, *J. Phys.Chem. A*, **118**, 7672 (2014)