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REMOVAL OF DEGENERACY IN THE TOPOLOGICAL INDICES OF COSPECTRAL GRAPHS USING EDGE WEIGHTED MOLECULAR GRAPHS

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Abstract

Two graphs having the same number of vertices connected in the same way are said to be isomorphic. Topological matrices representing such graphs will have the same eigen value spectrum. Hence isomorphic graphs are also known as co spectral or iso spectral graphs. There are certain molecular graphs representing chemically different substances which are found to be co spectral graphs. Therefore the molecular descriptors calculated using topological matrices will not be able to distinguish between these molecules. Under such circumstances, edge weighted topological matrices can be formulated so that, their eigen value spectrum will be unique. The edge weighted molecular graphs with bond length as the weight for the edges in adjacency and distance matrices distinguish between the molecules having similar molecular graphs. So different molecules having the same molecular graph will have the same topological indices, but the edge weighted adjacency and distance matrices have the ability to overcome this problem of degeneracy.

Keywords: Co spectral graphs, topological indices, edge weighted topological matrices.

Introduction

Graph theory is a branch of Mathematics that analyses any system on the basis of a fundamental quality known as connectivity between various objects or topology of the system. Graphs can be used to model many types of relations and processes in physical, biological, social and information systems. A chemical graph is a mathematical structure which provides a pictorial representation of a molecule, taking into account the internal connectivity of atoms in the molecule through bonds. The molecular connectivity determines a number of properties of the chemical systems. Therefore many predictions can be made regarding the physico-chemical properties of the molecules using chemical graph theory.

Nenad Trinajstic [1] has shown that many quantum mechanical results can be derived or rederived using spectral properties of associated graphs. Saraswathi Vishveshwara, K.V.Brinda and N.Kannan [2] have used graph spectral properties to study the protein structure, protein dynamics and protein-protein interactions. Mathavi Manisekar and S.Lalitha have used the techniques of chemical graph theory to find the centre of amino acids [3]. G.Al Hagri, M.El. Marraki and M.Essalih [4] have shown the effectiveness of the degree distance of a graph as a successful structure descriptor and in the prediction of the boiling points and calculation of ultrasonic velocity in organic material. Roberto Todeschini and Viviana Consonni [5] have discussed a number of molecular descriptors with appropriate examples known till 2009. Chemical graph theory finds applications in reaction networks also Gábor Szederkényi [6] has illustrated that two different reaction networks with mass action kinetics may have the same differential equation description even if the source complexes are not the same in the reaction system.

Any chemical / molecular graph having N vertices can be represented by an NxN symmetric matrix, known as topological matrix. . There are different kinds of topological matrices like adjacency matrix, distance matrix, reciprocal distance matrix, Laplacian matrix and so on [7]. The set of eigen values of such a matrix is known as the spectrum of the graph and the sum of the absolute eigen values is termed as the energy of the graph.

The adjacency matrix [8]

The most simple and effective matrix of a molecular graph is the Adjacency matrix (A). The adjacency matrix of a molecular graph having N vertices is a square N x N symmetric matrix which is defined as

$$[A]_{ij} = \begin{cases} 1 \text{ if } i \neq j \text{ and } e_{ij} \in E(G) \\ 0 \text{ if } i=j \text{ or } e_{ij} \notin E(G) \end{cases} \quad (1)$$

where e_{ij} is the edge between i and j and E (G) is the set of edges of the graph G.

The Distance Matrix[8]

The distance matrix (D) of a molecular graph having N vertices is a real symmetric N x N square matrix, whose elements $[D]_{ij}$ represent the minimum distance or minimum length of the path between the vertices i and j in terms of the number of edges between them.

$$[D]_{\mathbf{ij}} = \begin{cases} \min (l (\mathbf{p}_{ij})) \quad \text{if} \quad i \neq j \\ 0 \text{ if } i = j \end{cases} \quad (2)$$

where p_{ij} is the number of edges separating the vertices i and j.

Vertex and edge weighted topological matrix

A vertex and edge weighted graph [1] is a graph having one or more vertices or edges which can be distinguished from the other vertices and edges. A number (the weight) may be assigned to each one of such vertices and edges in a weighted graph. Such weights for a vertex might represent for example the atomic weights, number of free electrons, etc., and for the edge, the bond lengths, number of bonds, the length of a route, the capacity of a line, the energy required to move between locations along a route, etc., depending on the problem in hand. The corresponding topological matrices are known as vertex or edge weighted matrices.

Co spectral graphs

Two graphs having the same number of vertices connected in the same way are said to be isomorphic. Topological matrices representing such graphs will have the same eigen value spectrum. Hence isomorphic graphs are also known as co spectral or iso spectral graphs [1]. There are certain molecular graphs representing chemically different substances which are found to be co spectral graphs. Therefore the molecular descriptors calculated using topological matrices will not be able to distinguish between these molecules. Under such circumstances, edge weighted topological matrices can be formulated so that, their eigen value spectrum will be unique. To illustrate this fact, a set of co spectral graphs representing the molecules Methane (CH_4), Carbon tetra fluoride (CF_4), Carbon tetra chloride (CCl_4), Carbon tetra bromide (CBr_4) and Carbon tetra iodide (CI_4) are considered. Fig.1 is the molecular graph of all the above mentioned molecules.

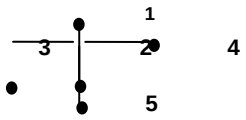

Fig.1

The atoms are labelled as 1,2,3,4 and 5. Atom 2 is carbon atom. Atoms 1,3,4, and 5 represent H, F, Cl, Br and I atoms in the respective molecules.

The adjacency matrix of this graph is

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

The eigen values of this matrix are -2, 0 ,0,0, 2.

The graph energy , E = 4, which is the same for all the five molecules, CH_4, CCl_4, CF_4, CBr_4 and CI_4. This degeneracy can be lifted if the edge weighted adjacency matrices are considered. Here, the actual bond length is substituted in the place of '1' in the adjacency matrix. The length of C – H bond is 1.14 Aº. The edge weighted adjacency matrix $A_{(EW)}$, thus formulated for CH_4 is given below.

$$A_{(EW)} = \begin{pmatrix} 0 & 1.14 & 0 & 0 & 0 \\ 1.14 & 0 & 1.14 & 1.14 & 1.14 \\ 0 & 1.14 & 0 & 0 & 0 \\ 0 & 1.14 & 0 & 0 & 0 \\ 0 & 1.14 & 0 & 0 & 0 \end{pmatrix}$$

Now the graph energy is 4.56. Table 1 gives the edge weighted adjacency matix energies of CH_4, CCl_4, CF_4, CBr_4 and CI_4 . These values are unique for each molecule.

Table 1:

S.No.	Molecule	BondLength (A°) [9]	Molecular weight	Edge weighted Adjacency matrix energy
1.	CH_4	1.14	16.04	4.56
2.	CF_4	1.35	88.00	5.40
3.	CCl_4	1.77	153.82	7.08
4.	CBr_4	1.94	331.63	7.76
5.	CI_4	2.13	519.60	8.52

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A graph is drawn between the molecular weights (x) and the corresponding energies(y) of edge weighted adjacency matrices. Fig.2 shows the linear relationship between the molecular weight and graph energy.

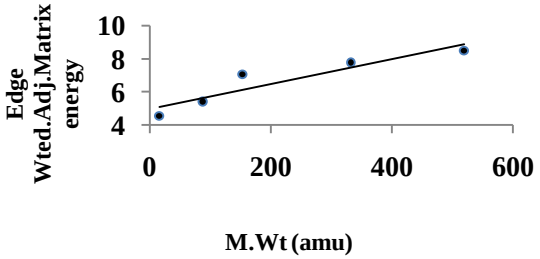

Fig.2. Edge weighted Adjacency Matrix Energy Vs Molecular weight

for CH_4, CF_4, CCl_4,CBr_4 and CI_4 molecules

The edge weighted adjacency matrix energies for the molecules Fluoromethane (**CH_3F),** Chloromethane **(CH_3Cl),** Bromomethane **(CH_3Br)** and Methyl iodide (**CH_3I)** are evaluated and given in Table 2.

Table 2:

S. No.	Molecule	Molecular weight	Edge weighted Adj, matrix energy
1.	CH_4	16.04	4.560
2.	CH_3F	34.03	4.784
3.	C H_3Cl	50.49	5.303
4.	C H_3Br	94.94	5.536
5.	C H_3I	141.94	5.808

A graph is drawn between the molecular weights (x) and the corresponding energies (y) of edge weighted adjacency matrices of chemical graphs of the molecules CH_4, CH_3F, CH_3Cl, CH_3Br and CH_3I. Fig.3 shows the linear relationship between the molecular weight and graph energy.

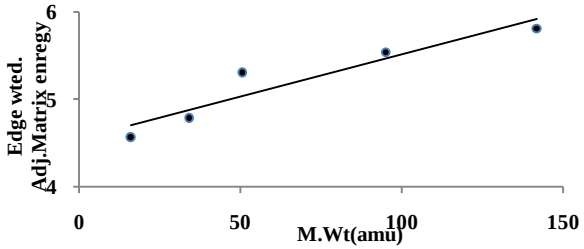

Fig.3 Edge weighted Adjacency Matrix Energy Vs Molecular weight

for CH_4, CH_3F, CH_3Cl, CH_3Br and CH_3I molecules

Similarly in formulating the edge weighted distance matrix, the appropriate bond lengths are added to get the distance between the vertices. Thus the degeneracy in Wiener index can be lifted.

The distance matrix of CH_4 is

$$D = \begin{pmatrix} 0 & 1 & 2 & 2 & 2 \\ 1 & 0 & 1 & 1 & 1 \\ 2 & 1 & 0 & 2 & 2 \\ 2 & 1 & 2 & 0 & 2 \\ 2 & 1 & 2 & 2 & 0 \end{pmatrix}$$

The energy of this matrix is 13.21. The Wiener number W, and Wiener index W are calculated using this matrix using the following definitions [5].

$$W = \tfrac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} d_{ij} \qquad (1)$$

$$\overline{W} = 2W / N(N-1) \quad (2)$$

Where N is the number of vertices and d_{ij} is the distance between the vertices in terms of number of edges. The values are : Wiener number = 16 and Wiener Index, W.I. = 1.6.

The edge weighted distance matrix of CH_4 is

$$D_{EW} = \begin{pmatrix} 0 & 1.14 & 2.28 & 2.28 & 2.28 \\ 1.14 & 0 & 1.14 & 1.14 & 1.14 \\ 2.28 & 1.14 & 0 & 2.28 & 2.28 \\ 2.28 & 1.14 & 2.28 & 0 & 2.28 \\ 2.28 & 1.14 & 2.28 & 2.28 & 0 \end{pmatrix}$$

The energy of this matrix is 15.06.

Table 3 gives the energies of the edge weighted distance matrix of CH_4, CF_4, CCl_4, CBr_4 and CI_4.

Table 3:

S.No.	Molecule	Molecular weight (amu)	Edge weighted Distance Matrix energy	Edge weighted	
				W.No.	W.I.
1.	CH_4	16.04	15.06	18.24	1.82
2.	CF_4	88.00	17.00	21.40	2.14
3.	CCl_4	153.80	23.38	28.32	2.83
4.	CBr_4	331.60	25.62	31.04	3.10
5.	CI_4	519.60	28.14	34.08	3.41

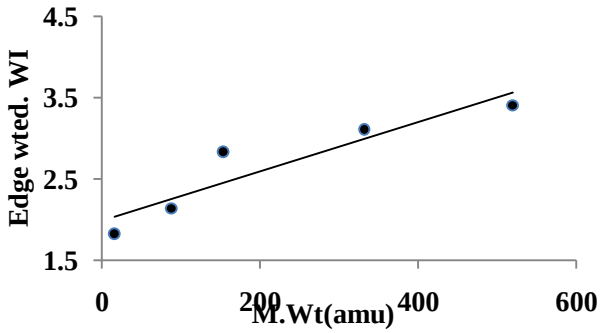

Fig: 4 Edge weighted Wiener index Vs Molecular weight for CH_4, CF_4, CCl_4,

A graph is drawn between the molecular weight and the Wiener index calculated using the edge weighted distance matrices. Fig. 4 shows this relationship.

CBr_4 and CI_4 molecules

Table 4 gives energies of the edge weighted distance matrices of the molecules CH_3F, CH_3Cl, CH_3Br, CH_3I, and the values of Wiener number and Wiener index for the same, which are proportional to the corresponding molecular weights.

Table 4:

S.No.	Molecule	Molecular weight (amu)	Edge weighted Dist. Matrix energy	Edge weighted	
				W.No.	W.I.
1.	CH_4	16.04	15.060	18.24	1.824
2.	CH_3F	34.03	15.764	19.08	1.908

3.	CH_3Cl	50.49	17.224	20.76	2.076
4.	CH_3Br	94.94	17.830	21.44	2.144
5.	CH_3I	141.94	18.510	22.20	2.220

From Fig.5 it is seen that the molecular weights and Edge weighted Wiener index of CH_4, CH_3F, CH_3Cl, CH_3Br and CH_3I molecules have a linear relationship with each other.

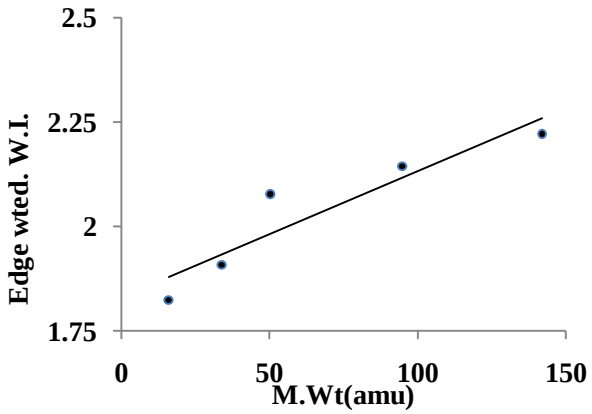

Fig. 5 Molecular weight Vs Edge weighted Wiener index

for CH_4, CH_3F, CH_3Cl, CH_3Br and CH_3I molecules

Conclusion

Thus it has been shown that the edge weighted graphs with bond length as the weight for the edges in adjacency and distance matrices distinguish between the molecules having similar molecular graphs.

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