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Molecular topological index of tree with equal number of vertices of a given degree

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Abstract. Adjacency between vertices, degree of the vertices and distance between every pair of vertices are the graph properties used in the calculation of molecular topological index. More the number of properties, the calculation complexity increases. In this paper we propose a method of determining the molecular topological index of trees with equal number of vertices of a given degree from triangular matrices. Also determining the molecular topological index of such trees from its subtree is also determined.

1. Introduction
Topological indices are calculated using graph properties. A topological index can be viewed as a value determined from a graph using graph properties like degree, distance,adjacency. These values are of use in determination of chemical properties. Different topological indices are used in different property determination. The Wiener and Wiener Topological Index is used in determination of boiling point of chemicals. Calculation of these indices depends on the techniques used. In general these indices are calculated using matrices. In this paper we provide a method to determine the Molecular Topological Index of trees having equal number of vertices of a given degree from a triangular matrix.

2. Preliminaries
Graph
In a mathematician's terminology, a graph is a collection of points and lines connecting some subset of them. The points of a graph are most commonly known as graph vertices, but may also be called nodes or simply points. Similarly, the lines connecting the vertices of a graph are most commonly known as graph edges, but may also be called arcs or lines [1]. A weighted graph is a graph in which each edge is assigned some numerical value called the weight of the graph. Snapshot – 1 [2] provides an example of graph.

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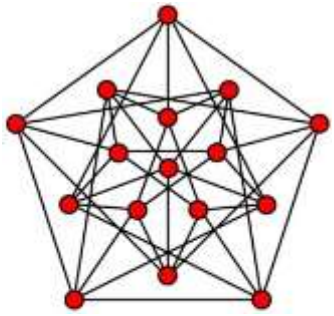


Snapshot – 1.

Path

In graph theory, a path in a graph is a finite or infinite sequence of edges which connect a sequence of vertices which, by most definitions, are all distinct from one another [3]. A path with n – vertices is denoted by P_n. Examples of paths with n = 1, 2, 3, 4 vertices are shown in Fig. 1.

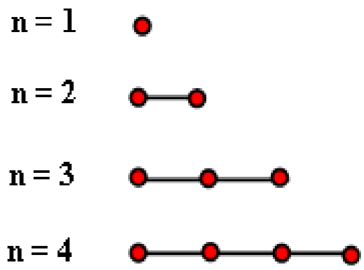
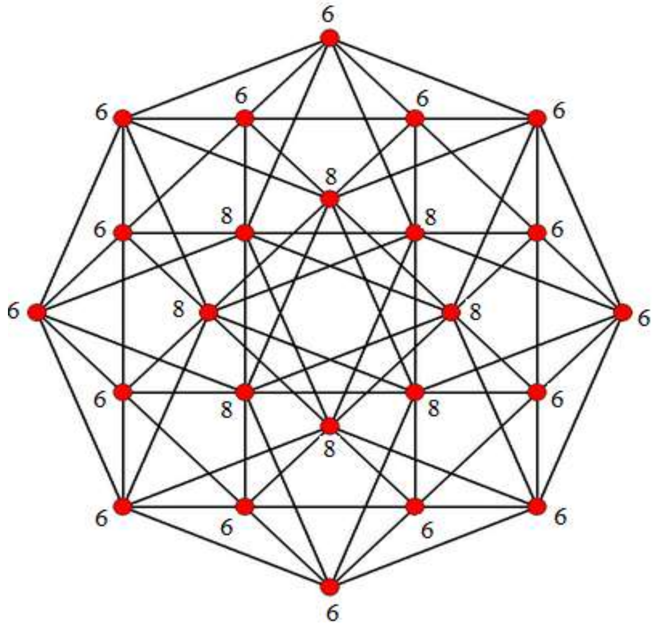


Figure 1.

Degree

In graph theory, the degree (or valency) of a vertex of a graph is the number of edges incident to the vertex, with loops counted twice. The degree of a vertex is denoted by d(G) or deg(G). The maximum degree of a graph G, denoted by Δ(G), and the minimum degree of a graph, denoted by δ (G) [4]. Snapshot – 2 provides an example of a graph with vertices labeled by degree [5].



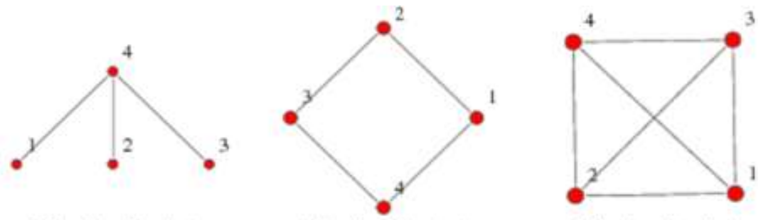
Snapshot – 2.

Adjacency matrix

The adjacency matrix of a graph G with n vertices and no parallel edges is an n by n symmetric binary matrix X = [x_{ij}] defined as follow

x_{ij}=1, if there is an edge between i^{th} and j^{th} vertices, and
= 0, if there is no edge between them[6]

Snapshot – 3 [7] provides an example for adjacency matrix.

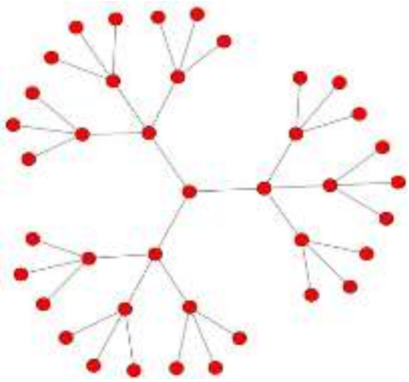


$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Snapshot – 3.

Tree

A tree is a connected graph in which any two vertices are connected by exactly one path [8].Snapshot – 4 provides an example of a tree [9].



Snapshot – 4.

Rooted tree

A rooted tree is a tree with a countable number of nodes, in which a particular node is distinguished from the others and called the root node[10]. In a rooted tree, the parent of a vertex is the vertex connected to it on the path to the root; every vertex except the root has a unique parent. A child of a vertex v is a vertex of which v is the parent. A descendent of any vertex v is any vertex which is either the child of v or is (recursively) the descendent of any of the children of v. A sibling to a vertex v is any other vertex on the tree which has the same parent as v[11]. Fig. 2 provides an example of a rooted tree. The root vertex is encircled.

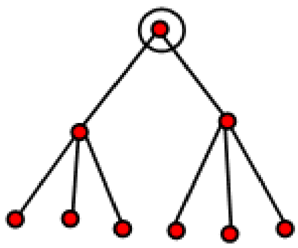


Figure 2.

Tree levels

The level of a tree as the number of parent nodes a tree node has. The root of the tree, therefore, is at level 0. Root's children are at level 1, etc. In general, each level of a binary tree can have, at most, 2^N nodes, where N is the level of the tree [12]. Fig. 3 provides an example of tree levels.

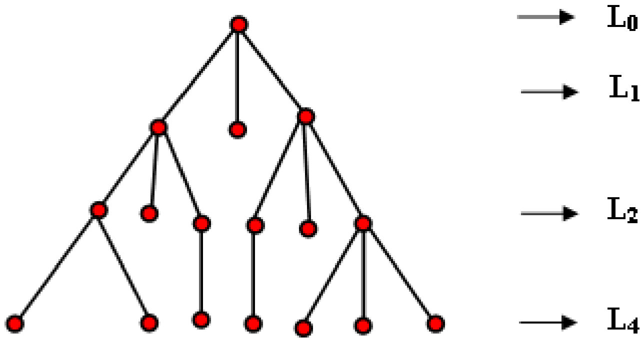


Figure3.

Molecular topological indices

The molecular topological index is a graph index defined by

$$\mathrm{MTI} = \sum_{i=1}^{n} E_i ,$$

where E_i are the components of the vector E = (A + D) d with A the adjacency matrix, D the graph distance matrix, and d, the vector of vertex degrees of a graph.The molecular topological index is well– defined only for connected graphs, being indeterminate for disconnected graphs having isolated nodes and infinity for all other disconnected graphs[13] . In [14] a selection of the most important graph descriptor's and topological indices including molecular matrices graph spectral moments graph polynomials and vertex topological indices is presented. In [15] the matrix expression topological index and atomic attribute of molecular topological structure are reviewed. In [16] topological indices are determined for some members isomers of decane. In [17] a focus on the theoretical analysis of topological indices expression for molecular structures is presented. In [18] the molecular topological index is extended to heterosystems.In this paper we determine the molecular topological index of degree symmetric trees.

3. Molecular topological index for a degree symmetric tree

To determine the Molecular Topological Index we use adjacency and distance matrices.We know that the adjacency and distance matrices are symmetric matrices. Since matrix multiplication is used in the calculation generally the symmetric properties of these matrices cannot be considered.We mean to insist here that in general when matrices are symmetric, the upper or lower triangular part of the matrix would be sufficient for calculations.This cannot be so in this case,since matrix multiplication is also implemented.We now track out trees for which the symmetric property of these matrices could benefit in molecular topological Index calculation.Let T be a tree with n vertices having equal number of vertices of any given degree.If n is odd,then T has n– 1 distinct pair of vertices with same degree.

3.1. Label assignment to the vertices

We know that, T has n vertices.When n is even,T has n/2 distinct pair of vertices with a given degree.Letn/2=k_1.Label the vertices as $v_1,v_2,\ldots,v_{k1}$ such that $(v_1,u_1),(v_2,u_2),\ldots,(v_{k1},u_{k1})$ have same degree. If n is odd,then we have (n– 1)/2 vertex pairs with same degree,so that k_1 = (n– 1)/2.We assign the vertex labels as 1,2,…, n in the following fashion $(u_1,v_1),(u_2,v_2),\ldots,(u_{k1},v_{k1})$ receives the label (1,n),(2,n– 1),…, (n/2,(n+1)/2),then n is even and (1,n),(2,n– 1),…,((n– 1)/2,(n+3)/2), when n is odd.

In case of odd number of vertices assign the label (n+1)/2 to the left over single vertex say vertex w. As an illustration, consider the following trees in Figure 4.

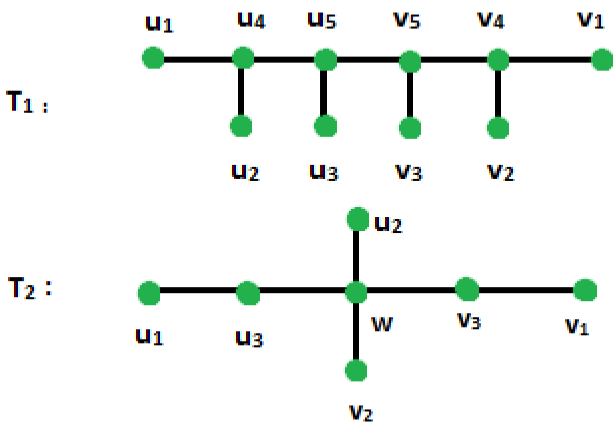


Figure 4.

T_1 has 6 vertices of degree 1 and 4 vertices of degree 3.T_1 has 10 vertices with 3 pairs (u_1,v_1),(u_2,v_2),(u_3,v_3) with degree 1 and 2 pair of vertices (u_4,v_4) and (u_5,v_5) with degree 3 each. As discussed assign the labels (1,10),(2,9),(3,8),(4,7),(5,6) to these pairs.The resulting labeled tree is seen in Figure 5.

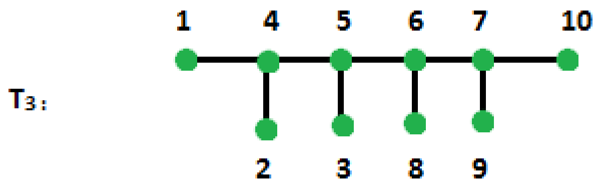


Figure 5.

T_2 has 7 vertices with 2pairs (u_1,v_1),(u_2,v_2) of degree 1 and 1 pair (u_3,v_3) with degree 2 and a single vertex w with degree 4 respectively.Assign the labels (1,7), (2,6),(3,5) to the pairs (u_1,v_1),(u_2,v_2), (u_3,v_3).Vertex w receives the label 4.The resulting labeled tree is seen in Figure 6.

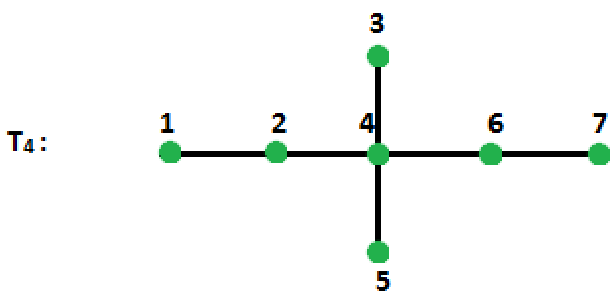


Figure 6.

We know that Adjacency and Distance matrix are n×nmatrices.Arrange the rows and columns of these matrices in the following order.

$u_1,u_2,\ldots,u_{k1},v_{k1},v_{k1-1},\ldots,v_2,v_1$,when n is even and $u_1,u_2,\ldots, u_{k1},w, v_{k1},v_{k1-1},\ldots,v_2,v_1$,when n is odd. The Adjacency and Distance matrices for trees T_3 and T_4 following this labeling is given below. Let us label the Adjacency matrix of any tree T_i as $A(T_i)$ and the Distance matrix of any tree as $D(T_i)$. We know that to find molecular topological index, we multiply matrix A+D with the degree sequence vector. Consider the degree sequence vector as in $[u_1\ u_2\ \ldots\ u_{k1}v_{k1}\ v_{k1-1}\ldots\ v_2\ v_1]^T$when n is even and $[u_1\ u_2\ \ldots\ u_{k1}\ \ w\ v_{k1}\ v_{k1-1}\ \ldots\ v_2\ v_1]^T$,when n is odd. For Trees T_3 and T_4, the degree sequence vector is $[1\ 1\ 1\ 3\ 3\ 3\ 3\ 1\ 1\ 1\ ]^T$ and $[1\ 1\ 2\ 4\ 2\ 1\ 1]^T$ respectively. We notice that the degree sequence vector is symmetric. We know that A+D is the symmetric matrix, since A+D is symmetric. We know that if A+D has n rows, then the row pair (1,n), (2,n– 1),…,(n/2,(n+1)/2), then n is even and (1,n),(2,n– 1),…,((n– 1)/2,(n+3)/2), when n is odd have the entries arranged in reverse orders. i.e., if row 1 entry is $a_1,a_2,\ldots,a_n$, then row n entry is $a_n,a_{n-1},\ldots,a_2,a_1$. Since the degree sequence vector v is symmetric, $u_1 \times v$ and $v_1 \times v$ will have the same value. Similarly, the other row pairs $(u_2,v_2),\ldots,(u_{k1},v_{k1})$ also will have same value when multiplied with degree vector. Hence it is sufficient to consider A+D to be a triangular matrix. From this we conclude that, when A+D is treated as a triangular matrix, (A+D) v = (½) (A+D)v , when (A+D) is regular matrix.For Trees T_1 and T_2, the Molecular Topological Index calculation is given below.

First we calculate Molecular Topological Index for tree T_1.

$$A(T_1)=\begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\end{array}\begin{array}{c}\begin{array}{cccccccccc}1&2&3&4&5&6&7&8&9&10\end{array}\\ \begin{bmatrix}0&0&0&1&0&0&0&0&0&0\\0&0&0&1&0&0&0&0&0&0\\0&0&0&0&1&0&0&0&0&0\\1&1&0&0&1&0&0&0&0&0\\0&0&1&1&0&1&0&0&0&0\\0&0&0&0&1&0&1&1&0&0\\0&0&0&0&0&1&0&0&1&1\\0&0&0&0&0&1&0&0&0&0\\0&0&0&0&0&0&1&0&0&0\\0&0&0&0&0&0&1&0&0&0\end{bmatrix}\end{array}$$

$$D(T_1)=\begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\end{array}\begin{array}{c}\begin{array}{cccccccccc}1&2&3&4&5&6&7&8&9&10\end{array}\\ \begin{bmatrix}0&2&3&1&2&3&4&4&5&5\\2&0&3&1&2&3&4&4&5&5\\3&3&0&2&1&2&3&3&4&4\\1&1&2&0&1&2&3&3&4&4\\2&2&1&1&0&1&2&2&3&3\\3&3&2&2&1&0&1&1&2&2\\4&4&3&3&2&1&0&2&1&1\\4&4&3&3&2&1&2&0&3&3\\5&5&4&4&3&2&1&3&0&2\\5&5&4&4&3&2&1&3&2&0\end{bmatrix}\end{array}$$

$$[(A(T_1)+D(T_1)]\,v(T_1)=\begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10\end{array}\begin{array}{c}\begin{array}{cccccccccc}1&2&3&4&5&6&7&8&9&10\end{array}\\ \begin{bmatrix}0&2&3&2&2&3&4&4&5&5\\2&0&3&2&2&3&4&4&5&5\\3&3&0&2&2&2&3&3&4&4\\2&2&2&0&2&2&3&3&4&4\\2&2&2&2&0&2&2&2&3&3\\3&3&2&2&2&0&2&2&2&2\\4&4&3&3&2&2&0&2&2&2\\4&4&3&3&2&2&2&0&3&3\\5&5&4&4&3&2&2&3&0&2\\5&5&4&4&3&2&2&3&2&0\end{bmatrix}\end{array}\begin{bmatrix}1\\1\\1\\3\\3\\3\\3\\1\\1\\1\end{bmatrix}=\begin{bmatrix}52\\52\\44\\38\\32\\32\\38\\44\\52\\52\end{bmatrix}=436$$

$$A(T_1) = \begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10 \end{array}\begin{array}{c} \begin{array}{cccccccccc} 1&2&3&4&5&6&7&8&9&10 \end{array} \\ \begin{bmatrix} 0&0&0&1&0&0&0&0&0&0\\ 0&0&0&1&0&0&0&0&0&0\\ 0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&1&1&0&0\\ 0&0&0&0&0&0&0&0&1&1\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0 \end{bmatrix} \end{array}$$

$$D(T_1) = \begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10 \end{array}\begin{array}{c} \begin{array}{cccccccccc} 1&2&3&4&5&6&7&8&9&10 \end{array} \\ \begin{bmatrix} 0&2&3&1&2&3&4&4&5&5\\ 0&0&3&1&2&3&4&4&5&5\\ 0&0&0&2&1&2&3&3&4&4\\ 0&0&0&0&1&2&3&3&4&4\\ 0&0&0&0&0&1&2&2&3&3\\ 0&0&0&0&0&0&1&1&2&2\\ 0&0&0&0&0&0&0&2&1&1\\ 0&0&0&0&0&0&0&0&3&3\\ 0&0&0&0&0&0&0&0&0&2\\ 0&0&0&0&0&0&0&0&0&0 \end{bmatrix} \end{array}$$

$$[(A(T_1)+D(T_1)]\ v(T_1) = \begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8\\9\\10 \end{array}\begin{array}{c} \begin{array}{cccccccccc} 1&2&3&4&5&6&7&8&9&10 \end{array} \\ \begin{bmatrix} 0&2&3&2&2&3&4&4&5&5\\ 0&0&3&2&2&3&4&4&5&5\\ 0&0&0&2&2&2&3&3&4&4\\ 0&0&0&0&2&2&3&3&4&4\\ 0&0&0&0&0&2&2&2&3&3\\ 0&0&0&0&0&0&2&2&2&2\\ 0&0&0&0&0&0&0&2&2&2\\ 0&0&0&0&0&0&0&0&3&3\\ 0&0&0&0&0&0&0&0&0&2\\ 0&0&0&0&0&0&0&0&0&0 \end{bmatrix} \end{array} \begin{bmatrix} 1\\1\\1\\3\\3\\3\\3\\1\\1\\1 \end{bmatrix} = \begin{bmatrix} 52\\50\\38\\32\\20\\12\\6\\6\\2\\0 \end{bmatrix} = 218$$

We now calculate Molecular Topological Index for tree T_2.

$$A(T_2) = \begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7 \end{array}\begin{array}{c} \begin{array}{ccccccc} 1&2&3&4&5&6&7 \end{array} \\ \begin{bmatrix} 0&1&0&0&0&0&0\\ 1&0&0&1&0&0&0\\ 0&0&0&1&0&0&0\\ 0&1&1&0&1&1&0\\ 0&0&0&1&0&0&0\\ 0&0&0&1&0&0&1\\ 0&0&0&0&0&1&0 \end{bmatrix} \end{array} \qquad D(T_2) = \begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7 \end{array}\begin{array}{c} \begin{array}{ccccccc} 1&2&3&4&5&6&7 \end{array} \\ \begin{bmatrix} 0&1&3&2&3&3&4\\ 1&0&2&1&2&2&3\\ 3&2&0&1&2&2&3\\ 2&1&1&0&1&1&2\\ 3&2&2&1&0&2&3\\ 3&2&2&1&2&0&1\\ 4&3&3&2&3&1&0 \end{bmatrix} \end{array}$$

$$[A\,(T_2)+D\,(T_2)].v\,(T_2)=\begin{bmatrix}0&2&3&2&3&3&4\\2&0&2&2&2&2&3\\3&2&0&2&2&2&3\\2&2&2&0&2&2&2\\3&2&2&2&0&2&3\\3&2&2&2&2&0&2\\4&3&3&2&3&2&0\end{bmatrix}.\begin{bmatrix}1\\2\\1\\4\\1\\2\\1\end{bmatrix}=\begin{bmatrix}28\\21\\24\\16\\24\\21\\28\end{bmatrix}=162$$

$$A\,(T_2)+D\,(T_2)=\begin{array}{c|ccccccc}&1&2&3&4&5&6&7\\\hline 1&0&1&0&0&0&0&0\\2&0&0&0&1&0&0&0\\3&0&0&0&1&0&0&0\\4&0&0&0&0&1&1&0\\5&0&0&0&0&0&0&0\\6&0&0&0&0&0&0&1\\7&0&0&0&0&0&0&0\end{array}+\begin{array}{c|ccccccc}&1&2&3&4&5&6&7\\\hline 1&0&1&3&2&3&3&4\\2&0&0&2&1&2&2&3\\3&0&0&0&1&2&2&3\\4&0&0&0&0&1&1&2\\5&0&0&0&0&0&2&3\\6&0&0&0&0&0&0&1\\7&0&0&0&0&0&0&0\end{array}$$

$$[A\,(T_2)+D\,(T_2)]\,v\,(T_2)=\begin{bmatrix}0&2&3&2&3&3&4\\0&0&2&2&2&2&3\\0&0&0&2&2&2&3\\0&0&0&0&2&2&2\\0&0&0&0&0&2&3\\0&0&0&0&0&0&2\\0&0&0&0&0&0&0\end{bmatrix}.\begin{bmatrix}1\\2\\1\\4\\1\\2\\1\end{bmatrix}=\begin{bmatrix}28\\19\\17\\8\\7\\2\\0\end{bmatrix}=81$$

4. Molecular topological index for a degree symmetric tree

Let T be a tree with n vertices having equal number of vertices of a given tree.

Step 1 Let the vertices of T as $u_1,u_2,\ldots,u_{k1},v_{k1},v_{k1-1},\ldots,v_2,v_1$,when n is even and $u_1,u_2,\ldots,u_{k1},w,v_{k1},v_{k1-1},\ldots,v_2,v_1$,when n is odd such that $(u_1,v_1),(u_2,v_2),\ldots,(u_{k1},v_{k1})$ have same degree.

Step 2 Assign labels to the vertices of T as follows

(u_1, v_1) (u_2, v_2), …, (u_{k1}, v_{k1}) , when n is even

↓ ↓ ↓ ↓ ↓ ↓

1 n 2 n-1 n/2 (n+1)/2

(u_1, v_1) (u_2, v_2) , …, (u_{k1}, v_{k1}) , w , when n is odd

↓ ↓ ↓ ↓ ↓ ↓ ↓

1 n 2 n-1 (n-1)/2(n+3)/2(n+1)/2

Step 3 Arrange rows and columns of adjacency and distance matrix as $u_1,u_2,\ldots,u_{k1},v_{k1},v_{k1-1},\ldots,v_2,v_1$,when n is even and $u_1,u_2,\ldots,u_{k1},w,v_{k1},v_{k1-1},\ldots,v_2,v_1$,when n is odd.

Step 4 Consider A+D as a triangular matrix.

Step 5 Determine (A+D) v

Step 6 Formula A (A+D) vwhen A+D is triangular = ½ (A+D) v ,when A+D is the usual sum of the distance and adjacency matrices.

If tree T is not a tree with equal number of vertices of a given degree, then this result need not be true.As an illustration, we consider the tree in Figure 7.

T_5 :

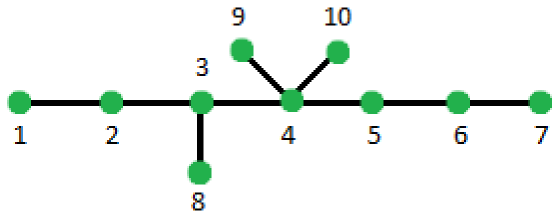


Figure 7.

In $T_{5,}$ we do not have equal number of vertices of a given degree.

A (T_5) =

	1	2	3	4	5	6	7	8	9	10
1	0	1	0	0	0	0	0	0	0	0
2	1	0	1	0	0	0	0	0	0	0
3	0	1	0	1	0	0	0	1	0	0
4	0	0	1	0	1	0	0	0	1	1
5	0	0	0	1	0	1	0	0	0	0
6	0	0	0	0	1	0	1	0	0	0
7	0	0	0	0	0	1	0	0	0	0
8	0	0	1	0	0	0	0	0	0	0
9	0	0	0	1	0	0	0	0	0	0
10	0	0	0	1	0	0	0	0	0	0

D (T_5) =

	1	2	3	4	5	6	7	8	9	10
1	0	1	2	3	4	5	6	3	4	4
2	1	0	1	2	3	4	5	2	3	3
3	2	1	0	1	2	3	4	1	2	2
4	3	2	1	0	1	2	3	2	1	1
5	4	3	2	1	0	1	2	3	2	2
6	5	4	3	2	1	0	1	4	3	3
7	6	5	4	3	2	1	0	5	4	4
8	3	2	1	2	3	4	5	0	3	3
9	4	3	2	1	2	3	4	3	0	2
10	4	3	2	1	2	3	4	3	2	0

$$[A(T_5) + D(T_5)]\, V(T_5) = \begin{bmatrix} 0 & 2 & 2 & 3 & 4 & 5 & 6 & 3 & 4 & 4 \\ 2 & 0 & 2 & 2 & 3 & 4 & 5 & 2 & 3 & 3 \\ 2 & 2 & 0 & 2 & 2 & 3 & 4 & 2 & 2 & 2 \\ 3 & 2 & 2 & 0 & 2 & 2 & 3 & 2 & 2 & 2 \\ 4 & 3 & 2 & 2 & 0 & 2 & 2 & 3 & 2 & 2 \\ 5 & 4 & 3 & 2 & 2 & 0 & 2 & 4 & 3 & 3 \\ 6 & 5 & 4 & 3 & 2 & 2 & 0 & 5 & 4 & 4 \\ 3 & 2 & 2 & 2 & 3 & 4 & 5 & 0 & 3 & 3 \\ 4 & 3 & 2 & 2 & 2 & 3 & 4 & 3 & 0 & 2 \\ 4 & 3 & 2 & 2 & 2 & 3 & 4 & 3 & 2 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 2 \\ 2 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 57 \\ 43 \\ 34 \\ 30 \\ 37 \\ 46 \\ 61 \\ 46 \\ 43 \\ 43 \end{bmatrix} = 440$$

$$A(T_5) = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{array} \begin{array}{c} \begin{array}{cccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$$D(T_5) = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{array} \begin{array}{c} \begin{array}{cccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{array} \\ \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 3 & 4 & 4 \\ 0 & 0 & 1 & 2 & 3 & 4 & 5 & 2 & 3 & 3 \\ 0 & 0 & 0 & 1 & 2 & 3 & 4 & 1 & 2 & 2 \\ 0 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 4 & 3 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 4 & 4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$$[A(T_5) + D(T_5)]\, V(T_5) = \begin{bmatrix} 0 & 2 & 2 & 3 & 4 & 5 & 6 & 3 & 4 & 4 \\ 0 & 0 & 2 & 2 & 3 & 4 & 5 & 2 & 3 & 3 \\ 0 & 0 & 0 & 2 & 2 & 3 & 4 & 2 & 2 & 2 \\ 0 & 0 & 0 & 0 & 2 & 2 & 3 & 2 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 2 & 2 & 3 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 4 & 3 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 4 & 4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 2 \\ 2 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 57 \\ 1 \\ 28 \\ 17 \\ 13 \\ 12 \\ 13 \\ 6 \\ 2 \\ 0 \end{bmatrix} = 189$$

Thus for tree T_5, **Formula A** is not satisfied.

5. Molecular topological index for a degree symmetric tree from its subtree

In this section we propose a method of determining the molecular topological index of a tree from its subtree and triangular matrices.

5.1 Tree reduction

Find a longest path $P_m$that is a subtree of the tree such that

- Removal of the path will not disconnect the tree.
- $T - \{P_m\}$ has at least 1 vertex of degree 1 and $(m - 1)$ vertices of degree 2.

5.2 Tree labeling

Let the longest path removed be $P_m$ie., a path with m vertices. Label the vertices of this path as $u_1, u_2, \ldots, u_m$. Label the remaining vertices ofT as discussed section 3. Arrange the rows and columns of

the matrices A & D and vector v as discussed in section 3.We now develop a procedure to determine the Molecular topological index of T which is degree symmetric from its sub tree T– $\{P_m\}$.
As an illustration consider tree T in Figure 8

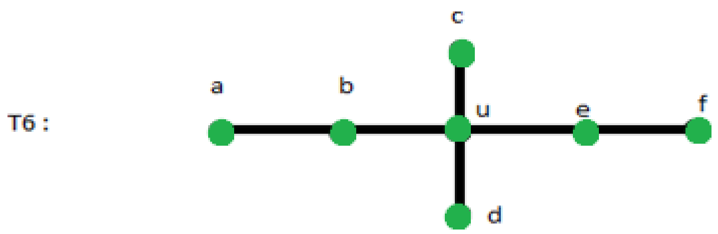


Figure 8.

We can remove a path of length 2 attached to vertex u.Note that if we remove path a,b then we have 1 vertex of degree 1 and 1 vertex of degree 2 in $T_6 - \{a\} - \{b\}$. Label the vertices a and b as u_1,u_2.
The remaining vertices can be labeled as discussed in Section 3.1.
Tree T_6 with labels assigned is seen in Figure 9.

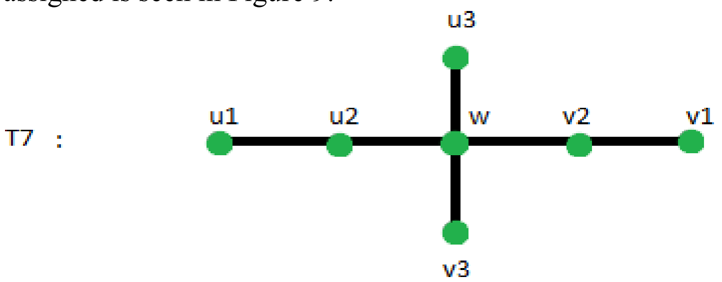


Figure 9.

As discussed in Section 3, the tree with labels assigned is as seen in Figure 10.

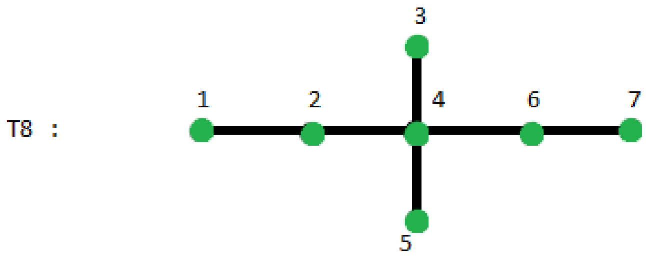


Figure 10.

5.3 Modified distance matrix

The reduced tree after removing longest possible path from any vertex as discussed in Section 5.1 is considered. For our tree $T_8$the reduced tree T_9 is seen in Figure 11.

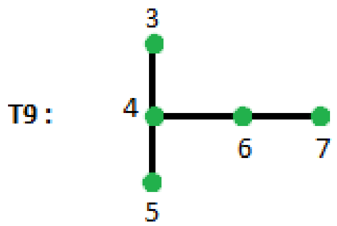


Figure 11.

The modified distance matrix for the reduced tree T− $\{P_m\}$ is determined as proposed in [19].
For T_9 the modified distance matrix is determined as follows

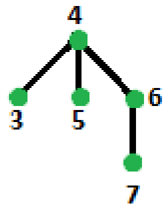


Figure 12.

Label of 4=$\sum_{i=1}^{m} i = \sum_{i=1}^{2} i$ = 1+2 = 3
Label of 3,5,6 = $\sum_{i=1}^{m} i$ + m = 3+2 = 5
Label of 7 = $\sum_{i=1}^{m} i$ + 2m = 3 + 2(2) = 7.
Therefore the modified Distance matrix D(T_9)=

$$\begin{array}{c|ccccc} & 3 & 4 & 5 & 6 & 7 \\ \hline 3 & 5 & 1 & 2 & 2 & 3 \\ 4 & 0 & 3 & 1 & 1 & 2 \\ 5 & 0 & 0 & 5 & 2 & 3 \\ 6 & 0 & 0 & 0 & 5 & 1 \\ 7 & 0 & 0 & 0 & 0 & 7 \end{array}$$

5.4 Modified adjacency matrix

Determine the Adjacency matrix ofT− $\{P_m\}$.Let T− $\{P_m\}$ be rooted at vertex u. We know that u is adjacent to a vertex say v in P_m. This means that there is an adjacency between vertices u and v which should be considered in molecular topological index determination.So in matrix A(T− $\{P_m\}$) , the (u,u) entry in matrix A(T− $\{P_m\}$) is considered as 1.Therefore for T_9 the modified Adjacency matrix A(T_9)=

$$\begin{array}{c|ccccc} & 3 & 4 & 5 & 6 & 7 \\ \hline 3 & 0 & 1 & 0 & 0 & 0 \\ 4 & 0 & 1 & 1 & 1 & 0 \\ 5 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 1 \\ 7 & 0 & 0 & 0 & 0 & 0 \end{array}$$

5.5 Modified degree vector

We have an edge between u and v in the original tree T contributing 1 degree to vertex u.This degree need not to be considered for Molecular topological index calculation of T− $\{P_m\}$.If the degree of u in T− $\{P_m\}$ is k ,then in the degree vector for T− $\{P_m\}$ consider degree of vertex u as k+1. For T_9, the modified degree sequence is $[\ 1\ 4\ 1\ 2\ 1\ ]^T$.
Determine [A(T− $\{P_m\}$) + D(T− $\{P_m\}$)]v(T− $\{P_m\}$). i.e.,we determine the Molecular topological index of T− $\{P_m\}$ using the modified distance,adjacency,degree vector as discussed in section 5.3,5.4,5.5.
For T_9, the Molecular topological index is

$$[\,A(T_9)+D(T_9)\,]\,v(T_9) = \begin{array}{c|ccccc} & 3 & 4 & 5 & 6 & 7 \\ \hline 3 & 5 & 2 & 2 & 2 & 3 \\ 4 & 0 & 4 & 2 & 2 & 2 \\ 5 & 0 & 0 & 5 & 2 & 3 \\ 6 & 0 & 0 & 0 & 5 & 2 \\ 7 & 0 & 0 & 0 & 0 & 7 \end{array} \begin{bmatrix} 1 \\ 4 \\ 1 \\ 2 \\ 1 \end{bmatrix} = 77$$

5.6 Molecular topological index of path P_m

Path P_m is removed from tree T. The adjacency between vertex u and v is considered in tree T– $\{P_m\}$ as modified adjacency matrix.The distance values are also incorporated in modified distance matrix of T– $\{P_m\}$.We now calculate the Molecular topological index of path P_m .When the edge uv is removed,the degree contribution of the edge of vertex u is considered in T– $\{P_m\}$.Now the degree contribution of this edge to vertex v need to be considered.To incorporate this the (v,v) entry in the degree vector will always be considered as 2, that is in the degree sequence vector of path P_m is $[1\ 2\ 2\ 2 \ldots 2]^T$.The Molecular topological index of path P_m is calculated as usual using the degree vector as $[1\ 2\ 2 \ldots 2]^T$.For the Tree T_8 the path removed is 1,2. For this the molecular topological index is calculated as follows.

$$A + D = \begin{matrix} & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 0 & 0 \end{matrix} + \begin{matrix} & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 0 & 0 \end{matrix}$$

$$(A + D)v = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 0 \end{bmatrix} = 12$$

5.7 Molecular topological index for degree symmetric tree from reduced tree

Step 1 Let T be a treewith n vertices.
Step 2 Remove a path P_m as discussed in Section 5.1.
Step 3 Label the vertices of T as discussed in Section 5.2.
Step 4 Determine the triangular matrix as discussed in Section 5.3.
Step 5 Finalize the modified adjacency matrix,distance matrix ,degree sequence vector as discussed in Section 5.3,5.4,5.5.
Step 6 Determine Molecular topological index of path P_m as discussed in Section 5.6.
Step 7Formula B– Molecular topological index of tree T = [A(T– $\{P_m\}$) + D(T– $\{P_m\}$)]v(T– $\{P_m\}$) + Molecular topological index of P_m (using modified degree vector).

The Molecular topological index for tree T_8 = 77 + 4 = 81 which matches with the Molecular topological index calculated in Section 3for tree T_4.So we conclude that **Formula C**– Moleculartopological index of tree T = 2{[A(T– $\{P_m\}$) + D(T– $\{P_m\}$)]v(T– $\{P_m\}$) + Molecular topological index of P_m}.Thus for the tree T_8 the molecular topological index = 2 × 81 = 162.

6. Conclusion

To determine the molecular topological index we have to determine the adjacencymatrix, distance matrix and the vertex degree sequence. So the number of manual entries required is more in number. The proposed method provides a method to determine the molecular topological index of trees having equal number of vertices of a given degree using triangular matrices, which means that half of the manual calculation and entry is reduced. Moreover determining the index from reduced tree is developed, which further reduces the computational complexity of the algorithms developed.

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