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Computing the Cluj Index of a Type Dendrimer Nanostars

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Abstract

The Cluj index is a topological index that counts all the vertex proximities in a molecular graph. In this paper, the Cluj index is computed for dendrimer nanostructures of type 1-3.

1. Introduction

A single number, representing a chemical structure, in graph-theoretical terms, is called a topological descriptor. Being a structural invariant, it does not depend on the labeling or the pictorial representation of a graph. Despite the considerable loss of information by the projection in a single number of a structure, such descriptors found broad applications in the correlation and prediction of several molecular properties [1,2] and also in tests of similarity and isomorphism [3,4]. When a topological descriptor correlates with a molecular property, it can be denominated as molecular index or topological index (TI).

A graph**,** G = G (V, E) is a pair of two sets: V = V (G), a finite nonempty set of N points (i.e. vertices) and E = E (G), the set of Q unordered pairs of distinct points of V. Each pair of points (v_i, v_j) (or simply (i,j)) is a line (i.e. edge), $e_{i,j}$, of G if and only if $(i,j)\in E(G)$. In a graph, n equals to the cardinality, $|V|$, of the set V while e is identical to |E|. A graph with n points and e lines is called a (n, *e*) graph. Two vertices are adjacent if they are joined by an

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edge. If two distinct edges are incident with a common vertex, then they are adjacent edges. The angle between edges as well as the edge length is disregarded.

In an undirected connected acyclic graph, a given pair of vertices (*i,j*) is joined by a unique path p(*i,j*), that is, a continuous sequence of edges, with the property that all are distinct and any two subsequent edges are adjacent. The length of the path p(*i,j*) is equal to the number of edges in the path between vertices *i* and *j*.

In an undirected connected cycle-containing graph between any two vertices, there is at least one path connecting them. If more than one path connects a given pair of vertices (i,j), we denote the k^th^ path by the symbol $p_k(i,j)$. The shortest path joining vertices i and j is called geodesic and its length is the topological distance, $(\Delta)_{i,j}$. The longest path is the elongation and its length is equal to the detour distance, $(D)_{ij}$. The square arrays which collect the lengths of the two path types are called the distance matrix, denoted as Δ, and the detour matrix, denoted as D**,** respectively:

$$(D_e)_{ij} = \begin{cases} N_{e,P(i,j)}: & p(i,j) \text{ is a geodesic} \quad \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases} \qquad (1)$$

$$(\Delta_e)_{ij} = \begin{cases} N_{e,P(i,j)}: & p(i,j) \text{ is an elongation} \quad \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases} \qquad (2)$$

Where $N_{e,p(i,j)}$ is the number of edges on the shortest/longest path p(i,j). The subscript e in the symbols of the above matrices means that they are edge-defined, that is, their entries count edges on the path p (*i,j*).

When paths of length $1 \leq |p| \leq |p(i,j)|$ are counted on path p(*i,j*), another pair of matrices can be constructed

$$(D_p)_{ij} = \begin{cases} N_{p,P(i,j)}: & p(i,j) \text{ is a geodesic} \quad \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases} \qquad (3)$$

$$(\Delta_p)_{ij} = \begin{cases} N_{p,p(i,j)}: & p(i,j) \text{ is an elongation} \quad \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases} \qquad (4)$$

They are path-defined matrices and the number of paths $N_{e,p(i,j)}$ is obtained from entries $(\boldsymbol{M}_e)_{ij}$, $\boldsymbol{M}_e = \boldsymbol{D}_e$ or Δ_e, by:

$$N_{p,p(i,j)} = \left\{\left[(M_e)_{ij}\right]^2 + (M_e)_{ij}\right\}/2 \tag{5}$$

The asymmetric Cluj matrices $\boldsymbol{CJD}_u$ and $\boldsymbol{CJ}\Delta_u$ have been introduced by Diudea [5, 6]. These matrices are $n \times n$ square matrices and the subscript u denotes the unsymmetricity of matrices. The non-diagonal entries, $(\boldsymbol{M}_u)_{ij}$, $\boldsymbol{M}_u = \boldsymbol{CJD}_u$ or $\boldsymbol{CJ}\Delta_u$, in the two Cluj matrices are defined as:

$$(M_u)_{ij} = N_{i,p_k(i,j)} = max\left|V_{i,p_k(i,j)}\right| \tag{6}$$

$$V_{i,p_k(i,j)} = \{v | v \in V(G);\ D_{iv} < D_{jv};\ P_h(i,v) \cap P_k(i,j) = \{i\}:\quad P_k(i,j)\ is\ a\ geodesic\} \\ ;\ k = 1,2,\cdots;\ h = 1,2,\cdots \tag{7}$$

Or

$$V_{i,p_k(i,j)} = \{v | v \in V(G);\ \Delta_{iv} < \Delta_{jv};\ P_h(i,v) \cap P_k(i,j) = \{i\}:\quad P_k(i,j)\ is\ an\ elongation\} \\ ;\ k = 1,2,\cdots;\ h = 1,2,\cdots \tag{8}$$

Quantity $V_{i,pk(i,j)}$ denotes the set of vertices lying closer to vertex i than the vertex j, and are external with respect to path $p_{k(i,j)}$ (condition $p_h(i,v) \cap p_k(i,j) = \{i\}$). Since in cycle-containing structures, various shortest paths $p_k(i,j)$, in general, lead to various sets $V_{i,pk(i,j)}$, by definition, the (ij)-entries in the Cluj matrices are taken as $\max|V_{i,pk(i,j)}|$. The diagonal entries are zero. For paths $p_h(i,v)$, no restrictions related to their length are imposed. The above definitions, Eqs. (6)–(8), are valid for any connected graph.

The two Cluj matrices $\boldsymbol{M}_u$ allow the construction of the corresponding symmetric matrices $\boldsymbol{M}_p$ (defined on paths) and $\boldsymbol{M}_e$ (defined on edges) by:

$$\boldsymbol{M}_p = \boldsymbol{M}_u \bullet (\boldsymbol{M}_u)^T \tag{9}$$

$$\boldsymbol{M}_e = \boldsymbol{M}_p \bullet \boldsymbol{A} \tag{10}$$

where $\boldsymbol{A}$ is the adjacency matrix. The symbol $\bullet$ means the Hadamard matrix product, *i. e.*, $(\boldsymbol{M}_a \bullet \boldsymbol{M}_b)_{ij} = (\boldsymbol{M}_a)_{ij}\,(\boldsymbol{M}_b)_{ij}$ [7].

The Cluj indices are calculated as half-sum of the entries in a Cluj symmetric matrix, **M**, (**M = CJD, CJ**Δ)

$$IE\,(M) = (1/2)\sum_i \sum_j [M]_{ij}\,[A]_{ij} \tag{11}$$

$$IP(M) = (1/2)\sum_i \sum_j [M]_{ij} \tag{12}$$

The number defined on edge, *IE*, is an index while the number defined on path, *IP* is a hyper-index [8]. The Cluj Index of dendrimer nanostars computed recently in [9] and another topological index of a dendrimer is obtained in [10].

In this paper, we obtain the Cluj indices for a type of dendritic nanostructures.

2. Computing of IE_K (CJD) and IE_K (CJΔ) for a dendrimer of type 1-3

Figure 1 shows dendrimer of type 1-3 which has grown third stages.

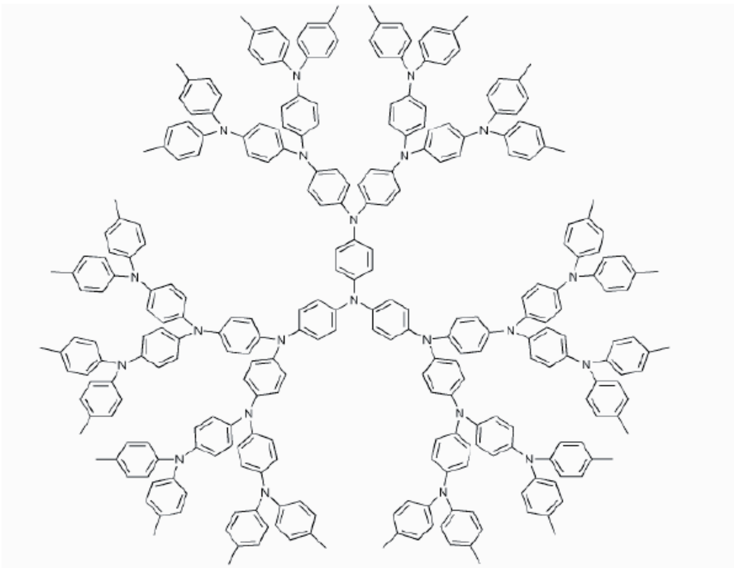

Figure1. Dendrimer of type 1-3 which has grown three stages

We denote IE_K (CJD) and IE_K (CJΔ) for the Cluj indices of k-connected hexagons according to there are two edges between each two hexagons and the first and the last hexagons have an external edge and the sum of entries in i^{th} row of $[CJD]_{ij}[A]_{ij}$ is called the valuation of i^{th} vertex and we denote it by v_i.

The main result of this section is the following theorem:

Theorem 2.1: The number of IE_K (CJD) for this type of dendrimer is:

$$IE_K(CJD) = \frac{1}{2}(35K^2 - K + 2(\sum_{i=1}^{K} 7(K+i)+1)), K \geq 2.$$

Proof: At first we compute IE_2 (CJD) of Figure 2.

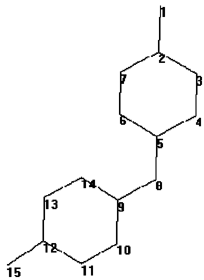

Figure 2. Tow connected hexagons

For this purpose, we need to compute the matrix CJD. For IE_2 (CJD), the matrix is

$$\begin{pmatrix}
0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
14 & 0 & 4 & 3 & 3 & 3 & 4 & 3 & 4 & 4 & 4 & 4 & 4 & 4 & 4 \\
11 & 11 & 0 & 4 & 3 & 3 & 2 & 4 & 4 & 5 & 5 & 5 & 5 & 5 & 5 \\
11 & 10 & 11 & 0 & 4 & 2 & 10 & 4 & 6 & 6 & 6 & 6 & 6 & 6 & 6 \\
10 & 10 & 10 & 11 & 0 & 11 & 10 & 7 & 7 & 7 & 7 & 7 & 7 & 7 & 7 \\
11 & 10 & 10 & 2 & 4 & 0 & 11 & 4 & 6 & 6 & 6 & 6 & 6 & 6 & 6 \\
11 & 11 & 2 & 3 & 3 & 4 & 0 & 4 & 4 & 5 & 5 & 5 & 5 & 5 & 5 \\
8 & 8 & 8 & 8 & 8 & 8 & 8 & 0 & 8 & 8 & 8 & 8 & 8 & 8 & 8 \\
7 & 7 & 7 & 7 & 7 & 7 & 7 & 7 & 0 & 11 & 10 & 10 & 10 & 11 & 10 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 4 & 4 & 0 & 11 & 10 & 10 & 2 & 11 \\
5 & 5 & 5 & 5 & 4 & 5 & 5 & 4 & 3 & 4 & 0 & 11 & 2 & 3 & 11 \\
4 & 4 & 4 & 4 & 4 & 4 & 4 & 3 & 3 & 3 & 4 & 0 & 4 & 3 & 14 \\
5 & 5 & 5 & 5 & 4 & 5 & 5 & 4 & 3 & 3 & 2 & 11 & 0 & 4 & 11 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 4 & 4 & 2 & 10 & 10 & 11 & 0 & 11 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0
\end{pmatrix}$$

We now compute the Cluj index of this graph (Figure 2) by its definition (IE (CJD) = (1/2) $\Sigma_i\Sigma_j$ [CJD] $_{ij}$ [A]$_{ij}$). Thus $[\mathbf{CJD}]_{ij}\,[\mathbf{A}]_{ij}$ is

$$\begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
14 & 0 & 4 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 11 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 11 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 11 & 0 & 11 & 0 & 7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 4 & 0 & 11 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 11 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 7 & 0 & 11 & 0 & 0 & 0 & 11 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 11 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 11 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 4 & 0 & 14 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 11 & 0 & 4 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 11 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0
\end{pmatrix}$$

We can compute IE_2 (CJD) with dividing the summation of rows by two and therefore IE_2 (CJD) =120.

Now, we analyze matrix based on this graph. The graph has 15 vertices that the valuation of vertex 1 and 15 is equal to 1, i.e., v_1 and v_{15} is equal to 1. In addition, v_2 and v_{12} are 22, v_5 and v_9 are 29, v_8 is 16 and the valuation of eight remaining vertices is equal to 15.

Now, we can compute IE_2 (CJD) regarding the valuation of these vertices. Thus $IE_2(CJD) = \frac{1}{2}(2\times 1 + 2\times 22 + 2\times 29 + 8\times 15 + 16) = 120$.

By the same procedure, we can compute IE_3 (CJD) of Figure 3.

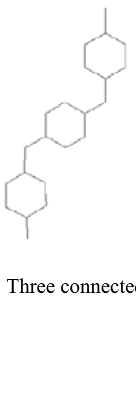

Figure 3. Three connected hexagons.

$$IE_3(CJD) = \frac{1}{2}(1\times 2 + 2\times 29 + 2\times 43 + 2\times 36 + 2\times 23 + 12\times 22) = 264 .$$

Now, suppose that there are k-connected hexagons, k≥2, according to there are two edges between each two hexagons and the first and the last hexagons have an external edge. The number of all vertices in this graph is equal to 6k+ (k+1) =7k+1.

We define the position and valuation of vertices as follows:

Vertices, connected to the first and the last hexagons, are called external vertices and the valuation of these vertices is 1. In all growth process, the number of these vertices is 2.

The vertices that are between two hexagons are called central vertices. The number and valuation of these vertices are (k-1) and 7k+2 respectively.

Now, in this graph vertices which are connected beside three vertices are called joining vertices. The number of these vertices in all growth process is 2k. Each pair of joining vertices has the same valuation and the value of each pairs is as follows:

$$7k+8, 7k+8+7, 7k+8+2\times 7, 7k+8+3\times 7, \ldots, 7k+8+(k-1)\times 7 .$$

Thus, the valuation of all joining vertices is equal to

$$\sum_{i=1}^{k}(7k+8)+7(i-1) = \sum_{i=1}^{k} 7(k+i)+1 .$$

The remainder vertices are 7k+1-(k-1+2k+2) =4k and the valuation of these vertices are equal to 7k+1 in all process growth. Thus we have

$$IE_k(CJD) = \frac{1}{2}(2\times 1 + (k-1)\times(7k+2) + 2\times(\sum_{i=1}^{k} 7(k+i)+1) + 4k\times(7k+1)) .$$

Therefore, $IE_k(CJD) = \frac{1}{2}(35k^2 - k + 2\times(\sum_{i=1}^{k} 7(k+i)+1)), k\geq 2$. ′

Theorem 2.2: The number of IE_K (CJΔ) for this type of dendrimer is:

$$IE_K(CJ\Delta) = \frac{1}{2}(7K^2 + 3K + 2(\sum_{i=0}^{K-1} 7(K+i)+4)), K \geq 2 .$$

Proof. The proof theorem is similar to Theorem 2.1 but the shortest path (*i.e.*, geodesic) is replaced by the longest path between two vertices *i* and *j*.

3. The Cluj index for dendrimer nanostructures of type 1-3.

We denote IE_n (CJD) and IE_n (CJΔ) for the Cluj indices of this type of dendrimer that has grown n stages.

Theorem 3.1: IE_n (CJD) of this type dendrimer is:

$$IE_n(CJD) = \frac{1}{2}(35K^2 - K + 2\times(\sum_{i=1}^{K} 7(K+i)+1))$$

where $K = 3(2^{n+1} - 1)$.

Proof: At first we compute IE_n (CJD) of this dendrimer which has grown three stages (Figure 1). Thus, we compute IE_n (CJD) of this nanostar in the n^{th} stage.

In Figure 4 we show the graph of a nucleus in dendrimer nanostructures of type 1-3

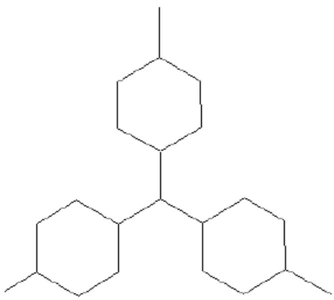

Figure 4. Nucleus

In the graph of Figure 4, we have three connected hexagons thus we can compute IE_0 (CJD) (IE (CJD) of nucleus) from Theorem 2.1. Hence, we have

$$IE_0(CJD) = \frac{1}{2}(35(3^2) - 3 + 2\times(\sum_{i=1}^{3} 7(3+i)+1)) = 264 \ .$$

As shown in Figure 1 in growth primary stage, 6 connected hexagons add to nucleus and hence this graph has 9 connected hexagons in the first growth. Thus, we have from Theorem 2.1

$$IE_1(CJD) = \frac{1}{2}(35(9^2) - 9 + 2\times(\sum_{i=1}^{9} 7(9+i)+1)) = 2304 \ .$$

Now, in the second growth stage, 12 connected hexagons add to the graph that has grown one stage. Therefore, in the second growth stage, all graphs have 21 connected hexagons. Thus, we have from Theorem 2.1

$$IE_2(CJD) = \frac{1}{2}(35(21^2) - 21 + 2\times(\sum_{i=1}^{21} 7(21+i)+1)) = 11559 .$$

In the third growth stage, 24 connected hexagons add to graph which has grown two stages. Therefore, in the third growth stage, all graphs have 45 connected hexagons. Thus, we have from Theorem 2.1

$$IE_3(CJD) = \frac{1}{2}(35(45^2) - 45 + 2\times(\sum_{i=1}^{45} 7(45+i)+1)) = 46431 .$$

Now, suppose that the graph of Figure 1 has grown n stages, thus, we compute IE_n (CJD) of this type dendrimer that has grown n stages. With consider growth process and examples as a result for computing IE_n (CJD) it is sufficient to obtain, how many connected hexagons add to nucleus in each stage of growth. Each stage growth process of connected hexagons is the same. In the first stage, 6 connected hexagons are added to nucleus and in the second stage, 12 connected hexagons are added to graph and in the third stage, 24 connected hexagons are added to graph. Therefore when the graph has grown n stages, 3×2^n connected hexagons in the n^{th} stage are added to graph. Thus, the number of all connected hexagons in the n^{th} stage is equal to

$$K = 3 + \sum_{i=1}^{n} 3\times 2^i = 3(2^{n+1} - 1) .$$

Therefore, we compute IE_n (CJD) of this type of dendrimer as follows:

$$IE_n(CJD) = \frac{1}{2}(35K^2 - K + 2\times(\sum_{i=1}^{K} 7(K+i)+1))$$

where $K = 3(2^{n+1} - 1)$.   ′

Theorem 3.2: IE_n (CJΔ) of this type of dendrimer is equal to:

$$IE_n(CJ\Delta) = \frac{1}{2}(7K^2 + 3K + 2\times(\sum_{i=0}^{K-1} 7(K+i)+4))$$

where $K = 3(2^{n+1}-1)$.

Proof: At first, we compute IE_n (CJΔ) of this type dendrimer that has grown three stages (Figure 1). Thus, we can compute IE_n (CJΔ) of this nanostar in the stage n. We have

$$IE_0(CJ\Delta) = \frac{1}{2}(7(3^2) + 3\times 3 + 2\times(\sum_{i=0}^{2} 7(3+i)+4)) = 116 \ .$$

As shown in Figure 1, in the first growth stage, 6 connected hexagons are added to the nucleus; therefore, we have 9 connected hexagons in the first growth. Thus, we have from Theorem 2.2

$$IE_1(CJ\Delta) = \frac{1}{2}(7(9^2) + 3\times 9 + 2\times(\sum_{i=0}^{8} 7(9+i)+4)) = 1054 \ .$$

Now, in the second growth stage, 12 connected hexagons are added to the graph that has grown one stage. Therefore, in the second growth stage, all graphs have 21 connected hexagons. Thus, we have from Theorem 2.2

$$IE_2(CJ\Delta) = \frac{1}{2}(7(21^2) + 3\times 21 + 2\times(\sum_{i=0}^{20} 7(21+i)+4)) = 3896 .$$

In the third growth stage, 24 connected hexagons are added to the graph that has grown two stages. Therefore, in the third growth stage, all graphs have 45 connected hexagons. Thus, we have from Theorem 2.2

$$IE_3(CJ\Delta) = \frac{1}{2}(7(45^2) + 3\times 45 + 2\times(\sum_{i=0}^{44} 7(45+i)+4)) = 14018 .$$

With considering growth process and examples as a result for computing IE_n (CJΔ) it is sufficient to obtain how many connected hexagons need add to the nucleus in each stage of growth. In Theorem 3.1, we computed K. Therefore, we compute IEn (CJΔ) of this type of dendrimer as follows:

$$IE_n(CJ\Delta) = \frac{1}{2}(7K^2 + 3K + 2\times(\sum_{i=0}^{K-1} 7(K+i)+4))$$

where $K = 3(2^{n+1}-1)$. ′

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