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Computing the Cluj index of the first type dendrimer nanostar

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The Cluj index ($IE(M)=(\frac{1}{2})\sum_i\sum_j[M]_{ij}[A]_{ij}$) is related with the Cluj matrices (M =CJD, CJΔ, CFD, CFΔ) but in all graphs: IE (CJD) = IE (CFD); IE (CJΔ) = IE (CFΔ). Thus for computation the Cluj index it is sufficient that we compute only IE (CJD) and IE (CJΔ). In this paper we compute IE (CJD) and IE (CJΔ) for the first type dendrimer nanostar.

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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 the cardinality, |V|, of the set V while Q is identical to |E|. A graph with N points and Q lines is called a (N, Q) graph (*i.e.,* a graph of order N and dimension Q). Two vertices are adjacent if they are joined by an 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 kth 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:

$$(\boldsymbol{D}_e)_{ij} = \begin{cases} N_{e,p(i,j)}: \text{ p}(i,j) \text{ is a geodesic if } i \neq j \\ 0 \quad \text{if } i = j \end{cases}$$

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

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

$$(\boldsymbol{D}_p)_{ij} = \begin{cases} N_{p,p(i,j)}: \text{ p}(i,j) \text{ is a geodesic if } i \neq j \\ 0 \quad \text{if } i = j \end{cases}$$

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

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:

$$N_{p,p(i,j)} = \{[(\boldsymbol{M}_e)_{ij}]^2 + (\boldsymbol{M}_e)_{ij}\}/2 \ .$$

The unsymmetric 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:

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

$$V_{i,p_k(i,j)} = \{v \mid v \in V(\mathrm{G});\ \boldsymbol{D}_{iv} < \boldsymbol{D}_{jv};\ \mathrm{p}_h(i,v) \cap \mathrm{p}_k(i,j) = \{i\} : \mathrm{p}_k(i,j) \text{ is a geodesic}\}\ ;\ k = 1,2,\ldots;\ h = 1,2\ldots$$

or

$$V_{i,p_k(i,j)} = \{v \mid v \in V(\mathrm{G});\ \Delta_{iv} < \Delta_{jv};\ \mathrm{p}_h(i,v) \cap \mathrm{p}_k(i,j) = \{i\} : \mathrm{p}_k(i,j) \text{ is an elongation}\}\ ;\ k = 1,2,\ldots;\ h = 1,2\ldots \quad (8)$$

Quantity $V_{i,pk(i,j)}$ denotes the set of vertices lying closer to vertex i than to vertex j, and are external with respect to path $\mathrm{p}_{k(i,j)}$ (condition $\mathrm{p}_h(i,v) \cap \mathrm{p}_k(i,j) = \{i\}$). Since in cycle-containing structures, various shortest paths $\mathrm{p}_k(i,j)$, 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 $\mathrm{p}_h(i,v)$, no restrictions related to their length are imposed.

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:

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

$$\boldsymbol{M}_e = \boldsymbol{M}_p \bullet \boldsymbol{A} \quad (10)$$

where $\boldsymbol{A}$ is the adjacency matrix. 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, CJΔ**)

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

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

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].

In this paper we obtain the Cluj indices for the first type dendrimer nanostar.

2. Results

Fig. 1 shows a first type dendrimer which has grown four stages.

We denote IE'_K (CJD) and IE'_K (CJΔ) for the Cluj indices of K-connected hexagons according to there are three edges between each two hexagons.

Theorem 1: IE'_K (CJD) for K-connected hexagons according to there are three edges between each two hexagons are:

$$IE_K(CJD) = \frac{1}{2}(64K^2 - 30K + 14 + 2(\sum_{i=3}^{K} 8i - 10)), K \geq 2$$

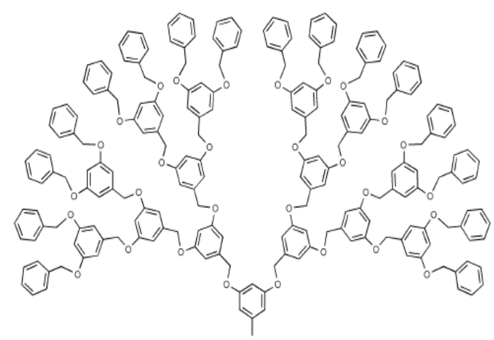

Fig. 1. A first type dendrimer which has grown four stages.

Theorem 2: IE'_K (CJΔ) for K-connected hexagons according to there are three edges between each two hexagons equal to:

$$IE_K(CJ\Delta) = \frac{1}{2}(16K^2 - 10K + 6 + 2(\sum_{i=0}^{K-2} 8(K+i+1)), K \geq 2.$$

3. Discussion and conclusions

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

Definition 1. The sum of entries in the i-th row of $[CJD]_{ij}[A]_{ij}$ is called valuation of i-th vertex (*i.e.,* v_i).

Definition 2. All of vertices which connected to the near of three vertices is called junction vertices.

Definition 3. The vertex is located out of hexagon called external vertex.

Theorem 3: IE_n (CJD) of the first type dendrimer is:

$$IE'_n(CJD) = (8K-2) + K' +$$
$$\frac{1}{2}(64K^2 - 30K + 14 + 2(\sum_{i=3}^{K} 8i - 10))$$

where $K=2^{n+1}-1$ and $K'=2^n$.

Proof: At first we compute IE_4 (CJD) of the first type dendrimer which has grown four stages (see Fig 1). Thus, we compute IE_n (CJD) of this nanostar from stages n.

As shown in Fig. 1, this graph is made out of a nucleus (see Fig. 2).

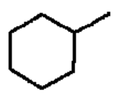

Fig. 2. Nucleus.

According the above definitions, the above nucleus is made out of one hexagon and one external vertex. Thus, the value of this external vertex is 1, the value of junction vertex is 14, the value of vertex to be opposite of junction vertex is 6 and four remainder vertices have the same value and equal to 7. Now, we can compute IE_0 (CJD) (IE (CJD) of nucleus). Thus, we have $IE_0(CJD) = \frac{1}{2}(6 + 4\times 7 + 14 + 1) = 25$.

As shown in Fig 1 in the growth primary we have IE_1 (CJD) =288 (by *TOPOCLUJ* software). Now we can without count the external edge computed IE'_3 (CJD) from theorem 1. Thus, we have IE'_3 (CJD) =264. Therefore we have

IE_1 (CJD) =24+264=24+IE'_3 (CJD).

Now, we have IE_2 (CJD) =1736 (by *TOPOCLUJ* software). But in this stage 4 connected hexagons add to the graph which has grown one stage. Therefore in the second growth stage all graphs have 7 connected hexagons. Thus, we have from Theorem 1, IE'_7 (CJD) =1678, therefore

IE_2 (CJD) =58+1678=58+IE'_7 (CJD).

Now, we have IE_3 (CJD) =6063 but in this stage 8 connected hexagons add to the graph which has grown two stages. Therefore in the third growth stage, all graphs have 15 connected hexagons. Thus, we have from Theorem 1, IE'_{15} (CJD) = 5937, and therefore IE_3 (CJD) =126+5937=126+IE'_{15} (CJD).

This time, we have IE_4 (CJD) =66236, but in this stage 16 connected hexagons add to graph which has grown three stages. Therefore in the fourth growth stage, all graphs have 31 connected hexagons. Thus, we have from Theorem 1, IE'_{31} (CJD) =65974, therefore IE_4 (CJD) =262+65974=262+IE'_{31} (CJD). Therefore, IE_4 (CJD) of the first type dendrimer which has grown four stages (see Fig 1) is equal to 66236.

Now, suppose that the graph of figure1 has grown $n\geq 1$ stages, thus we compute IE_n (CJD) of the first type dendrimer. With consider growth process that we have number of connected hexagons which in each stage add to the graph as follows:

In the first stage 2 hexagons, in the second stage $2^2=4$ connected hexagons, in the third stage $2^3=8$ connected hexagons and in the fourth stage $2^4=16$ connected hexagons add to graph. If number of connected hexagons which in each stage add to graph is called K', therefore we have $K'=2^n$.

If we denote the number of all hexagons in graph for all stages by K, then t we have

$$K = (\sum_{i=0}^{n-1} 2^{i+1}) + 1 = 2^{n+1} - 1.$$

Therefore we have

$$IE'_n(CJD) = (8K-2) + K' + IE_K(CJD).$$

Thus, we have

$$IE'_n(CJD) = (8K-2) + K' +$$
$$\frac{1}{2}(64K^2 - 30K + 14 + 2(\sum_{i=3}^{K} 8i - 10))$$

where $K=2^{n+1}-1$ and $K'=2^n$.

Definition 4. The sum of entries in i-th row of $[CJ\Delta]_{ij}[A]_{ij}$ is called valuation of i-th vertex (*i.e.,* v_i).

Theorem 4: IE_n (CJΔ) of the first type dendrimer is equal to:

$$IE_n(CJ\Delta) = 6K + (K' - 2) +$$
$$\frac{1}{2}(16K^2 - 10K + 6 + 2(\sum_{i=0}^{K-2} 8(K + i + 1)))$$

where $K=2^{n+1}-1$ and $K'=2^n$.

Proof: At first we compute IE_4 (CJΔ) of the first type dendrimer which has grown four stages (see Fig 1). Thus, we compute IE_n (CJΔ) of this nanostar from stages n.

In Fig. 2, the value of external vertex is equal to 1, value of junction vertex is equal to 10 and the value of five reminder vertices is equal to 2. Now, we can compute IE_0 (CJΔ) (IE (CJΔ) of nucleus). Thus, we have

$$IE_0(CJ\Delta) = \frac{1}{2}(1 + 10 + 5\times 2) = 11 .$$

As shown in Fig. 1, in the first growth, we have IE_1 (CJΔ) =150 (by *TOPOCLUJ* software). Now we can without count the external edges, computed IE'_3 (CJΔ) from Theorem 2. Thus, we have IE'_3 (CJΔ) =132. Therefore we have IE_1 (CJΔ) =18+132=24+IE'_3 (CJΔ).

Now, we have IE_2 (CJΔ) =908 (by *TOPOCLUJ* software). But in this stage 4 connected hexagons add to graph which has grown one stage. Therefore in the second stage of growth, all graphs have 7 connected hexagons. Thus, we have from Theorem 2, IE'_7 (CJΔ) =864, therefore IE_2 (CJΔ) =44+864=44+IE'_7 (CJΔ).

Now, we have IE_3 (CJΔ) =4344 but in this stage, 8 connected hexagons add to the graph which has grown two stages. Therefore in the third stage of growth all graphs have 15 connected hexagons. Thus, we have from Theorem 2, IE'_{15} (CJΔ) =4248, therefore IE_3 (CJΔ) =96+4248=96+IE'_{15} (CJΔ).

Thus, we have IE_4 (CJΔ) =37592 but in this stage 16 connected hexagons add to the graph which has grown three stages. Therefore in the fourth stage of growth, all graphs have 31 connected hexagons. Thus, we have from Theorem 2, IE'_{31} (CJΔ) =37392, therefore IE_4 (CJΔ) =200+37392=200+IE'_{31} (CJΔ). Therefore, IE_4 (CJΔ) of the first type dendrimer which has grown four stages (see Fig. 1) equal to 37592.

Therefore we have

$$IE_n(CJ\Delta) = 6K + (K' - 2) + IE'_K(CJ\Delta)$$

Thus, we have

$$IE_n(CJ\Delta) = 6K + (K' - 2) + \frac{1}{2}(16K^2 - 10K + 6 + 2(\sum_{i=0}^{K-2} 8(K+i+1)))$$

where $K=2^{n+1}-1$ and $K'=2^n$.

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