***MATCH***
*Communications in Mathematical and in Computer Chemistry*

MATCH Commun. Math. Comput. Chem. **62** (2009) 389-395

ISSN 0340 - 6253

# Computing the Cluj Index of Dendrimer Nanostars

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(Received October, 10 2008)

**Abstract**

The Cluj index is a topological index that counts all the vertex proximities in a molecular graph. It was proposed to complete the calculation of distances in cyclic graph, a domain non-covered by the Wiener matrices. In this paper, the Cluj index is computed for two types of dendrimer nanostructures by analyzing the constitutive substructures of these dendrimers.

## 1. Introduction

Topological indices are numerical descriptors derived from graphs. Such indices, for example those based on the distances in graph are widely used for establishing relationships between the molecular structure and their physicochemical properties. Usage of topological indices began in 1947 when Harold Wiener [1] introduced the number counting all the distances in a molecular graph (latter called the Wiener index) to study the thermodynamic properties of alkanes; in the last decade, other physicochemical properties of alcohols, amines and analogous compounds have been predicted by using topological indices [2].

The unsymmetric Cluj matrix, UCJ, has been introduced by Diudea [3, 4]. It is defined by using either the distance or the detour concept. The non-diagonal entries, $[UM]_{ij}$, M=CJD (Cluj-Distance) or CJΔ (Cluj-Detour), are defined as:

$$V_{i,p(i,j)_k} = \{v | v \in V(G); d_{iv} < d_{jv}; p(i,v)_h \cap p(i,j)_k = \{i\}\}; h, k = 1,2,... \quad (1)$$

$$[\mathbf{UCJ}]_{ij} = \max_{k=1,2,..} \left| V_{i,p(i,j)_k} \right| \quad (2)$$

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The set $V_{i,j,pk}$ consists of vertices $v$ lying *closer* to the vertex $i$ (condition $d_{iv}<d_{jv}$). This variant of Cluj matrices is called [5] "at least one path external to the path $(i,j)$", since at least one of the paths $(v,i)_h$ must be external with respect to the path $(i,j)_k$ **:** $(i, v)_h \cap p_k = \{i\}$ . In cycle-containing structures, more than one path $(i,j)_k$ may exist, thus supplying various sets $V_{i,j,pk}$ . By definition, the $(i,j)$-entry in the Cluj matrices is taken as $max \mid V_{i,j,pk} \mid$ The diagonal matrices are zero. The Cluj matrices are defined in any connected graph.

In trees, the non-diagonal entries count the paths going to $j$ through $i$, the number of which equals that of vertices located closer to $i$ than to $j$.

It happens that $V_{i,j,pk}$ be sets of disconnected vertices. This fact is undesirable when molecular graphs (which are always connected graphs) are investigated. If $V_{i,j,pk}$ is a real (connected) chemical fragment, the Cluj fragmental matrices are defined:

$$V_{i,p(i,j)_k} = \{v \mid v \in V(G); d(G_p)_{iv} < d(G_p)_{jv}; G_p = G - p(i,j)_k \}; k = 1,2,... \quad (3)$$

Such a fragment collects the vertex proximity of $i$ against any vertex $j$, joined by the path $p$, with the distances measured in the subgraph $G$-$p$.

This version is called "all path external to the path $(i,j)$," by the reason that all paths $(i,v)_h$ , $h$=1,2,... are external with respect to $p_k$ , since the last path was already cut off [6]. The diagonal entries are zero.

The Cluj matrices are defined in any graph and, except for some symmetric graphs, are unsymmetrical and can be symmetrized by the Hadamard multiplication with their transposes:

$$SM_P = UM \bullet (UM)^T \quad (4)$$

If the matrices calculated on edges (*i.e.*, on adjacent vertex pairs) are required, the matrices calculated from the paths must be multiplied by the adjacency matrix **A** (which has the non-diagonal entries 1 if the vertices are joined by an edge and zero, otherwise:

$$SM_e = SM_P \bullet A \quad (5)$$

The Cluj indices are calculated [7, 8] as half-sum of the entries in a Cluj symmetric matrix, M, (M=CJD, CJΔ, CFD, CFΔ), IE(M)=$(1/2)\sum_i\sum_j[M]_{ij}[A]_{ij}$, IP(M)=$(1/2)\sum_i\sum_j[M]_{ij}$ or an unsymmetrical Cluj matrix, by IE2(UM)=$(1/2)\sum_i\sum_j[UM]_{ij}[UM]_{ji}[A]_{ij}$, IP2(UM)=$(1/2)\sum_i\sum_j[UM]_{ij}[UM]_{ji}$.

The number defined on edge, IE, is an index while the number defined on path, IP is a hyper-index.

Note that the operators IE and IP , as well as IE2 and IP2 may be applied to both symmetric and unsymmetrical matrices. The edge defined indices are identical for the two versions of Cluj indices in all graphs: IE(CJD) = IE(CFD); IE(CJΔ) = IE(CFΔ) .

Dendrimers are large and complex molecules with tailored molecular structure. They are nearly perfect monodisperse macromolecules, with a regular and highly branched three-dimensional architecture. They consist of three major architectural components: core, branches and end groups. Dendrimers are produced in an iterative sequence of reaction steps [9]. The dendrimers in Figure are formulated by their molecular graphs.

A graph G consists of a set of vertices V(G) and a set of edges E(G). In a chemical graph, each vertex represents an atom of the molecule while the covalent bonds between atoms are represented by edges joining the corresponding vertices. The graphs derived from a chemical compound are often called a molecular graph, and can be a path, a tree or a cyclic graph.

In this paper we derived the Cluj indices for two types of dendritic nanostructures.

## 2. Computing the Cluj index of the first type nanostars

The main result of this section is the following theorem:

**Theorem2.1:** The Cluj index of the first type dendrimer nanostars is $I'_n=240+(145K'+I_{K'})$ where $K'=15+\sum_{i=3}^{n}2^i$ , if n=1 than, K'=7 and if n=2 than, K'=15.

**Proof:** We compute the Cluj index of the first type dendrimer nanostar which has grown four stages. Thus, we compute the Cluj index of this nanostar from stages n.

Figure 1 shows the first-type dendrimer nanostar which was grown four stages.

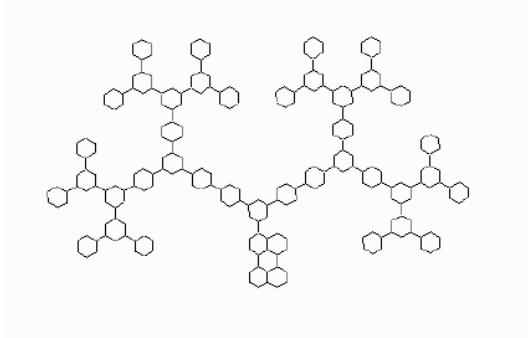

Figure 1. The first type dendrimer nanostar, grown up to the four stage

At first we consider two connected hexagons (Figure 2) and compute the Cluj index of this graph by its definition (IE(CJD)= $(1/2)\Sigma_i\Sigma_j[CJD]_{ij}[A]_{ij}$). Therefore $IE_2(CJD)=78$ (index 2 is number of hexagons), for simplicity we denote IE(CJD) by I.

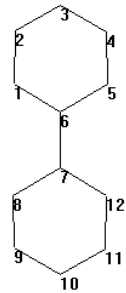


Figure 2. Two connected hexagons

Now, we compute the Cluj index of three connected hexagons (Figure 3). We have $I_3=78+6(6\times3-1)=180$.

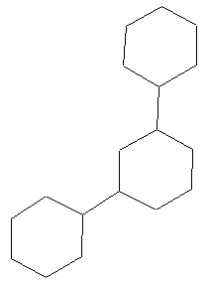

Figure 3. Three connected hexagons

In continuing, we consider four connected hexagons (Figure 4). We have $I_4 =180+6(6\times4-1)+6=324$.

Now, suppose $h_k$ is K-connected hexagons , $k \geq 3$ , then for obtaining the Cluj index of hk we have :

$I_{hK}= I_K = I_{K-1}+6(6K-1)+(K-3)\times6$. Therefore

$$I_K=I_{K-1}+6(7K-4) \qquad (6)$$

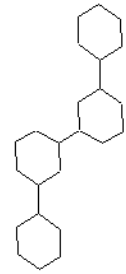

Figure 4. Four connected hexagons

Now, we compute the Cluj index of the first type nanostar which was grown four stages. At first we compute the Cluj index of the nucleus (Figure 5). Thus we have $I'_0$= 240 (i.e., IE(CJD) of nucleus).

As shown in Figure 1, the growing at the primary stage 7 hexagons adds to the nucleus. Thus the Cluj index of the primary stage is: $I'_1$=240+(6×(6×4×7))+7+738=2263, where the number 738 is the Cluj index of 7 connected hexagons, obtained by relation (6).

The growing at the second stage 8 hexagons will add to the graph, which has grown one stage. Therefore we have

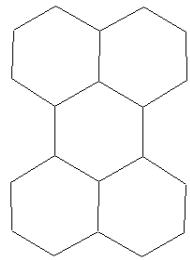

Figure 5. The nucleus of dendrimer

$I'_2$=240+(6×(6×4×15))+15+4680=7095 where the number 4680 is the Cluj index of 15 connected hexagons.

The grown of this nanostar in the first and second stage is different with other stages but the grown in the third stage is the same therefore we can compute the number of hexagons which add to the graph. Taking K the number of connected hexagons, at the growing i-stage we have

$K=2^i$, $i \geq 3$. Thus in the third stage of growing, 23 connected hexagons are add to the graph (which has 15 connected hexagons). Therefore $I'_3=240+(6\times(6\times4\times23))+23+11040=14615$ where the number 11040 is the Cluj index of 23 connected hexagons.

Now, at the fourth stage growing, 24 hexagons are added to the graph, which will have 23 connected hexagons. Therefore we have $I'_4=240+(6\times(6\times4\times39))+39+31824=37719$ where number 31824 is the Cluj index of 39 connected hexagons.

Thus, we obtain the Cluj index of the first type dendrimer nanostar, at the $n^{th}$ growing stage:

$I'_n=240+(145K'+I_{K'})$ Where $K'=15+\sum_{i=3}^{n} 2^i$ , if n=1 than, $K'=7$ and if n=2 than, $K'=15$.

## 3. Computing the Cluj index of the second type nanostar

The main result of this section is the following theorem:

**Theorem 3.1:** The Cluj index of the second type dendrimer nanostars is $I''_n= I_{K''-1}+6(7K''-4)$ where $K''=2^{n+2}-3$.

**Proof:** We compute the Cluj index of the second type dendrimer nanostar, grown up to the third stage. Figure.6 shows a second-type dendrimer nanostar.

As shown in Figure.6, there are 5 connected hexagons in the first stage, therefore from relation (6) we have $I''_1=I_5=I_4+6(7\times5-4)=510$. Now, there are 13 connected hexagons in the second stage, thus by relation (6) the Cluj index is $I''_2=I_{13}=I_{12}+6(7\times13-4)= 3510$.

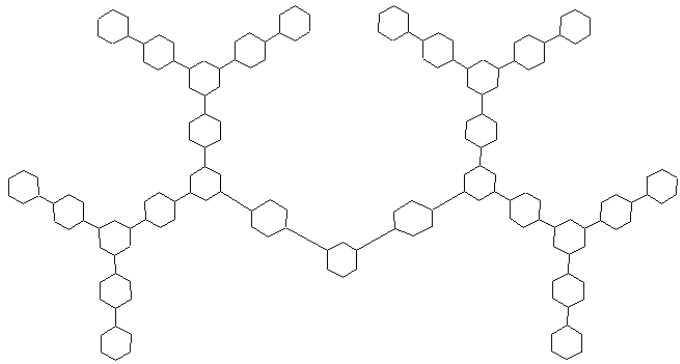

Figure 6. A second type dendrimer nanostar, three stages grown

In the third stage, there are 29 connected hexagons thus the Cluj index is $I''_3=I_{29}=I_{28}+6(7\times29-4)=17574$. As a result, the Cluj index of this nanostar dendrimer, grown up to the third stage is $I''_3=17574$.

Now, suppose this type of dendrimer was grown n stages. Then, to compute the Cluj index of this nanostar is sufficient to know how many hexagons are added to the central hexagon in a given growing stages. As shown in Figure 6, at the first stage, $2^2$ hexagons are added to the central hexagon. Thus, there are 5 connected hexagons in the first stage and $2^3$ hexagons are added at the second stage growing. Thus, we have 13 connected hexagons in the second stage. At the third stage, $2^4$ hexagons are added to the graph at the second stages. Thus, we have 29 connected hexagons. The growing of this nanostar follows the same rule in each stage. Taking K" as the number of hexagons added in the i-stage, we have $K''=1+\sum_{i=1}^{n}2^{i+1}=2^{n+2}-3$.

Thus we compute the Cluj index of the second-type of dendrimer nanostars by formula: $I''_n=I_{K''-1}+6(7K''-4)$ where $K''=2^{n+2}-3$.

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