OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 3, No. 10, October 2009, p. 1076 - 1079

Relations between clar structures, clar covers and sextet-rotations of dendrimer nanostars

K. AMINI, A. R. ASHRAFI*
Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, Iran

In this paper, the notions of Clar cover and Clar polynomial of hexagonal systems are extended to nanostar dendrimer graphs. We compute the number of Clar covers, Clar polynomial and Kekule index of four type of dendrimer nanostars.

(Received June 23, 2009; accepted September 29, 2009)

Keywords: Clar cover, Clar polynomial, Kekule index, Dendrimer nanostars

1. Introduction

Let G = (V,E) be a graph without loops and multiple edges. Let n and m be the number of vertices and edges of G, respectively. Such a graph will be referred to as an (n, m)-graph. A perfect matching of G is a set of independent edges of G covering all vertices of G.

A dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. For some time, dendrimers have received much hype as controllable tunable nanoscale materials, yet a question mark still remains. The nanostar dendrimer is part of a new group of macromolecules with great applications but first its mathematical properties must be understood. Here, a nanostar dendrimer is a connected plane graph, in which each interior face is a regular hexagon and there are no common vertices or edges between hexagons [1-3].

By IUPAC terminology, a representation of an aromatic molecular entity with fixed alternating single and double bonds, in which interactions between multiple bonds are assumed to be absent, called a Kekule structure. The number of Kekule structures of a graph G is denoted by K(G) [4]. In mathematics, a Kekule structure for a graph G usually named a perfect matching of G [5]. In graph theory language, a perfect matching of a graph H is a set of pairwise disjoint edges that cover all vertices of H. A bipartite graph is a graph whose vertex set V can be partitioned into two disjoint subsets V_1 and V_2 such that any edge e=uv $\in$ E(G) joins V_1 with V_2. It is well-known that a graph is bipartite if and only if all of its cycles have even length.

If H and G are graphs in which V(H) $\subseteq$ V(G) and E(H) $\subseteq$ E(G) then we call H to be a subgraph of G. H is called a spanning subgraph of G, if V(H) = V(G). If H is a spanning subgroup of G then we write $H \leq_{ss} G$. A spanning subgraph of H is called a Clar cover if each of its components is either a hexagon or K_2. A Clar cover of H is called a Clar structure if the set of hexagons is maximal (in the sense of set-inclusion) within all Clar covers of H. The number of Clar structures and Clar covers without alternating hexagons are denoted by cs(G) and cc(G), respectively. In this paper we are interested in dendrimer nanostar graphs that possess perfect matchings. The Clar polynomial of a of a hexagonal system H can be defines as $\rho(x,H) = \Sigma_{i\geq 0}\rho(i,H)x^i$, where $\rho(i,H)$ is the number of Clar structures containing i cycles. If G is a dendrimer nanostar then we apply the same definition as hexagonal systems to define the Clar polynomial of G. An alternating hexagon for a Clar cover C is a hexagon such that its edges are alternatively contained in C and G – C. We encourage the reader papers [6-12] and references therein for background materials as well as basic computational techniques.

In this paper we only consider connected graphs. Our notation is standard and mainly taken from [13,14].

2. Results and discussion

The aim of this section is to compute the sextet rotation, Clar structures, Clar covers and Kekule index of four dendrimer nanostars $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$, Figs. 1-4, where n is the number of layers of the nanostar dendrimer graph under consideration. We notice that if cs(G) = cc(G) then it is possible to compute easily the Clar polynomial of G.

For convenience, any nanostar dendrimer G considered, is assumed to be placed in the plane so that one of its edge directions is vertical, Fig. 5. Following Zhou, Zhang and Gutman [12], the peaks and valleys of G are coloured black and white, respectively, and all cycles considered are assumed to be oriented clockwise. Suppose M is a perfect matching for G. A cycle C of G is called M-alternating if its edges belong alternately in M and G - M. An M-alternating cycle C of H is said to be proper if each edge of C belonging to M goes from a white vertex to a black vertex, and improper otherwise. The sextet rotation, transforming all proper sextets of a Kekulé structure into improper sextets, results in a directed tree with one root, which is denoted by R(G).

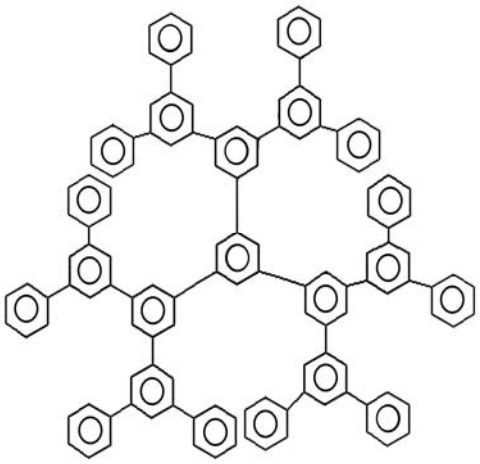

Fig. 1. The molecular graph of $NS_1[2]$.

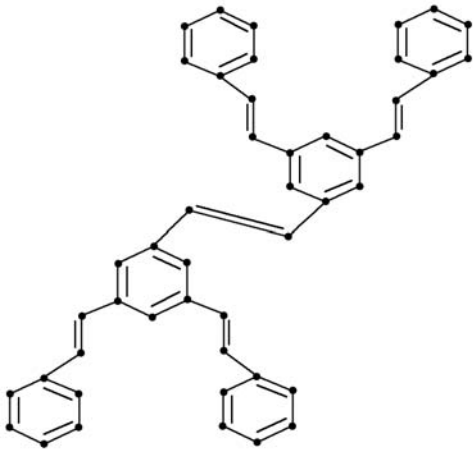

Fig. 2. The molecular graph of $NS_2[1]$.

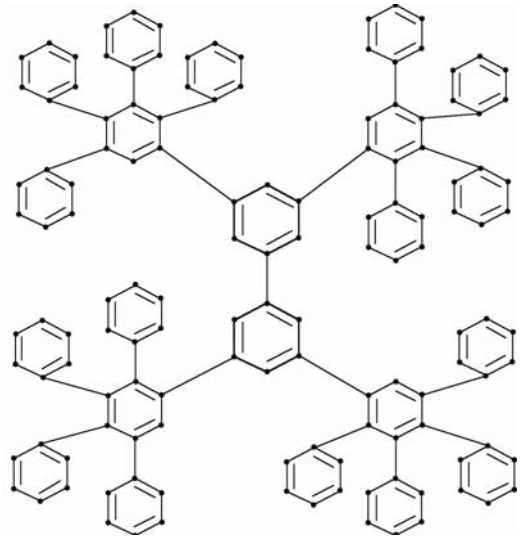

Fig. 3. The molecular graph of $NS_3[1]$.

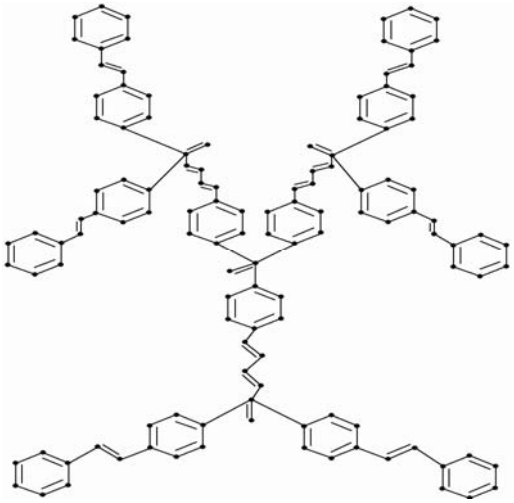

Fig. 4. The core of $NS_4[n]$.

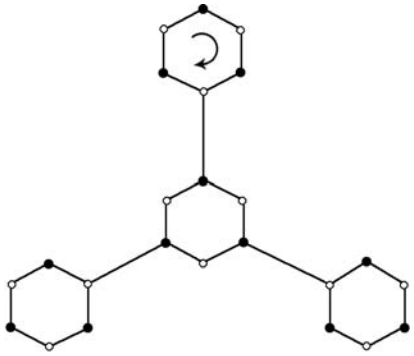

Fig. 5. The Core of $NS_1[n]$.

The root perfect matching of G is the unique perfect matching without proper sextets**.** Consider a non-root perfect matching M_i. By a sextet rotation, one can obtain another perfect matching M_j from M_i. This process is denoted by equation $R(M_i) = M_j$. We now correspond a directed tree R(G) to G. The vertices of R(G) are the perfect matching of G and two vertices M_i and M_j are adjacent if and only if $R(M_i) = M_j$.

Example. Consider the core of $NS_1[n]$. In Fig. 6, all of perfect matchings of this graph are depicted. In Fig. 7, the sextet rotation tree of this graph is drawn.

In what follows, the number of Kekule structures of a graph G is denoted by K(G). Our discussion shows that the following theorem is correct:

Theorem 1. The sextet rotation tree T_i of the dendrimer nanostar $NS_i[n]$, $1 \le i \le 4$, is a rooted directed tree with only one vertex of out-degree 0 and the number of leaves of T_i is $K(NS_i[n]) - 1$.

Gao and Zhang [14], proved that a perfect matching M of a hexagonal system H corresponds to a non-leaf of R(H) if and only if each proper M-alternating hexagon (if such exists) intersects some improper M-alternating hexagon. By our generalization of these concepts to nanostar dendrimer, one can prove the following result:

Corollary. Let G denote one of the nanostar dendrimers of Figs. 1-4 and M be a perfect matching of G with only M-alternating hexagons. Then every perfect matching of G, other than M, is corresponded to leaf of R(G).

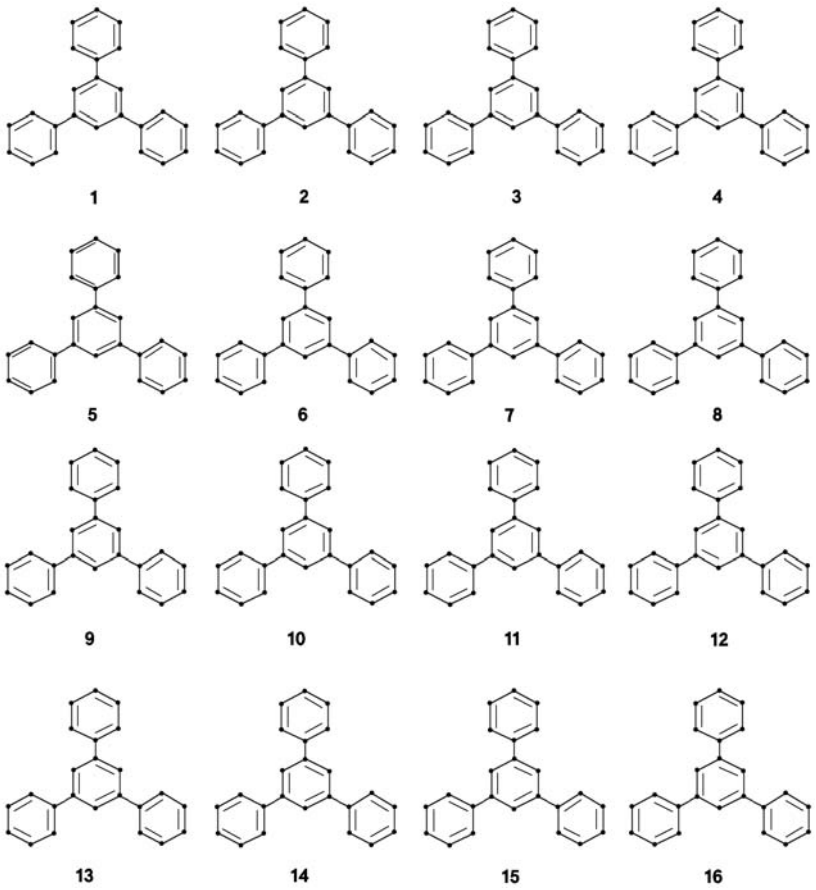

Fig. 6. The perfect matching of the core of $NS_1[n]$.

It is clear that a perfect matching for a graph G is a Clar cover of G. If we add the edges of each hexagon to initial perfect matching, then we find a Clar cover containing hexagons. This shows that our nanostar dendrimers has exactly one Clar structure. For a graph G, the number of Clar covers of G is denoted by $C_0(G)$.

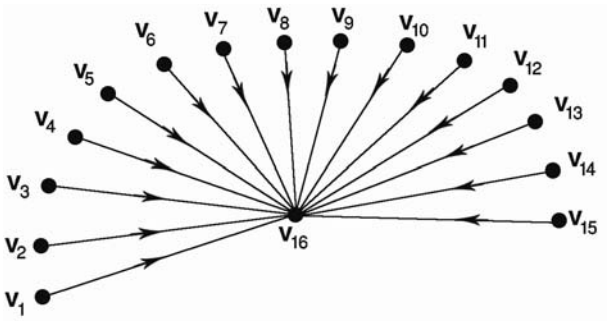

Fig. 7. The sextet rotation tree of the core of $NS_1[n]$.

Theorem 1. The following statements are hold:

a) $C_0(NS_1[n]) = 3^{6.2^n - 2}$,

b) $C_0(NS_2[n]) = 3^{2^{n+2}-2}$,

c) $C_0(NS_3[n]) = 3^{5.2^{n+2}-18}$,

d) $C_0(NS_4[n]) = 3^{3(2^{n+2}+1)}$.

Proof. The proof is straightforward and follows from our last discussion and the molecular graph of $NS_i[n]$, $1 \leq i \leq 4$.

Consider a given Clar cover T of a nanostar dendrimer G. If there is a hexagon h outside T we add h to T to obtain another Clar cover strictly containing T. This process can be continued to obtain the unique Clar structure of G. This shows that in a nanostar dendrimer G, cc(G) = cs(G) = 1. The following simple lemma is crucial in our next results.

Lemma 1. Suppose h(G) denotes the number of hexagons in a nanostar dendrimer G. Then the following are hold:

a) $h(NS_1[n]) = 3.2^{n+1} - 2$,
b) $h(NS_2[n]) = 2^{n+2} - 2$,
c) $h(NS_3[n]) = 10.2^{n+1} - 18$,
d) $h(NS_4[n]) = 6.2^{n+1} + 3$.

Proof. The proof is straightforward and follows from the molecular graph of $NS_i[n]$, $1 \le i \le 4$.

We now compute the Clar polynomial of four types of nanostar dendrimers introduced in this paper. Since the Clar structure of a nanostar dendrimer is unique, the Clar polynomial is a monomial.

Theorem 2. The following statements are hold:

a) $\rho(NS_1[n]) = x^{6.2^n - 2}$,
b) $\rho(NS_2[n]) = x^{2^{n+2} - 2}$,
c) $\rho(NS_3[n]) = x^{5.2^{n+2} - 18}$,
d) $\rho(NS_4[n]) = x^{3(2^{n+2}+1)}$.

Proof. The proof is straightforward and follows from our last discussion and the molecular graph of $NS_i[n]$, $1 \le i \le 4$.

Let G be a non-acyclic graph. The number of components and perfect matchings of G are denoted by c(G) and m(G), respectively. The perfect matching index of G is defined as $\pi(G) = \frac{\log_2 m(G)}{z(G)}$, where z(G) = |E(G)| - |V(G)| + c(G) is called the cyclic number of G. In the case of molecular graph, π(G) is called the Kekule index of G and is denoted by κ(G).

Lemma 2. The number of Kekule structures of our nanostar dendrimers are as follows:

a) $K(NS_1[n]) = 28^{n+1}$,
b) $K(NS_2[n]) = 2^{2^{n+2}-2}$,
c) $K(NS_3[n]) = \frac{1}{262144}.2^{10.2^{n+1}}$,
d) $K(NS_4[n]) = 82^{62(n+1)}$.

In the following table, the number of edges and vertices of our nanostar dendrimers are computed.

Table 1. The number of vertices and edges of $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_1[n]$.

$\lvert V(NS_1[n])\rvert = 18.2^{n+1} - 12$	$\lvert E(NS_1[n])\rvert = 21.2^{n+1} - 15$
$\lvert V(NS_2[n])\rvert = 2^{n+6} - 24$	$\lvert E(NS_2[n])\rvert = 9.2^{n+2} - 21$
$\lvert V(NS_3[n])\rvert = 15.2^{n+3} - 108$	$\lvert E(NS_3[n])\rvert = 35.2^{n+2} - 127$
$\lvert V(NS_4[n])\rvert = 3.2^{n+5} + 26$	$\lvert E(NS_4[n])\rvert = 27.2^{n+2} + 28$

We are now ready to prove one of our main results related to the Kekule index of these nanostars. We have:

Theorem 2. The Kekule indices of $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ are computed as follows:

a) $\kappa(NS_1[n]) = (n+1)(2 + \log_2^7)/(3.2^{n+1} - 2)$,
b) $\kappa(NS_2[n]) = (2^{n+1} - 1)/(2 - 7.2^{n+1})$,
c) $\kappa(NS_3[0n]) = (10.2^{n+1} - \log_2^{262144})/(10.2^{n+1} - 19)$,
d) $\kappa(NS_4[n]) = 62(n+1).\log_2^{82}/(6.2^{n+1} + 2)$.

Proof. The proof follows from definition of Kekulé index, Lemmas 1,2, Theorems 1,2 and Table 1.

References

[1] A. R. Ashrafi, H. Saati, J. Comput. Theoret. Nanosci. **5**, 681 (2008).
[2] A. R. Ashrafi, M. Mirzargar, Indian J. Chem. **47A**, 535 (2008).
[3] H. Yousefi-Azari, A. R. Ashrafi, A. Bahrami, J. Yazdani, Asian J. Chem. **20**, 15 (2008).
[4] R. Swinborne-Sheldrake, W. C. Herndon, I. Gutman, Tetrahedron Lett. **16**, 755 (1975).
[5] H. Sachs, Combinatorica **4**, 89 (1984).
[6] W. C. Herndon, H. Hosoya, Tetrahedron **40**, 3987 (1984).
[7] H. Zhang, F. Zhang, Discr. Appl. Math. **105,** 291 (2000).
[8] S. El-Basil, Theor. Chim. Acta **70**, 53 (1986).
[9] I. Gutman, in: Proceedings of the 4th Yougoslav seminar on Graph theory, Novi Sad, 51, 1983.
[10] N. Ohkami, A. Motoyama, H. Hosoya, I. Gutman, Tetrahedron **37**, 1113 (1981).
[11] Z. Chen, Chem Phys Lett. **115**, 291 (1985).
[12] S. Zhou, H. Zhang, I. Gutman, Disc. Appl. Math. **156**, 1809 (2008).
[13] I. Gutman, S. J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer-Verlag, Berlin, 1989.
[14] N. Trinajstic, Chemical graph theory, 2nd edn, CRC Press, Boca Raton, FL, 1992.
[15] X. Guo, F. Zhang, J. Math. Chem, **12**, 163 (1993).

[*]Corresponding author: ashrafi@kashanu.ac.ir