OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 4, No. 6, June 2010, p. 877 - 880

Clar structures, Clar covers and Kekule index of dendrimer nanostars

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In an earlier paper, the present authors extended the notions of Clar cover and Clar polynomial of hexagonal systems to nanostar dendrimers. In this paper, we compute the number of Clar covers, Clar polynomial and Kekule index of four types of dendrimer nanostars.

(Received March 26, 2010; accepted June 16, 2010)

Keywords: Clar structure, Clar polynomial, Kekule index

1. Introduction

A dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. 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. The topological study of these macromolecules is the aim of this article, see [1-6] for details.

Let G = (V,E) be a molecular graph with n vertices and m edges. 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. 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) [7]. In mathematics, a Kekule structure for a graph G usually named a perfect matching of G [8]. Kekule structures have numerous applications in chemistry [9-14]. For instance, various Kekule-structure-related models for approximating the Dewar resonance energy (DRE) of benzenoid hydrocarbons have been proposed, see [7,15] for details.

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. A spanning subgraph of H of a graph G is called a Clar cover if each of its components is either a hexagon or K_2. A hexagon belonging to a Clar cover is often indicated by drawing a circle inside this hexagon. For example in Figure 1, four Clar covers containing two alternating hexagons are shown. 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(H) and cc(H), respectively.

The Clar polynomial of a hexagonal system H can be defined 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 H is a dendrimer nanostar then we apply the same definition as hexagonal systems to define the Clar polynomial of H. An alternating hexagon for a Clar cover C is a hexagon such that its edges are alternatively contained in C and G – C.

In this paper we are interested in dendrimer nanostar graphs that possess perfect matchings. Throughout this paper we only consider connected graphs. Our notation is standard and mainly taken from [16].

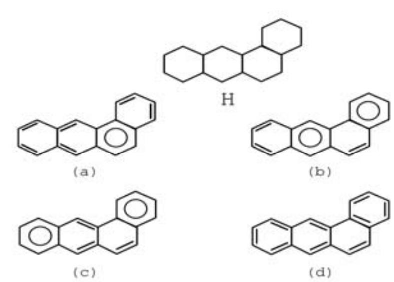

Fig. 1. A Hexagonal system H and four Clar covers, one containing the two alternating hexagons.

2. Main 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. 2-5, where n is the number of layers of the nanostar dendrimer graph under consideration. We notice that if cs(H) = cc(H) then it is possible to compute easily the Clar polynomial of H, since it can be solved by contracting all Clar covers without alternating hexagons.

Following Zhou, Zhang and Gutman [14], 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 cycle 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.

It is clear that a perfect matching M for a graph H is a Clar cover of H, because any perfect matching of H is a spanning subgraph that its all of components are K_2. Every hexagon in these dendrimer nanostars is an alternating hexagon. Thus M is a Clar cover with alternating hexagon. If in the perfect matching M, select all of edges in a hexagon instead of 3 alternating edges K_2 in a hexagon, we make a Clar cover without alternating hexagons. For a graph H, the number of Clar covers of H is denoted by $C_0(H)$.

Lemma 1. The number of vertices and edges of NSi[n], $1 \le i \le 4$, is:

a) $|V(NS_1[n])| = 24.2^n - 4$ and $|E(NS_1[n])| = 27.2^n - 5$,

b) $|V(NS_2[n])| = 16.2^{n+1} - 4$ and $|E(NS_2[n])| = 18.2^{n+1} - 5$,

c) $|V(NS_3[n])| = 52.2^n - 12$ and $|E(NS_3[n])| = 58.2^n - 13$,

d) $|V(NS_4[n])| = 96.2^{n-1} - 60$ and $|E(NS_4[n])| = 105.2^{n-1} - 66$.

Theorem 1. The following statements are hold:

a) $C_0(NS_1[n])$ =,
b) $C_0(NS_2[n])$ =,
c) $C_0(NS_3[n]) = 16^{2^n}$,
d) $C_0(NS_4[n]) = 3^{13+3(2^n-4)}$, n≥2.

Proof. The parts (a), (b) and (c) are easy consequences of the Figs. 2-4. Every hexagon of a Clar cover has three different forms. To prove the part (d), we must calculate the number of hexagons. In fact, $C_0(NS_4[n]) = 3^{h(NS_4[n])}$, where n ≥ 2. From the Fig. 9, one can see that $h = 13 + \sum_{i=1}^{n-1} 3.2^i$, proving the theorem.

Notice that the growth of the nanostar dendrimer $NS_3[n]$ depicted in Figs. 3 and 8, is different from other nanostar dendrimers presented in this paper.

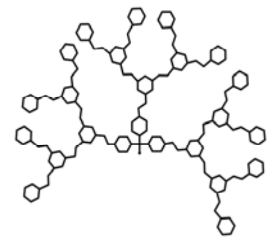

Fig. 2. The molecular graph of $NS_1[n]$ for n=3.

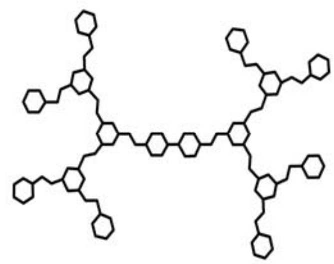

Fig. 3. The molecular graph of $NS_2[n]$ for n=2.

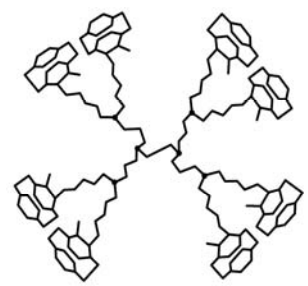

Fig. 4. The molecular graph of $NS_3[n]$ for n=2.

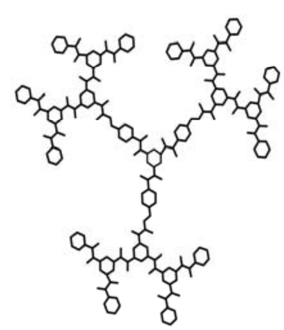

Fig. 5. The molecular graph of $NS_4[n]$ for n=3.

Lemma 2. Suppose h(H) denotes the number of hexagons in a nanostar dendrimer H. Then the following are hold:

a) $h(NS_1[n]) = 3.2^n$,
b) $h(NS_2[n]) = 2^{n+2}$,
c) $h(NS_3[n]) = 2^{n+2}$,
d) $h(NS_4[n]) = 13+3(2^n - 4)$, n≥2.

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

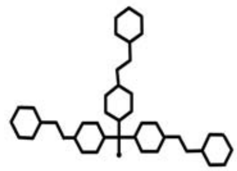

Fig. 6. The Core of $NS_1[n]$.

Theorem 2. For dendrimer nanostars $NS_1[n]$, $NS_2[n]$ and $NS_4[n]$, cc = cs = 1 and for dendrimer nanostar $NS_3[n]$, cc = cs = 4^{2^n}.

Proof. Consider a given Clar cover C of dendrimer nanostars $NS_1[n]$, $NS_2[n]$ or $NS_4[n]$. If there is a hexagon h outside C, we add h to C as a hexagon component in Clar cover C to obtain another Clar cover strictly containing C. This process can be continued to obtain the unique Clar structure of $NS_i[n]$, i = 1, 2, 4. This shows that in dendrimer nanostars $NS_1[n]$, $NS_2[n]$ and $NS_4[n]$, cc = cs = 1.

We now consider the dendrimer shape molecule $NS_3[n]$. From Fig. 8, the core of this molecule has exactly four similar branches, each of which can be given four different forms for Clar cover, Fig. 10. Hence by a simple counting method, cc = cs = 4^{2^n}. This completes the proof.

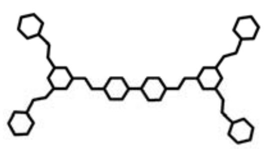

Fig. 7. The Core of $NS_2[n]$.

We now compute the Clar polynomial of four types of dendrimer nanostars nanostars $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$. Since, the Clar structure of the dendrimer nanostars $NS_1[n]$, $NS_2[n]$ and $NS_4[n]$ are unique, the Clar polynomial is a monomial. The number of cycles in a Clar structure is equivalent to the number of hexagon components in a Clar structure. Hence for dendrimer nanostars $NS_i[n]$, i = 1, 2, 4, the Clar polynomial is $\rho(x,NS_1[n]) = x^{h(NS_i[n])}$, since cc = cs = 1.

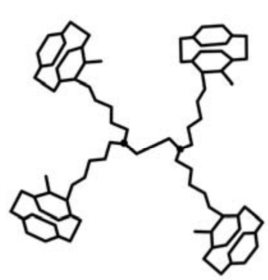

Fig. 8. The Core of $NS_3[n]$.

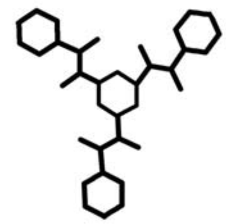

Fig. 9. The Core of $NS_4[n]$.

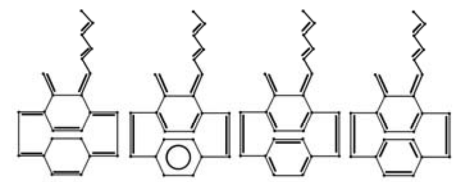

Fig. 10. Four different forms of branches of the molecule in calculation of Clar covers.

Theorem 3. The following statements are hold:

a) $\rho(x, NS_1[n]) = x^{3.2^n}$,

b) $\rho(x, NS_2[n]) = x^{2^{n+2}}$,

c) $\rho(x, NS_3[n]) = 2^{n+1}x + \binom{2^{n+1}}{2}x^2 + \binom{2^{n+1}}{3}x^3 + \ldots + x^{2^{n+1}}$,

d) $\rho(x, NS_4[n]) = x^{13+3(2^n-4)}$.

Proof. The parts (a), (b) and (d) are obtained from our discussion before stating the theorem. To prove (c), we notice that each branch of $NS_3[n]$ has exactly one hexagon and the molecule is containing 2^{n+1} branches, proving the result.

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 $\pi(G) = \dfrac{\log_2 m(G)}{z(G)}$, 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 it is denoted by κ(G). In particular, when G is a hexagonal system, z(G) is the number of hexagons and therefore, the Kekule index is also considered by some chemists as a measure of resonance energy per hexagon. It is well known that $\kappa(G) \le 1$ [16].

Lemma 3. The number of Kekule structures of four dendrimer nanostars $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ are as follows:

a) $K(NS_1[n]) = 64^{2^{n-1}}$,

b) $K(NS_2[n]) = 2^{2^{n+2}}$,

c) $K(NS_3[n]) = 9^{2^n}$,

d) $K(NS_4[n]) = 2^{13+3(2^n-4)}, n \ge 2$.

We are now ready to state our final main results related to the Kekule index of these nanostars:

Theorem 4. The Kekule index of dendrimer nanostars $NS_1[n]$, $NS_2[n]$, $NS_3[n]$ and $NS_4[n]$ are computed as follows:

a) $\kappa(NS_1[n]) = 6.2^{n-1}/(3.2^{n+1}-2)$,

b) $\kappa(NS_2[n]) = 2^{n+2}/(2-7.2^{n+1})$,

c) $\kappa(NS_3[n]) = 2^{n+1}.\log_2^3/(10.2^{n+1}-19)$,

d) $\kappa(NS_4[n]) = 13+3(2^n-4)/(6.2^{n+1}+2), n \geq 2$.

Proof. The proof follows from definition and Lemmas 1 and 3.

References

[1] K. Amini, A. R. Ashrafi, Optoelectron. Adv. Mater.-Rapid Comm. **3**(4), 356 (2009).

[2] A. R. Ashrafi, H. Saati, J. Comput. Theoret. Nanosci. **5**(4), 681 (2008).

[3] H. Yousefi-Azari, A. R. Ashrafi, A. Bahrami, J. Yazdani, Asian J. Chem. **20** (1), 15 (2008).

[4] A. R. Ashrafi, M. Mirzargar, Indian J. Chem. **47A** (4), 535 (2008).

[5] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Indian J. Chem. **47A**(10), 1503 (2008).

[6] A. R. Ashrafi, M. Mirzargar, Util. Math. **77,** 249 (2008).

[7] R. Swinborne-Sheldrake, W. C. Herndon, I. Gutman, Tetrahedron Lett. **16**, 755 (1975).

[8] H. Sachs, Combinatorica **4**, 89 (1984).

[9] H. Sachs, P. Hansen, M. Zheng, MATCH Commun. Math. Comput. Chem. **33**, 169 (1996).

[10] S. El-Basil, Theor. Chim. Acta **70**, 53 (1986).

[11] L. J. Schaad, B. A. Hess, Chem. Rev. **101**, 1465 (2001).

[12] I. Gutman, Covering hexagonal systems with hexagons, in: Proceedings of the 4th Yougoslav seminar on Graph theory, Novi Sad, 1983, pp. 51–60.

[13] H. Zhang, F. Zhang, Discrete Appl. Math. **105**, 291 (2000).

[14] S. Zhou, H. Zhang, I. Gutman, Discrete Appl. Math. **156**, 1809 (2008).

[15] W. C. Herndon, H. Hosoya, Tetrahedron **40**, 3987 (1984).

[16] I. Gutman, S. J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer-Verlag, Berlin, 1989.

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