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Eccentric Connectivity Index of Hexagonal Belts and Chains

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Abstract

We present explicit formulae for the eccentric connectivity index of zigzag and armchair hexagonal belts and the corresponding open chains.

1 Introduction

The eccentric connectivity index is a graph invariant that has been used over the course of last decade for modeling and predicting various properties of chemical compounds [4, 8, 9, 10, 12]. In spite of its satisfactory performance, the mathematical properties of this index remained unexplored until very recently, when a number of papers appeared almost simultaneously [14, 6, 2]. Those papers are mostly concerned with extremal graphs and values, reporting along the way also some explicit formulae for various classes of graphs. In the present note we consider some chemically interesting graphs, such as the zigzag and armchair hexagonal belts and the corresponding open hexagonal chains, and establish explicit formulae for the values of the eccentric connectivity index of such graphs. The presented results could be viewed as stepping stones toward explicit formulae for carbon nanotubes and tubular fullerenes.

2 Definitions and preliminaries

All graphs in this paper are finite, simple and connected. For terms and concepts not defined here we refer the reader to any of several standard monographs such as, e.g., [5] or [13]. Some terms are borrowed from the chemistry of benzenoid compounds; for an introduction to the graph-theoretic aspects of this area we recommend reference [1].

Let G be a graph on n vertices. We denote the vertex and the edge set of G by $V(G)$ and $E(G)$, respectively. For two vertices u and v of $V(G)$ we define their **distance** $d(u, v)$ as the length of a shortest path connecting u and v in G. For a given vertex u of $V(G)$ its **eccentricity** $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. Hence, $\varepsilon(u) = \max_{v \in V(G)} d(u, v)$. The maximum eccentricity over all vertices of G is called the **diameter** of G and denoted by $D(G)$. The **eccentric connectivity index** $\xi(G)$ of a graph G is defined as

$$\xi(G) = \sum \delta_u \varepsilon(u),$$

where δ_u denotes the degree of vertex u, i. e., the number of its neighbors in G.

Let us consider the graph L_h shown in Fig. 1. It is a planar and bipartite graph with h hexagonal faces. It is immediately clear that L_h has $n = 4h + 2$ vertices and $m = 5h + 1$ edges. This graph is called a **linear polyacene** on h hexagons. By identifying the two

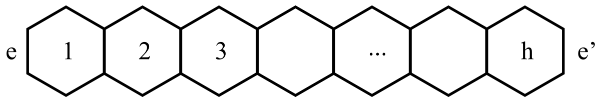

Figure 1: A linear polyacene.

edges denoted by e and e' one obtains a closed belt made of h hexagons. We denote such a belt by Z_h and call it a **zigzag hexagonal belt**. The belt could be viewed as a (very short) nanotube of zigzag type, hence the name. In order to avoid degeneracy we assume that the number of hexagons in a zigzag belt is at least three. It is easily seen that $|V(Z_h)| = 4h$ and $|E(Z_h)| = 5h$.

Consider now the graph F_h shown in Fig. 2. It is called a **fibonacene** on h hexagons. (The name is derived from the fact that the Fibonacci numbers appear as the counting sequence for perfect matchings in such graphs.) By identifying the edges e and e' we again obtain a closed hexagonal belt. Such belts are called **armchair belts**, again after the nanotubes obtained by stacking several such belts. We denote the armchair belt on

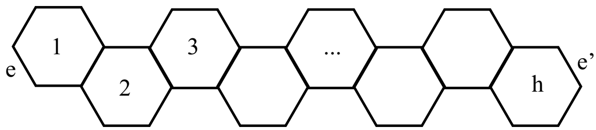

Figure 2: A fibonacene.

h hexagons by A_h. Obviously, armchair belts on h hexagons exist for all even $h \geq 4$; the case $h = 2$ leads to a degeneracy, and an odd number of hexagons introduces notational and technical complications and will not be considered here. Again, $|V(F_h)| = 4h + 2$, $|E(F_h)| = 5h + 1$, $|V(A_h)| = 4h$ and $|E(A_h)| = 5h$. Whenever there is no possibility of confusion we will use n and m for the number of vertices and edges, respectively, of graphs under consideration.

3 Hexagonal belts

Now we can derive the formulae for the eccentric connectivity index for our graphs. We start with the belts. In both types of belts we consider here there are two types of vertices, distinguished by their degree. As all vertices of a given degree are equivalent, our task boils down to computing the eccentricity of any two vertices of different degrees in the considered belt. We denote a vertex of degree i by v_i for $i = 2, 3$, and its eccentricity in a graph G by $\varepsilon_G(v_i)$, for $G = Z, A$. The subscript h is omitted for notational simplicity.

Proposition 1

$\varepsilon_Z(v_2) = h + 1\,;\ \varepsilon_Z(v_3) = h + 1\,;\ \varepsilon_A(v_2) = h$ for $h \geq 6\,;\ \varepsilon_A(v_3) = h\,.$

Proof

We consider the case of Z_h first. Let h be even. Then the eccentricity of a vertex of degree 2 from the upper border of Z_n is obviously achieved on the diametrally opposite vertex (again of degree 2) from the lower border. Any shortest path between those two vertices must include exactly one of vertical edges; the remaining edges in such a path must sum to the number of hexagons. Hence, $\varepsilon_Z(v_2) = h+1$ for h even. The situation is completely analogous for vertices of degree 3. For an odd h, the eccentricity of a vertex of degree 2 is achieved on the diametrally opposite vertex of degree 3 on the other border, and again all shortest paths have length $h+1=n/4+1$.

In case of A_h we always have h even. The eccentricity of a vertex of degree 2 is achieved on the diametrally opposite vertex of degree 2, and any shortest path is of length $h=n/4$. Similarly, the eccentricity of a vertex of degree 3 is achieved on a vertex of degree 3 on the opposite border, and the length of ant shortest path is again $h=n/4$.

For the exceptional case $h=4$ we have $\varepsilon_A(v_2)=5$. ■

Corollary 2
$\xi(Z_h)=\frac{5}{8}n(n+4)\,;\ \xi(A_h)=\frac{5}{8}n^2\,.$

Proof
In both Z_h and A_h there are $n/2$ vertices of degree 2 and $n/2$ vertices of degree 3. Hence $\xi(Z_h)=(h+1)(2+3)\frac{n}{2}=\frac{5n}{2}(h+1)=\frac{5}{8}n(n+4)$. The claim for A_h follows by the same arguments. ■

4 Open chains

The case of open chains is more complicated since the vertices of a given degree are no more equivalent and the border effects must be taken into account.

We consider first the zigzag open chain L_h. Her the equivalence classes are of size 4, with one exception. The exceptional class consists of two vertices from the vertical symmetry axis of L_h. For h odd those two vertices are of degree two, for h even they are of degree three. It is easy to see, by inspection, that in both cases their eccentricity is equal to $h+1$. Let us assume that h is odd. Then the exceptional class is made of two vertices of degree two, and their contribution to $\xi(L_h)$ is equal to $4(h+1)$.

Each of the remaining h classes consists of four vertices arranged symmetrically with respect to the horizontal and to the vertical symmetry axis. One of the classes is made from four vertices of degree two making the endpoints of two lateral vertical edges. Since each of those vertices has the eccentricity $2h+1$, the total contribution of this class to $\xi(L_h)$ is equal to $8(2h+1)$.

Now consider a class containing four vertices of degree three at distance i from the vertical symmetry axis. The integer i must be odd; the smallest value of i is 1, the largest value is $h-2$. By adding the value of i to the eccentricity of the vertices of the exceptional class one obviously obtains the eccentricity of a vertex from the considered class. The total contribution of all $\frac{h-1}{2}$ such classes is then obtained by summing the expressions $4 \cdot 3 \cdot (h+1+i)$ over all odd values of i from 1 to $h-2$.

The remaining $\frac{h-1}{2}$ classes consisting of vertices of degree 2 at the distance j from the vertical symmetry axis can be treated in a similar manner. Here j is even, the eccentricity of a vertex from a class at the distance j is given by $h+1+j$, and their total contribution is obtained by summing the expressions $4 \cdot 2 \cdot (h+1+j)$ over all even j from 2 to $h-1$.

Now we can add all the contributions and obtain the explicit formula for $\xi(L_h)$:

$$\xi(L_h) = 4(h+1) + 8(2h+1) + 12 \sum_{\substack{i=1 \\ i \text{ odd}}}^{h-2} (h+1+i) + 8 \sum_{\substack{j=2 \\ j \text{ even}}}^{h-1} (h+1+j) = 15h^2 + 14h + 3\,.$$

The result can be also expressed in terms of the number of vertices: $\xi(L_h) = (15/16)\,n^2 - n/4 - 1/4$.

Now consider the case of L_h for even h. Here the exceptional class and all classes at even distance from it contain vertices of degree three, while the classes at odd distances from the exceptional class contain vertices of degree two. The eccentricity of both vertices from the exceptional class is again $h+1$, but their total contribution is greater then in the case of odd h, and it is equal to $6(h+1)$. The eccentricity of the rightmost and the leftmost vertices of degree two is again $2h+1$, and the total contribution of this class is the same as in the case of odd h, i.e, $8(2h+1)$. The classes at even and odd distances now contribute $12 \sum_{\substack{j=2 \\ j \text{ even}}}^{h-2} (h+1+j)$ and $8 \sum_{\substack{i=1 \\ i \text{ odd}}}^{h-1} (h+1+i)$, respectively, and the final formula for even h is given by

$$\xi(L_h) = 6(h+1) + 8(2h+1) + 12 \sum_{\substack{j=2 \\ j \text{ even}}}^{h-2} (h+1+j) + 8 \sum_{\substack{i=1 \\ i \text{ odd}}}^{h-1} (h+1+i) = 15h^2 + 14h + 2.$$

In terms of number of vertices, $\xi(L_h) = \frac{1}{16}(15n^2 - 4n - 20)$.

Now we can summarize our results for L_h.

Proposition 3
$\xi(L_h) = 15h^2 + 14h + 2 - \frac{1-(-1)^h}{2}$. ■

It remains to consider armchair belts on h hexagons. The situation for an odd h is shown in Fig. 3. Now the vertical symmetry axis does not contain any vertices, and the distance

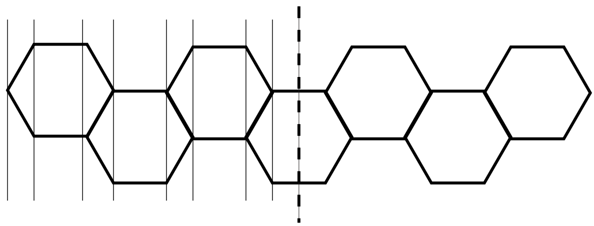

Figure 3: With the proof of Proposition 4.

classes are arranged symmetrically with respect to this axis. The left halves of the classes are indicated by thin vertical lines in Fig. 3. One of the classes contains only two vertices, farthest from the symmetry axis, both of them of degree two and the eccentricity $2h+1$. Its contribution to $\xi(F_h)$ is equal to $4(2h+1)$. Of the remaining h classes, one contains four vertices of degree two and eccentricity $2h$; its contribution is equal to $16h$. The sum of degrees of vertices in each of the remaining $h-1$ classes is equal to 10. Each such class contains four vertices, and their eccentricities vary from $h+1$ to $2h-1$ with step one. By summing their contributions we can conclude that $\xi(F_h) = 15h^2 + 9h + 4$ if the number h of hexagons is odd.

Finally, the case of even h in F_h is illustrated in Fig. 4. Again, the left half-classes are

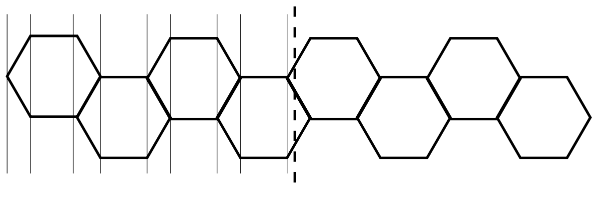

Figure 4: With the proof of Proposition 4.

indicated by thin vertical lines, and again none of the vertices lie on the symmetry axis (indicated by a thick dashed line). Now the result follows along the same lines as in the case of odd h, since the contributions of all classes are the same as in the odd case.

Proposition 4

$\xi(F_h) = 15h^2 + 9h + 4.$ ■

Now one can easily derive also the formulae in terms of the number of vertices by substituting $(n-2)/4$ for h in the above expressions.

5 Compression ratio

It is intuitively clear that closing an open hexagonal chain and thus forming the corresponding belt will decrease the eccentric connectivity index. The decrease can be quantified by considering the ratio of the eccentric connectivity indices for closed and open chains. Such quotient is called the **compression ratio**. Since we are interested in this quantity for large values of h (and hence n), it suffices to consider only the asymptotic behavior.

It follows from the above discussion that the eccentric connectivity index of open chains behaves asymptotically as $\frac{15}{16}n^2$, while for closed belts of both types the asymptotic behavior is given by $\frac{5}{8}n^2$. Hence in both cases the compression ratio is equal to 2/3. It is interesting to observe that the same compression ratio appears for the eccentric connectivity indices of path and cycles [2]. It indicates that the asymptotic behavior of this quantity is dominated by the number of monomer units in linear and circular polymers, and depends but weakly on the internal structure of monomers. It would be interesting to look at some polymers made of monomers with richer internal structure and to see whether this observation remains valid.

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References

[1] S. J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1988.

[2] T. Došlić , M. Saheli, D. Vukičević, Eccentric connectivity index: extremal graphs and values, to appear.

[3] H. Dureja, A. K. Madan, Superaugmented eccentric connectivity indices: new–generation highly discriminating topological descriptors for QSAR/QSPR modeling, *Med. Chem. Res.* **16** (2007) 331–341.

[4] S. Gupta, M. Singh, A. K. Madan, Application of graph theory: relationship of eccentric connectivity index and Wiener's index with anti–inflammatory activity, *J. Math. Anal. Appl.* **266** (2002) 259–268.

[5] F. Harary, *Graph Theory*, Addison–Wesley, Reading, 1969.

[6] A. Ilić, I. Gutman, Eccentric connectivity index of chemical trees, *MATCH Commun. Math. Comput. Chem.*, to appear.

[7] V. Kumar, S. Sardana, A. K. Madan, Predicting anti–HIV activity of 2,3-diaryl-1,3-thiazolidin-4-ones: computational approaches using reformed eccentric connectivity index, *J. Mol. Model.* **10** (2004) 399–407.

[8] V. Kumar, A. K. Madan, Application of graph theory: prediction of cytosolic phospholipase A_2 inhibitory activity of propan-2-ones, *J. Math. Chem.* **39** (2006) 511–521.

[9] V. Lather, A. K. Madan, Application of graph theory: topological models for prediction of CDK-1 inhibitory activity of aloisines, *Croat. Chem. Acta* **78** (2005) 55–61.

[10] V. Lather, A. K. Madan, Predicting dopamine receptors binding affinity of N-[4-(4-Arylpiperazin-1-yl)butyl]Aryl carboxamides: computational approach using topological descriptors, *Curr. Drug Discov. Tech.* **2** (2005) 115–121.

[11] S. Sardana, A. K. Madan, Application of graph theory: relationship of molecular connectivity index, Wiener's index and eccentric connectivity index with diuretic activity, *MATCH Commun. Math. Comput. Chem.* **43** (2001) 85–98.

[12] V. Sharma, R. Goswami, A. K. Madan, Eccentric connectivity index: a novel highly discriminating topological descriptor for structure–property and structure–activity studies, *J. Chem. Inf. Comput. Sci.* **37** (1997) 273–282.

[13] D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, 1996.

[14] B. Zhou, Z. Du, On eccentric connectivity index, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 181–198.