JOURNAL OF MATHEMATICAL NANOSCIENCE

JMNS

Vol. 2, No. 1, 2012, 29-36

Remarks on atom bond connectivity index

SOMAYYEH NIK-ANDISH

Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I R. Iran

ABSTRACT. A topological index is a function *Top* from $\sum$ into real numbers with this property that *Top*(*G*) = *Top*(*H*), if *G* and *H* are isomorphic. Nowadays, many of topological indices were defined for different purposes. In the present paper we present some properties of atom bond connectivity index.

Keywords: atom bond connectivity index, matching, clique number.

Journal of Mathematical Nano Science

1. INTRODUCTION

A topological index is a graphic invariant used in structure-property correlations. So many topological indices have been introduced and many mathematician works in this area, see [1,2]. One of the most important topological indices is the connectivity index, χ introduced in 1975 by Milan Randić [3]. Recently Estrada *et al.* [4,5] introduced atom-bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cyclo-alkanes. This index is defined as follows:

$$ABC(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}},$$

where $d_G(u)$ stands for the degree of vertex u.

An r-matching of G is a set of r edges of G which no two of them have common vertex. The maximum number of edges in a matching of a graph G is called the matching number of G and denoted by $\mu(G)$.

2. Main Results and Discussion

The aim of this section is to present some bounds of ABC index. The first Zagreb index [6] is defined as $M_1(G)=\sum_{uv\in E} d_G(u)+d_G(v)$, where $d_G(u)$ denotes the degree of vertex u. The modified second Zagreb index $M_2^*(G)$ is equal to the sum of the products of the reciprocal of the degrees of pairs of adjacent vertices of the underlying molecular graph G, that is

$$M_2^*(G)=\sum_{uv\in E}\frac{1}{d_G(u)d_G(v)}.$$

Theorem 1 [7]. Let G be a connected graph with n vertices, p pendent vertices, m edges, maximal degree Δ and minimal non-pendent vertex degree δ_1. Let M_1 and $M_2^*(G)$ be the first and modified second Zagreb indices of G. Then

$$ABC(G)\le p\sqrt{1-\frac{1}{\Delta}}+\sqrt{[M_1-2m-p(\delta_1-1)](M_2^*-\frac{p}{\Delta}}).$$

Corollary 1 [7]. With the same notation as in Theorem 1,

$$ABC(G)\le\sqrt{(M_1-2m)M_2^*},$$

with equality if and only if G is regular or bipartite semiregular.

Theorem 2 (Nordhaus–Gaddum-type) [8]. Let G be a simple connected graph of order n with connected complement $\bar{G}$. Then

$$ABC(G)+ABC(\bar{G})\ge\frac{2^{3/4}n(n-1)\sqrt{k-1}}{k^{3/4}(\sqrt{k}+\sqrt{2})} \qquad (1)$$

where $k = \max\{\Delta, n - \delta - 1\}$, and where Δ and δ are the maximal and minimal vertex degrees of G. Moreover, equality in (1) holds if and only if $G \approx P_4$.

Theorem 3 [8]. Let G be a simple connected graph of order n with connected complement $\overline{G}$. Then

$$ABC(G)+ABC(\overline{G})\le(p+\overline{p})\sqrt{\frac{n-3}{n-2}}\left(1-\sqrt{\frac{2}{n-2}}\right)+\binom{n}{2}\sqrt{\frac{2}{k}-\frac{2}{k^2}} \qquad (2)$$

where p, $\overline{p}$ and $\delta_1,\overline{\delta}_1$ are the number of pendent vertices and minimal non–pendent vertex degrees in G and $\overline{G}$, respectively, and $k = min\{\delta_1,\overline{\delta}_1\}$. Equality holds in (2) if and only if $G \approx P_4$ or G is an r-regular graph of order $2r + 1$.

Graphene is the first two-dimensional material observed so far. It is a planar sheet of carbon atoms that are densely packed in a honeycomb crystal lattice. Graphene is the main element of some carbon allotropes including graphite, charcoal, carbon nanotubes, and fullerenes, see Figure 1.

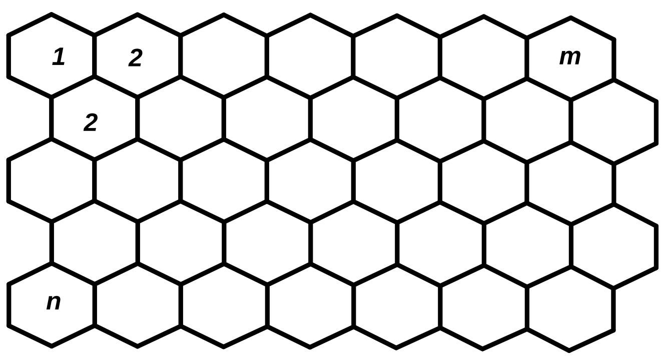

Figure 1. 2 – Dimensional graph of graphene sheet.

In the following examples we compute these topological indices for some graphene sheets that will serve as basic building blocks in the considered graphene graphs. Denoted by $G(m, n)$ means a graphene sheet with n rows and m columns.

Example 1. Consider graph $G(2,2)$ shown in Figure 2. There exist six edges with endpoint of degrees 2, ive edges with endpoint of degrees 3 and eight edges with endpoint of degrees 2, 3. This implies:

$$ABC(G(2,2))=\frac{14}{\sqrt{2}}+\frac{10}{3} \text{ and } ABC_3(G(2,2))=14\times8+5\times\frac{729}{64}=112+\frac{3645}{64}.$$

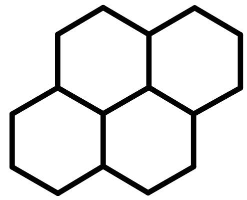

Figure 2. A 2 - Dimensional graph of $G(2, 2)$.

Example 2. Suppose $G(3,2)$ be a graphene sheet with 3 columns and 2 rows (depicted in Figure 3). By counting endpoint degrees one can see easily,

$$ABC(G(3,2)) = \frac{1}{\sqrt{2}} \times 18 + \frac{2}{3} \times 9 = 6 + 9\sqrt{2} \text{ and } ABC_3(G(3,2)) = 18 \times 8 + 9 \times \frac{729}{64}.$$

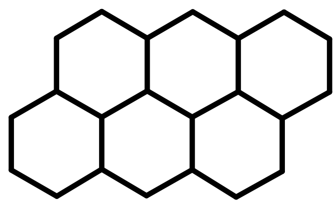

Figure 3. A 2 - Dimensional graph of $G(3, 2)$.

Example 3. Let $G(2, 3)$ be a graphene sheet depicted in Figure 4. By counting it's endpoint degrees, it is easy to check that

$$ABC(G(2,3)) = \frac{1}{\sqrt{2}} \times (8+9) + \frac{2}{3} \times 10 = \frac{17}{\sqrt{2}} + \frac{20}{3} \text{ and } ABC_3(G(3,2)) = 17 \times 8 + 10 \times \frac{729}{64}.$$

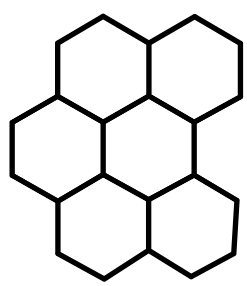

Figure 4. A 2 - Dimensional graph of $G(2, 3)$.

Example 4. Finally for graph $G(3, 3)$ depicted in Figure 5, it is easy to check that

$ABC(G(3,3)) = \frac{1}{\sqrt{2}} \times (12+9) + \frac{2}{3} \times 17 = \frac{21}{\sqrt{2}} + \frac{34}{3}$ and $ABC_3(G(3,2)) = 21 \times 8 + 17 \times \frac{729}{64}$.

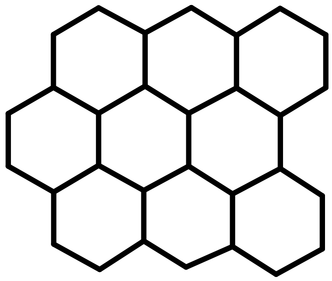

Figure 5. A 2 - Dimensional graph of $G(2, 3)$.

Consider now the graph G of a graphene sheet shown in Figure 1. One can partition the edge set $E(G)$ to three sets, $E(G) = A \cup B \cup C$ where

- $A = \{uv \in E(G),\ deg(u)=deg(v)=2\}$,
- $B = \{uv \in E(G),\ deg(u)=deg(v)=3\}$,
- $C = \{uv \in E(G),\ deg(u)=2, deg(v)=3\}$.

So $|A| + |B| + |C| = |E|$. It is easy to see that

$$|E(G)| = \begin{cases} \lceil n/2 \rceil (5m+1) + \lfloor n/2 \rfloor (m+3) & 2 \nmid n \\ \lceil n/2 \rceil (5m+1) + \lfloor n/2 \rfloor (m+3) + 2m - 1 & 2 \mid n \end{cases},$$

and $|A| = n+4, |C| = 4m+2n-4$. Hence, $|B| = |E| - |A| - |C|$. This implies

$$ABC(G) = \frac{1}{\sqrt{2}}(|A|+|B|) + \frac{2}{3}|B|.$$

Replacing $|A|$, $|B|$ and $|C|$ by their values we proved the following Theorem:

Theorem 5. Consider a graphene sheet $G(m,n)$ depicted in Figure 1. Then,

$$ABC(G) = \begin{cases} \frac{2}{3}\left(\lceil n/2 \rceil (5m+1) + \lfloor n/2 \rfloor (m+3) - 4m - 3n\right) + \frac{1}{\sqrt{2}}(4m+3n) & 2 \nmid n \\ \frac{2}{3}\left(\lceil n/2 \rceil (5m+1) + \lfloor n/2 \rfloor (m+3) - 2m - 3n - 1\right) + \frac{1}{\sqrt{2}}(4m+3n) & 2 \mid n \end{cases}.$$

Let $\alpha(G)$, $\chi(G)$ and $\omega(G)$ be independent set, chromatic number and clique number of *G*, respectively.

Theorem 6[9].

(a)
$$\frac{n}{\alpha(G)} \le \chi(G) \le n-\alpha(G)-1,$$

(b)
$$\chi(G) \le \left[\frac{n+\omega(G)}{2}\right].$$

If $G \cong K_2$ then $ABC(G) = 0$. Hence, suppose $G \ncong K_2$. Since for two distinct vertices *u*,*v*, $du, dv \le \Delta(G)$, then

$$d_G u d_G v \le \Delta^2(G) \Rightarrow \frac{1}{d_G u d_G v} \ge \frac{1}{\Delta(G)}.$$

On the other hand by using Vizing's theorem $\chi'(G) \ge \Delta(G)$ and so $\frac{1}{\chi'(G)} \le \frac{1}{\Delta(G)}$. Since $G \ncong K_2$ thus $d_G u + d_G v \ge 3$. It follows that

$$ABC(G) \ge \frac{\sum_{uv\in E(G)}\sqrt{du+dv-2}}{\Delta(G)} \ge \frac{\sum_{uv\in E(G)}\sqrt{du+dv-2}}{\chi'(G)} \ge \sum \frac{1}{\chi'(G)} = \frac{|E(G)|}{\chi'(G)}. \quad (1)$$

It is well-known that for a non empty graph *G*, $\chi'(G) = \chi(L(G))$ where $L(G)$ is dual of *G*. This implies that equation (1) can be simpli ied as

$$ABC(G) \ge \frac{m}{\chi(L(G))} = \frac{m}{\chi'(G)} \quad (2)$$

According to Theorem 6(*a*),

$$\frac{n}{\alpha(G)} \le \chi(G) \le n-\alpha(G)-1.$$

Hence

$$\frac{m}{\alpha(L(G))} \le \chi(L(G)) \le m - \alpha(L(G)) - 1.$$

It follows that

$$\frac{m}{m - \alpha(L(G)) - 1} \le \frac{m}{\chi(L(G))} \le \alpha(L(G)) = \mu(G)$$

and by using equation (2) we conclude that

$$ABC(G) \ge \frac{m}{\chi(L(G))} \ge \frac{m}{m - \alpha(L(G)) - 1}.$$

So, we proved the following theorem

Theorem 4. Let $\mu(G)$ be the matching number of G, then

$$\frac{m}{m - \mu(G) - 1} \le \mathrm{ABC}(G).$$

Further, if G has a perfect matching, then

$$ABC(G) \ge \frac{2m}{2m - n - 2}.$$

According to Theorem 6(*b*)

$$\chi(G) \le \left[\frac{n + \omega(G)}{2}\right]$$

and so

$$ABC(G) \ge \frac{m}{\chi(L(G))} \ge \left[\frac{2m}{m + \omega(L(G))}\right].$$

References

1. H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.*,**69** (1947), 17-20.
2. B. Zhou and Z. Du, Minimum Wiener indices of trees and unicyclic graphs of given matching number, *MATCH Commun. Math. Comput. Chem.,* **63(1)** (2010), 101 – 112.
3. M. Randić, On characterization of molecular branching, J. Am. Chem. Soc., 97 (1975), 6609-6615.
4. E. Estrada, L. Torres, L. Rodríguez and I. Gutman, An atom-bond connectivity index: modeling the enthalpy of formation of alkanes, Indian J. Chem., 37A (1998), 849-855.
5. E. Estrada, Atom-bond connectivity and the energetic of branched alkanes, Chem. Phys. Lett., 463 (2008), 422-425.
6. I. Gutman, and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17 (1972), 535-538.
7. K. Ch. Das, Atom-bond connectivity index of graphs, Disc. Appl. Math., 158 (2010), 1181-1188.
8. K. C. Das, I. Gutman and B. Furtula, On atom-bond connectivity index, Chem. Phys. Lett., 511 (2011), 452–454.
9. G. Chartrand and P. Zhang, Chromatic Graph Theory, Chapman and Hall/CRC, 2008.

Journal of Mathematical Nano Science