Scientific paper

Maximal Unicyclic Graphs With Respect to New Atom-bond Connectivity Index

Kinkar Ch. Das,[1] Kexiang Xu[2] and Ante Graovac[3]

[1] Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea.

[2] College of Science, Nanjing University of Aeronautics & Astronautics, Nanjing, Jiangsu, PR China

[3] Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia

* Corresponding author: E-mail: kinkardas2003@googlemail.com

Received: 23-04-2012

Abstract

The concept of atom-bond connectivity (ABC) index was introduced in the chemical graph theory in 1998. The atom-bond connectivity (ABC) index of a graph G defined as

$$ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}},$$

where E(G) is the edge set and d_i is the degree of vertex v_i of G. Very recently Graovac et al.[1] define a new version of the ABC index as

$$ABC_2(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{n_i + n_j - 2}{n_i n_j}},$$

where n_i denotes the number of vertices of G whose distances to vertex v_i are smaller than those to the other vertex v_j of the edge $e = v_iv_j$, and n_j is defined analogously. In this paper we determine the maximal unicyclic graphs with respect to new atom-bond connectivity index (ABC_2).

Keywords: Unicyclic graph, Atom-bond connectivity (ABC) index, New atom-bond connectivity (ABC_2) index, Upper bound

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry using mathematical methods to discuss and predict molecular properties without necessarily referring to quantum mechanics.[2–4] Chemical graph theory is a branch of mathematical chemistry which applies graph theory in mathematical modeling of chemical phenomena.[5] This theory has an important effect on the development of the chemical sciences.

Topological indices are numbers associated with chemical structures derived from their hydrogen-depleted graphs as a tool for compact and effective description of structural formulas which are used to study and predict the structure-property correlations of organic compounds. Molecular descriptors play significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place.[6] One of the best known and widely used is the connectivity index, χ, introduced in 1975 by Milan Randić.[7] Estrada et al. proposed a new index, known as the atom-bond connectivity index (ABC).[8] This index is defined as

$$ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}},$$

Where $E(G)$ is the edge set and d_i is the degree of vertex v_i of G. The ABC index has proven to be a valuable predictive index in the study of the heat of formation in alkanes.[8–9] The maithematical properties of this index was reported. [10–19]

Let $G = (V,E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. A vertex of a graph is said to be pendent if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendent if one of its vertices is a pendent vertex. We denote by C_n and P_n, the cycle and the path on n vertices, respectively, throughout this paper. For other undefined notations and terminology from graph theory, the readers are suggested to refer.[20]

Let G be a connected graph and $e = v_iv_j$ be an edge of G. The number of vertices of G whose distance to the vertex v_i is smaller than the distance to the vertex v_j is denoted by $n_i = n_i(e|G)$. Analogously, $n_j = n_j(e|G)$ is the number of vertices of G whose distance to the vertex v_j is smaller than to v_i. Graovac et al.[1] define a new version of the ABC index as

$$ABC_2(G) = \sum_{v_iv_j\epsilon E(G)} \sqrt{\frac{n_i + n_j - 2}{n_in_j}}.$$

Example 1.1. Dendrimers are nanostructures that can be precisely designed and manufactured for a wide variety of applications, such as drug delivery, gene delivery and diagnostics etc. Let $D[n]$ be a dendrimer where n is the step of growth in it.

Note that, in $D[n]$, there are $4(1 + 2 + \ldots + 2^{n-1}) + 1 = 4(2^n - 1) + 1$ vertices and $4(2^n - 1)$ edges. By the definition of (ABC_2)-index, we find that

$$\sqrt{\frac{1}{2^{n-i}-1} + \frac{1}{3(2^n-1)+1+2^{n-1}+\cdots+2^{n-i}} - \frac{1}{(2^{n-i}-1)[3(2^n-1)+1+2^{n-1}+\cdots+2^{n-i}]}}$$

$$= \sqrt{\frac{3(2^n-1)+2^n-2}{(2^{n-i}-1)[3(2^n-1)+1+2^{n-1}+\cdots+2^{n-i}]}}$$

$$= \sqrt{\frac{2^{n+2}-5}{(2^{n-i}-1)[3(2^n-1)+1+2^{n-1}+\cdots+2^{n-i}]}}.$$

For the edges linking the vertices on ith layer and the ones on $(i + 1)$ th layer each of which occurs 2^{i+2} times. When n = 1, $D[n]$ is just star S_5. So we have $ABC_2(D[1]) = ABC_2(S_5) = 2\sqrt{3}$. Set

$$\Delta_i = \sqrt{\frac{2^{n+2}-5}{(2^{n-i}-1)[3(2^n-1)+1+2^{n-1}+\cdots+2^{n-i}]}} \quad \text{for } i = 1, 2, \ldots, n-1.$$

Therefore, for $n \geq 2$, we have

$$ABC_2(D[n]) = 4\sqrt{\frac{1}{2^n-1} + \frac{1}{3(2^n-1)+1} - \frac{2}{(2^n-1)[3(2^n-1)+1]}} + \sum_{i=1}^{n-1} 2^{i+2}\Delta_i$$

$$= 4\sqrt{\frac{2^{n+2}-5}{(2^n-1)[3(2^n-1)+1]}} + \sum_{i=1}^{n-1} 2^i\Delta_i.$$

For example, we have

$$ABC_2(D[2]) = 4\sqrt{\frac{11}{30}} + 8\sqrt{\frac{11}{12}} = 4\left(\sqrt{\frac{11}{30}} + \sqrt{\frac{11}{3}}\right)$$

and

$$ABC_2(D[3]) = 4\sqrt{\frac{27}{154}} + 8\sqrt{\frac{27}{78}} + \sqrt{\frac{27}{28}}.$$

Example 1.2. Any connected graph with maximum degree not exceeding 4 is called molecular graph. Any (molecular) graph is called conjugated if it has a perfect matching. Conjugated unicyclic graphs have some important applications in chemistry, especially mathematical chemistry. Conjugated hydrocarbon molecules considered in the Hückel molecule orbital theory are usually represented by the carbon-atom skeleton graphs with perfect matching, of which all vertices have degrees not more than 4. For more details of chemical applications of conjugated molecular graphs, see [21, 22, 23]. Let $U(k)$ be the set of conjugated unicyclic graphs of order $2k$. Two conjugated unicyclic molecular graphs, denoted by $U_1(k)$ and $U_2(k)$, are shown in Fig. 1.

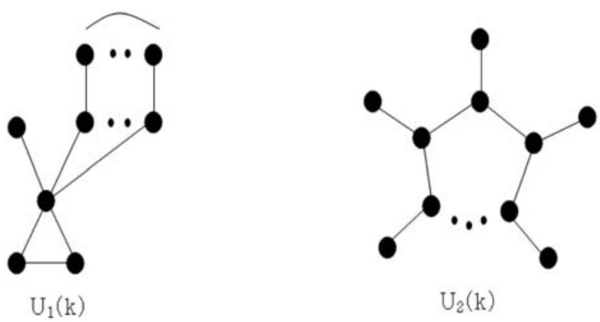

Figure 1. Two graphs $U_1(k)$ and $U_2(k)$.

Now we will calculate the ABC_2 index of $U_1(k)$ and $U_2(k)$ as follows:

$$ABC_2(U_1(k)) = (k-1)\sqrt{\frac{2k-2}{2k-1}} + (k-2)\sqrt{\frac{1}{2}} + 2\sqrt{\frac{2k-4}{2k-3}}.$$

$$ABC_2(U_2(k)) = k\sqrt{2k-2}\left(\frac{1}{\sqrt{2k-1}} + \frac{1}{k}\right)$$

when k is even and

$$ABC_2(U_2(k)) = k\left(\sqrt{\frac{2k-2}{2k-1}} + \sqrt{\frac{2k-4}{(k-1)^2}}\right)$$

when k is odd.

The goal of this paper is to determine the maximal unicyclic graphs with respect to new atom-bond connectivity index (ABC_2).

2. Some Lemmas

In this section, we shall list some results that will be needed in the next section.

Lemma 2.1. *Let* $n \geq 8$ *be a positive integer. Then*

$$\sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} > \sqrt{\frac{n-4}{n-3}} + \sqrt{2} \quad \text{for } 8 \leq n \leq 15$$

and

$$\sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} < \sqrt{\frac{n-4}{n-3}} + \sqrt{2} \quad \text{for } n \geq 16.$$

Proof: We have

$$\sqrt{\frac{n-3}{n-5}}=\sqrt{1+\frac{2}{n-5}}\le 1+\frac{1}{n-5}.$$

Using the above result, we get

$$\begin{aligned}(\sqrt{3}+1)n-4\sqrt{3}-3-\sqrt{3}(n-3)\sqrt{\frac{n-3}{n-5}} &\\ \ge(\sqrt{3}+1)n-4\sqrt{3}-3-\sqrt{3}(n-3)\left(1+\frac{1}{n-5}\right) &\\ =\frac{n^2-(8+2\sqrt{3})n+15+8\sqrt{3}}{n-5} & \qquad (1)\\ =\frac{(n-4-\sqrt{3})^2-4}{n-5}. &\end{aligned}$$

Let us consider a function

$$f(x)=\sqrt{\frac{x-4}{x-3}}+\sqrt{2}-\sqrt{\frac{2}{3}}-\sqrt{\frac{x-5}{x-4}}-\sqrt{\frac{x-3}{3(x-4)}},$$

$x\ge 8.$

Then

$$f'(x)=\frac{\left((\sqrt{3}+1)x-4\sqrt{3}-3\right)\sqrt{x-5}-\sqrt{3(x-3)^3}}{2\sqrt{3(x-5)(x-3)^3(x-4)^3}}$$

$$=\frac{\sqrt{x-5}\left((\sqrt{3}+1)x-4\sqrt{3}-3-\sqrt{3}(x-3)\sqrt{\frac{x-3}{x-5}}\right)}{2\sqrt{3(x-5)(x-3)^3(x-4)^3}}$$

$$\ge\frac{(x-4-\sqrt{3})^2-4}{2\sqrt{3(x-5)^2(x-3)^3(x-4)^3}}>0$$

as $x\ge 8$ and by (1).

Thus $f(x)$ is an increasing function for $x\ge 8$. Since $f(15)<0$ and $f(16)>0$,we get the required result.

Lemma 2.2. *Let $n\ge 7$ be a positive integer. Then*

$$\sqrt{\frac{3}{4}}+\sqrt{\frac{n-6}{n-5}}+\sqrt{\frac{n-3}{4(n-5)}}>\sqrt{\frac{2}{3}}+\sqrt{\frac{n-5}{n-4}}+\sqrt{\frac{n-3}{3(n-4)}}\ \text{ for } n=9 \qquad (2)$$

and

$$\sqrt{\frac{3}{4}}+\sqrt{\frac{n-6}{n-5}}+\sqrt{\frac{n-3}{4(n-5)}}\le\sqrt{\frac{2}{3}}+\sqrt{\frac{n-5}{n-4}}+\sqrt{\frac{n-3}{3(n-4)}}\ \text{ for } n\ne 9. \qquad (3)$$

Moreover, the equality holds in (3) if and only if $n=8$.

Proof: For $n=7$,

$$\sqrt{\frac{3}{4}}+\sqrt{2}\approx 2.28<2.3\approx 2\sqrt{\frac{2}{3}}+\frac{2}{3}$$

and (3) holds. For $n=8$ the equality holds in (3). For $n=9$,

$$2\sqrt{\frac{3}{4}}+\sqrt{\frac{3}{8}}\approx 2.344>2.343\approx\sqrt{\frac{2}{3}}+\sqrt{\frac{4}{5}}+\sqrt{\frac{2}{5}}$$

and (2) holds. We have

$$\sqrt{\frac{3}{4}}+\sqrt{\frac{4}{5}}+\sqrt{\frac{7}{20}}\approx 2.352<2.353\approx\sqrt{\frac{2}{3}}+\sqrt{\frac{5}{6}}+\sqrt{\frac{7}{18}}\ \text{ for } n=10,$$

$$\sqrt{\frac{3}{4}}+\sqrt{\frac{5}{6}}+\sqrt{\frac{1}{3}}\approx 2.356<2.359\approx\sqrt{\frac{2}{3}}+\sqrt{\frac{6}{7}}+\sqrt{\frac{8}{21}}\quad\text{ for } n=11,$$

$$\sqrt{\frac{3}{4}}+\sqrt{\frac{6}{7}}+\sqrt{\frac{9}{28}}\approx 2.359<2.364\approx\sqrt{\frac{2}{3}}+\sqrt{\frac{7}{8}}+\sqrt{\frac{3}{8}}\quad\text{ for } n=12$$

and

$$\sqrt{\frac{3}{4}}+\sqrt{\frac{7}{8}}+\sqrt{\frac{5}{16}}\approx 2.36<2.368\approx\sqrt{\frac{2}{3}}+\sqrt{\frac{8}{9}}+\sqrt{\frac{10}{27}}\ \text{ for } n=13.$$

Now it remains to prove this lemma for $n\ge 14$. For this, let us consider a function

$$f(x)=\frac{(x-8)\sqrt{x-3}}{(x-5)\sqrt{x-4}},\ x\ge 14.$$

Then

$$f'(x)=\frac{(x-8)\sqrt{x-3}}{(x-5)\sqrt{x-4}}\times\frac{(2x-4)(3x-13)-(x-4)(x-5)}{2(x-3)(x-4)(x-5)(x-8)}>0$$

as $x\ge 14$ and $(2x-4)(3x-13)>(x-4)(x-5)$.

Thus we have $f(x)$ is an increasing function for $x\ge 14$ and hence $f(x)\ge 0.699$ for $x\ge 14$.

Now,

$$\sqrt{\frac{n-3}{3(n-4)}}-\sqrt{\frac{n-3}{4(n-5)}}=$$

$$\sqrt{n-3}\left[\frac{1}{\sqrt{3(n-4)}}-\frac{1}{\sqrt{4(n-5)}}\right]$$

$$=\sqrt{n-3}\left[\frac{\sqrt{4(n-5)}-\sqrt{3(n-4)}}{\sqrt{12(n-4)(n-5)}}\right]$$

$$=\frac{(n-8)\sqrt{n-3}}{\sqrt{12(n-4)(n-5)}\left(\sqrt{4(n-5)}+\sqrt{3(n-4)}\right)}$$

$$\ge\frac{(n-8)\sqrt{n-3}}{8\sqrt{3}(n-5)\sqrt{n-4}}$$

as $4(n-5)>3(n-4)$

$$\ge 0.0504>\sqrt{\frac{3}{4}}-\sqrt{\frac{2}{3}}\ \text{ as } n\ge 14 \text{ and } f(x)\ge 0.699.$$

Using the above result

$$\sqrt{\frac{n-6}{n-5}}<\sqrt{\frac{n-5}{n-4}}\quad\text{for } n\ge 6,$$

we get the required result (3) for $n\ge 14$

Lemma 2.3. Let x, n be positive integers with $(n-3)/2\le x\le n-6$. Then

$$\sqrt{\frac{x}{x+1}}+\sqrt{\frac{n-3-x}{n-2-x}}+\sqrt{\frac{n-3}{(x+1)(n-2-x)}}\le$$

$$\sqrt{\frac{3}{4}}+\sqrt{\frac{n-6}{n-5}}+\sqrt{\frac{n-3}{4(n-5)}}$$

with equality holding if and only if x = n–6.

Proof: First we assume that $n \geq 12$. Now we have to prove the following two claims.

Claim 1. Let x,n be positive integer numbers with $(n–3)/2 \leq x \leq n – 6$, $n \geq 12$. Also let r be a positive integer number such that $x + r = n – 3$. Then

(i) $\sqrt{(x+r)xr} > n$

and

(ii) $(x+r)\sqrt{(x+r)xr} > 3(xr+x+r)+1$.

Proof of Claim 1 (i). Since $(n–3)/2 \leq x \leq n – 6$ and $x + r = n – 3$, we have $x \geq r \geq 3$. Again since both x and r are integers with $x + r = n – 3$, then the minimum value of xr is $3(n – 6)$. Now we have to show that

$$\sqrt{3(n-3)(n-6)} > n,$$

that is, $2n^2 – 27n + 54 > 0$, that is, $n \geq 12$, which, evidently, is always obeyed.

Proof of Claim 1 (ii). Now,

$$3(\mathrm{xr}+\mathrm{x}+\mathrm{r})+1 \leq 3(\mathrm{x}+\mathrm{r})+3\sqrt{\mathrm{xr}}\,\frac{\mathrm{x}+\mathrm{r}}{2}+1$$

by Arithmetic-Geometric Mean Inequality

$$< 3(x+r)\left(2+\frac{\sqrt{xr}}{2}\right)$$

$$= 3(x+r)\sqrt{4+2\sqrt{xr}+\frac{xr}{4}} \tag{5}$$

$$\leq 3(x+r)\sqrt{\frac{xr}{4}+n+1} \quad \text{as } 2\sqrt{xr} \leq x+r = n-3.$$

Now we have to show that

$$\frac{n-3}{9}xr \geq \frac{xr}{4}+n+1 \quad \text{as } x+r=n-3,$$

that is,

$$\left(\frac{n-3}{9}-\frac{1}{4}\right)xr \geq n+1,$$

that is, $\geq n + 1$

$$\left(\frac{n-3}{9}-\frac{1}{4}\right)xr \geq \left(\frac{n-3}{9}-\frac{1}{4}\right)3(n-6)$$

as $xr \geq 3(n – 6)$, that is, $4n^2 – 57n + 114 \geq 0$, that is, $n \geq 12$, which, evidently, is always obeyed.

Claim 2. Let x, n be positive integer numbers with $(n–3)/2 \leq x \leq n – 6$, $n \geq 12$. Then

$$\frac{1}{\sqrt{x(x+1)^3}}-\frac{1}{\sqrt{(n-3-x)(n-2-x)^3}}+\frac{\sqrt{n-3}(2x-n+3)}{\sqrt{(x+1)^3(n-2-x)^3}} > 0. \tag{6}$$

Proof of Claim 2. Let r be a positive integer number such that $x + r = n – 3$. Since $(n–3)/2 \leq x \leq n – 6$ and $x + r = n – 3$, we have $x \geq r \geq 3$. Now,

$$\left(\sqrt{x(x+1)^3}+\sqrt{r(r+1)^3}\right)(x-r)\sqrt{(n-3)xr}$$
$$\geq (x(x+1)+r(r+1))(x-r)\sqrt{(x+r)xr}$$
$$> (x-r)(n(x^2+r^2)+3(xr+x+r)+1)$$

by **Claim 1** (i) and (ii)

$$= (x-r)\big((n-3)(x^2+r^2)+3(x^2+xr+r^2)+3(x+r)+1\big)$$

$$= (x^4-r^4)+3(x^3-r^3)+3(x^2-r^2)+(x-r)$$

as $x + r = n – 3$

$$= x(x+1)^3 - r(r+1)^3.$$

From the above inequality, we can easily get

$$\sqrt{x(x+1)^3}-\sqrt{r(r+1)^3} < (x-r)\sqrt{(n-3)xr},$$

that is,

$$\sqrt{(n-3-x)(n-2-x)^3}-\sqrt{x(x+1)^3}+(2x-n+3)\sqrt{(n-3)x(n-3-x)} > 0.$$

From the above, we get the required result (6).

Let us consider a function

$$\mathrm{f}(\mathrm{x}) = \sqrt{\frac{\mathrm{x}}{\mathrm{x}+1}}+\sqrt{\frac{\mathrm{n}-3-\mathrm{x}}{\mathrm{n}-2-\mathrm{x}}}+\sqrt{\frac{\mathrm{n}-3}{(\mathrm{x}+1)(\mathrm{n}-2-\mathrm{x})}},$$
$$\frac{n-3}{2} \leq x \leq n-6,\ n \geq 12.$$

Then we have

$$f'(x) = \frac{1}{2\sqrt{x(x+1)^3}}-\frac{1}{2\sqrt{(n-3-x)(n-2-x)^3}}+\frac{(2x-n+3)\sqrt{n-3}}{2\sqrt{(x+1)^3(n-2-x)^3}} > 0 \text{ as } \frac{n-3}{2} \leq x \leq n-6,$$

and by **Claim 2**.

Thus $f(x)$ is strictly increasing function for $(n–3)/2 \leq x \leq n – 6$, $n \geq 12$. Hence we get the required result (4) for $n \geq 12$. Moreover, the equality holds in (4) if and only if $x = n – 6$.

Next we assume that $n \leq 11$. Since $(n–3)/2 \leq x \leq n – 6$, we have $n \geq 9$. Thus $(n,x) = (9,3)$ or $(10, 4)$ or $(11, 5)$. For $(n,x) = (9,3)$, the equality holds in (4). For $(n,x) = (10,4)$, the equality holds in (4). For $(n,x) = (11,4)$,

$$\sqrt{\frac{4}{5}}+\sqrt{\frac{4}{5}}+\sqrt{\frac{8}{25}} \approx 2.354 < 2.356 \approx \sqrt{\frac{3}{4}}+\sqrt{\frac{5}{6}}+\sqrt{\frac{1}{3}}$$

and (4) holds. Moreover, for $(n,x) = (11, 5)$, the equality holds in (4). This completes the proof.

Theorem 2.4. Let x, n be positive integer numbers with $(n–3)/2 \leq x \leq n – 4$.

(i) If $n = 7$, then

$$\sqrt{\frac{\mathrm{x}}{\mathrm{x}+1}}+\sqrt{\frac{\mathrm{n}-3-\mathrm{x}}{\mathrm{n}-2-\mathrm{x}}}+\sqrt{\frac{\mathrm{n}-3}{(\mathrm{x}+1)(\mathrm{n}-2-\mathrm{x})}} \leq 2\sqrt{\frac{2}{3}}+\frac{2}{3} \tag{7}$$

with equality holding in (7) if and only if $x = 2$.

(ii) If $n = 8$, then

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \le \sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{5}{12}} \quad (8)$$

with equality holding in (8) if and only if $x = 3$.

(iii) If $n = 9$, then

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \le \sqrt{3} + \sqrt{\frac{3}{8}} \quad (9)$$

with equality holding in (9) if and only if $x = 3$.

(iv) If $10 \le n \le 15$, then

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \le \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} \quad (10)$$

with equality holding in (10) if and only if $x = n - 5$.

(v) If $n \ge 16$, then

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \le \sqrt{2} + \sqrt{\frac{n-4}{n-3}} \quad (11)$$

with equality holding in (11) if and only if $x = n - 4$.

Proof: (i) Since n = 7, we have either $x = 2$ or $x = 3$. We have

$$\sqrt{\frac{3}{4}} + \sqrt{2} \approx 2.28 < 2.3 \approx 2\sqrt{\frac{2}{3}} + \frac{2}{3}.$$

Using the above result, we get the required result (7). Moreover, the equality holds in (7) if and only if $x = 2$.

(ii) Since $n = 8$, we have either $x = 3$ or $x = 4$. We have

$$\sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{5}{12}} \approx 2.328 < 2.309 \approx \sqrt{\frac{4}{5}} + \sqrt{2}.$$

Using the above result, we get the required result (8). Moreover, the equality holds in (8) if and only if $x = 3$.

(iii) Since $n = 9$, we have either $x = 3$ or $x = 4$ or $x = 5$. We have

$$\sqrt{\frac{5}{6}} + \sqrt{2} \approx 2.327 < 2.343 \approx \sqrt{\frac{2}{3}} + \sqrt{\frac{4}{5}} + \sqrt{\frac{2}{5}} < 2.344 \approx \sqrt{3} + \sqrt{\frac{3}{8}}.$$

Using the above result, we get the required result (9). Moreover, the equality holds in (9) if and only if $x = 3$.

(iv) If $x = n - 5$, then the equality holds in (10).

Otherwise, $x \ne n - 5$. Since $10 \le n \le 15$, by **Lemmas** 2.1, 2.2 and 2.3, we get

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \le \sqrt{\frac{3}{4}} + \sqrt{\frac{n-6}{n-5}} + \sqrt{\frac{n-3}{4(n-5)}}$$

$$< \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} > \sqrt{2} + \sqrt{\frac{n-4}{n-3}}.$$

(v) If $x = n - 4$, then the equality holds in (11). Otherwise, $x \ne n - 4$. Since $n \ge 16$, by **Lemmas** 2.1, 2.2 and 2.3, we get

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \le \sqrt{\frac{3}{4}} + \sqrt{\frac{n-6}{n-5}} + \sqrt{\frac{n-3}{4(n-5)}}$$

$$< \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} < \sqrt{2} + \sqrt{\frac{n-4}{n-3}}.$$

This completes the proof.

3. Upper Bound on the ABC_2 Index of Unicyclic Graphs

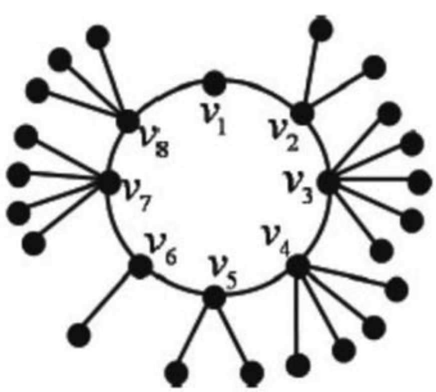

Figure 2. S(0, 2, 5, 4, 2, 1, 4, 3).

Now we turn to determine the maximal new atom-bond connectivity index (ABC_2) among all connected unicyclic graphs of order n. Let $S(m_1, m_2, \ldots, m_k)$ be a unicyclic graph of order n with girth k and $n - k$ pendent vertices, where m_i is the number of pendent vertices adjacent to i-th vertex of the cycle. We consider that the vertices in the cycle are numbered clockwise (see Fig. 2). Clearly, $\sum_{i=1}^{k} m_i = n - k$ and $S(0, 0, \ldots, 0) = C_n$. The cycle of a unicyclic graph G is denoted by $C(G)$. Denote by C'_4 is a unicyclic graph of order 5 obtained from cycle C_4 with one pendent edge attached to any one vertex of cycle C_4. Denote by C'_3, is a unicyclic graph of order 5 obtained from cycle C_3 with one end of path P_3 attached to any one vertex of cycle C_3.

Let G be a connected graph of order n. For $2 \le l \le n_j \le n_i$, $v_i v_j \in E(G)$,

$$\frac{1}{n_i}+\frac{1}{n_j}-\frac{2}{n_in_j}=\frac{1}{n_i}+\frac{1}{n_j}\left(1-\frac{2}{n_i}\right)\le\frac{1}{n_i}+\frac{1}{l}\left(1-\frac{2}{n_i}\right)\ \text{as}\ n_j\ge l$$
$$=\frac{1}{l}+\frac{1}{n_i}\left(1-\frac{2}{l}\right)$$
$$\le\frac{2}{l^2}(l-1)\quad\text{as}\quad n_i\ge l.$$

Thus we have

$$\sqrt{\frac{1}{n_i}+\frac{1}{n_j}-\frac{2}{n_in_j}}\le\frac{1}{l}\sqrt{2(l-1)}\tag{12}$$

with equality holding if and only if $n_i = n_j = l$.

Moreover, for pendent edge $v_iv_j \in E(G)$,

$$\sqrt{\frac{1}{n_i}+\frac{1}{n_j}-\frac{2}{n_in_j}}=\sqrt{\frac{n-2}{n-1}}.\tag{13}$$

Lemma 3.1. Suppose that v_iv_j is a cut-edge of connected unicyclic graph G of order n (>3), but v_iv_j is not a pendent edge. Let v_i denote the vertex obtained from identifying v_i and v_j in G_{vivj}, and $G^1 = G_{vivj} + v_iv_j$ (See, Fig. 3). Then $ABC_2(G) < ABC_2(G^1)$.

Proof: Denote by

$$ABC_2(G,v_rv_s)=\sqrt{\frac{1}{n_r}+\frac{1}{n_s}-\frac{2}{n_rn_s}}\ .$$

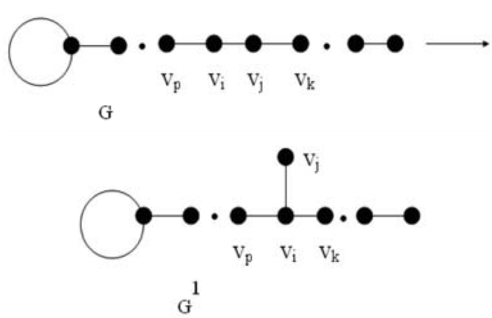

Figure 3. Two graphs G and G^1.

Then we have

$$ABC_2(G)=\sum_{v_rv_s\in E(G)}ABC_2\left(G,v_rv_s\right).$$

From given condition we get $ABC_2(G, v_rv_s) = ABC_2(G^1, v_rv_s)$, $v_rv_s \neq v_iv_j$.

Moreover, for $v_iv_j \in E(G)$, $n_i \ge 2$ and $n_j \ge 2$ as v_iv_j is not a pendent edge in G. Thus we have

$$ABC_2(G,v_iv_j)=\sqrt{\frac{1}{n_i}+\frac{1}{n_j}-\frac{2}{n_in_j}}\le\sqrt{\frac{1}{2}}.$$

Moreover, v_iv_j is a pendent edge in G^1 and hence

$$ABC_2(G^1,v_iv_j)=\sqrt{\frac{1}{n_i}+\frac{1}{n_j}-\frac{2}{n_in_j}}=\sqrt{\frac{n-2}{n-1}}.$$

Now we have

$$ABC_2(G^1)-ABC_2(G)=\sum_{v_rv_s\in E(G^1)}ABC_2\left(G^1,v_rv_s\right)-\sum_{v_rv_s\in E(G)}ABC_2\left(G,v_rv_s\right)$$
$$=ABC_2(G^1,v_iv_j)-ABC_2(G,v_iv_j)$$
as $ABC_2(G^1,v_rv_s)=ABC_2(G,v_rv_s),\ v_rv_s\neq v_iv_j$
$$\ge\sqrt{\frac{n-2}{n-1}}-\sqrt{\frac{1}{2}}>0\quad\text{as}\quad n>3.$$

Theorem 3.2. Let G be a connected unicyclic graph of order n (>3) with girth k. Then

$$ABC_2(G)\le ABC_2\left(S(m_1,\ m_2,\dots,\ m_k)\right)\tag{14}$$

with equality holding if and only if $G \cong S(m_1, m_2, ..., m_k)$.

Proof: If G is isomorphic to $S(m_1, m_2, ..., m_k)$, then the equality holds in (14). Otherwise, $G \not\cong S(m_1, m_2, ..., m_k)$. Then there exists a non-pendent edge v_iv_j in G such that $v_iv_j \notin E(C(G))$. We consider the transformation defined in **Lemma** 3.1. Then by **Lemma** 3.1, we have $ABC_2(G) < ABC_2(G^1)$, that is, we have increased the value of (ABC_2)-index. If G^1 is $S(m_1, m_2, \dots, m_k)$, then we are done. Otherwise, we continue the same transformation for sufficient number of times, we arrive at $S(m_1, m_2, \dots, m_k)$. This completes the proof.

Now we give an upper bound on the ABC_2 – index of unicyclic graph G in terms of order n.

Theorem 3.3. Let G be a connected unicyclic graph of order n (> 3).

(i) If $n = 4$, then

$$ABC_2(G)\le 2\sqrt{2}\tag{15}$$

with equality holding in (15) if and only if $G \cong C_4$.

(ii) If $n = 5$, then

$$ABC_2(G)\le\sqrt{3}+\frac{3}{\sqrt{2}}\tag{16}$$

with equality holding in (16) if and only if $G \cong S(1, 1, 0)$.

(iii) If $n = 6$, then

$$ABC_2(G)\le 3\sqrt{\frac{4}{5}}+\sqrt{2}+\sqrt{\frac{2}{3}}\tag{17}$$

with equality holding in (17) if and only if $G \cong S(2, 1, 0)$.

(iv) If $n = 7$, then

$$ABC_2(G)\le(n-3)\sqrt{\frac{n-2}{n-1}}+2\sqrt{\frac{2}{3}}+\frac{2}{3}\tag{18}$$

with equality holding in (18) if and only if $G \cong S(2, 2, 0)$.

(v) If $n = 8$, then

$$ABC_2(G)\le(n-3)\sqrt{\frac{n-2}{n-1}}+\sqrt{\frac{2}{3}}+\sqrt{\frac{3}{4}}+\sqrt{\frac{5}{12}}\tag{19}$$

with equality holding in (19) if and only if $G \cong S(3, 2, 0)$.

(vi) If $n = 9$, then

$$ABC_2(G) \le (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{3} + \sqrt{\frac{3}{8}} \tag{20}$$

with equality holding in (20) if and only if $G \cong S(3, 3, 0)$.

(vii) If $10 \le n \le 15$, then

$$ABC_2(G) \le (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} \tag{21}$$

with equality holding in (21) if and only if $G \cong S(n-5, 2, 0)$.

(viii) If $n \ge 16$, then

$$ABC_2(G) \le (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{2} + \sqrt{\frac{n-4}{n-3}} \tag{22}$$

with equality holding in (22) if and only if $G \cong S(n-4, 1, 0)$.

Proof: If $n = 4$, then $G \cong C_4$ or $G \cong S(1, 0, 0)$. We have

$$ABC_2(S(1,0,0)) = \sqrt{2} + \sqrt{\frac{2}{3}} < 2\sqrt{2} = ABC_2(C_4).$$

From the above, we get the required result (15). Moreover, the equality holds in (15) if and only if $G \cong C_4$. If $n = 5$, then $G \cong C_5$ or $G \cong C_4'$ or $G \cong S(1, 1, 0)$, or $G \cong S(2, 0, 0)$, or $G \cong C_3'$. Now we have

$$ABC_2(C_3') = \sqrt{\frac{3}{4} + \frac{1}{\sqrt{2}}} + 2\sqrt{\frac{2}{3}} \approx 3.206 < 3.365 \approx \sqrt{3} + 2\sqrt{\frac{2}{3}} = ABC_2(S(2,0,0)) < ABC_2(C_5) = \frac{5}{\sqrt{2}} \approx 3.535 < 3.694 \approx \sqrt{\frac{3}{4}} + 2\sqrt{2} = ABC_2(C_4') < 3.853 \approx \sqrt{3} + \frac{3}{\sqrt{2}} = ABC_2(S(1,1,0)).$$

From the above, we get the required result (16). Moreover, the equality holds in (16) if and only if $G \cong S(1, 1, 0)$. Otherwise, $n \ge 6$. Let G be a connected unicyclic graph of order n with girth k. Then $k \ge 3$. We consider two cases (a) $k \ge 4$, (b) $k = 3$.

Case (a): $k \ge 4$. In this case there are at most $n - 4$ pendent edges and at least 4 non-pendent edges in unicyclic graph G. Since $k \ge 4$, for each non-pendent edge $v_iv_j \in E(G)$, $n_i \ge 2$ and $n_j \ge 2$ as G is unicyclic graph. For each non-pendent edge $v_iv_j \in E(G)$, by (12),

$$\sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} \le \sqrt{\frac{1}{2}} < \sqrt{\frac{n-2}{n-1}} \quad \text{as } n > 3. \tag{23}$$

Using the above result and by (13), we get

$$\begin{aligned} ABC_2(G) &= \sum_{v_iv_j \in E(G), d_i=1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} + \sum_{v_iv_j \in E(G), d_id_j \ne 1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} \\ &\le (n-4)\sqrt{\frac{n-2}{n-1}} + \frac{4}{\sqrt{2}} \\ &< (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3}{\sqrt{2}}. \end{aligned} \tag{24}$$

Case (b): $k = 3$. By **Theorem** 3.2, we get $ABC_2(G) \le ABC_2(S(m_1, m_2, m_3))$. Moreover, the equality holds if and only if $G \cong S(m_1, m_2, m_3)$. Without loss of generality, we can assume that $m_1 \ge m_2 \ge m_3 \ge 0$, $m_1 + m_2 + m_3 = n - 3$. Now we consider the following three subcases:

Subcase (i): $m_1 \ge m_2 \ge m_3 \ge 1$. For each non-pendent edge $v_iv_j \in E(S(m_1, m_2, m_3))$, $n_i \ge 2$ and $n_j \ge 2$. By (12), we get

$$\sqrt{\frac{1}{p+1} + \frac{1}{q+1} - \frac{2}{(p+1)(q+1)}} + \sqrt{\frac{1}{q+1} + \frac{1}{r+1} - \frac{2}{(q+1)(r+1)}} + \sqrt{\frac{1}{r+1} + \frac{1}{p+1} - \frac{2}{(r+1)(p+1)}} \le \frac{3}{\sqrt{2}}.$$

Using the above result, we get
$ABC_2(G) \le ABC_2(S(m_1, m_2, m_3))$

$$\begin{aligned} &= \sum_{v_iv_j \in E(S(m_1,m_2,m_3)), d_i=1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} + \sum_{v_iv_j \in E(S(m_1,m_2,m_3)), d_id_j \ne 1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} \\ &\le (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3}{\sqrt{2}}. \end{aligned} \tag{25}$$

Subcase (ii): $m_2 = m_3 = 0$. There are exactly one non-pendent edge $v_iv_j \in E(S(n-3, 0, 0))$ such that $n_i = 1$ and $n_j = 1$ and hence

$$\sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} = 0.$$

Also there are exactly two non-pendent edges $v_iv_j \in E(S(n-3, 0, 0))$ such that $n_i = 1$ and $n_j = n - 2$ and hence

$$\sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} = \sqrt{\frac{n-3}{n-2}}.$$

Thus we have $ABC_2(G) \le ABC_2(S(n-3, 0, 0))$

$$= \sum_{v_iv_j \in E(S(n-3,0,0)), d_i=1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} + \sum_{v_iv_j \in E(S(n-3,0,0)), d_id_j \ne 1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}}$$

$$= (n-3)\sqrt{\frac{n-2}{n-1}} + 2\sqrt{\frac{n-3}{n-2}} < (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3}{\sqrt{2}}. \qquad (26)$$

Subcase (iii): $m_3 = 0$. In this subcase $m_1 + m_2 = n - 3$, $m_1 \ge m_2 \ge 1$, that is, $(n-3)/2 \le m_1 \le n-4$. Now, $ABC_2(G) \le ABC_2(S(m_1, m_2, 0))$

$$= \sum_{v_iv_j \in E(S(m_1,m_2,0)), d_i=1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}} + \sum_{v_iv_j \in E(S(m_1,m_2,0)), d_id_j \ne 1} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}}$$

$$= (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{m_1}{m_1+1}} + \sqrt{\frac{m_2}{m_2+1}} + \sqrt{\frac{1}{m_1+1} + \frac{1}{m_2+1} - \frac{2}{(m_1+1)(m_2+1)}}$$

$$= (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{m_1}{m_1+1}} + \sqrt{\frac{n-3-m_1}{n-2-m_1}} + \sqrt{\frac{n-3}{(m_1+1)(n-2-m_1)}}.$$

From the above result and by **Theorem** 2.4, we get the following:

If $n = 6$, then

$$ABC_2(G) \le ABC_2(S(m_1, m_2, 0)) = ABC_2(S(2,1,0)) = 3\sqrt{\frac{4}{5}} + \sqrt{2} + \sqrt{\frac{2}{3}}$$

with equality holding if and only if $G \cong S(2, 1, 0)$.

If $n = 7$, then

$$ABC_2(G) \le ABC_2(S(m_1, m_2, 0)) \le 4\sqrt{\frac{5}{6}} + 2\sqrt{\frac{2}{3}} + \frac{2}{3}$$

with equality holding if and only if $G \cong S(2, 2, 0)$.

If $n = 8$, then

$$ABC_2(G) \le ABC_2(S(m_1, m_2, 0)) \le 5\sqrt{\frac{6}{7}} + \sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{5}{12}}$$

with equality holding if and only if $G \cong S(3, 2, 0)$.

If $n = 9$, then

$$ABC_2(G) \le ABC_2(S(m_1, m_2, 0)) \le 6\sqrt{\frac{7}{8}} + \sqrt{3} + \sqrt{\frac{3}{8}}$$

with equality holding if and only if $G \cong S(3, 3, 0)$.

If $10 \le n \le 15$, then

$$ABC_2(G) \le ABC_2(S(m_1, m_2, 0)) \le (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}}$$

with equality holding if and only if $G \cong S(n-5, 2, 0)$.

If $n \ge 16$, then

$$ABC_2(G) \le ABC_2(S(m_1, m_2, 0)) \le (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{2} + \sqrt{\frac{n-4}{n-3}}$$

with equality holding if and only if $G \cong S(n-4, 1, 0)$.

Now we have

$$\frac{3}{\sqrt{2}} \approx 2.121 < 2.23 \approx \sqrt{2} + \sqrt{\frac{2}{3}} < 2.3 \approx 2\sqrt{\frac{2}{3}} + \frac{2}{3} < 2.328 \approx \sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{5}{12}},$$

$$\frac{3}{\sqrt{2}} \approx 2.121 < 2.344 \approx \sqrt{3} + \sqrt{\frac{3}{8}} < 2.353 \approx \sqrt{\frac{2}{3}} + \sqrt{\frac{5}{6}} + \sqrt{\frac{7}{18}} \le \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}}$$

by **Theorem** 2.4 and $n \ge 10$

and

$$\frac{3}{\sqrt{2}} < \sqrt{2} + \sqrt{\frac{n-4}{n-3}}$$

for $n \ge 6$. Using the above results, we get

$$ABC_2(G) \le ABC_2(S(2,1,0)) = 3\sqrt{\frac{4}{5}} + \sqrt{2} + \sqrt{\frac{2}{3}} > 3\sqrt{\frac{4}{5}} + \frac{3}{\sqrt{2}} \quad \text{for} \quad n = 6,$$

$$ABC_2(G) \le ABC_2(S(2,2,0)) = 4\sqrt{\frac{5}{6}} + 2\sqrt{\frac{2}{3}} + \frac{2}{3} > 4\sqrt{\frac{5}{6}} + \frac{3}{\sqrt{2}} \quad \text{for} \quad n = 7,$$

$$ABC_2(G) \le ABC_2(S(3,2,0)) = 5\sqrt{\frac{6}{7}} + \sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{5}{12}} > 5\sqrt{\frac{6}{7}} + \frac{3}{\sqrt{2}} \quad \text{for} \quad n = 8,$$

$$ABC_2(G) \le ABC_2(S(3,3,0)) = 6\sqrt{\frac{7}{8}} + \sqrt{3} + \sqrt{\frac{3}{8}} > 6\sqrt{\frac{7}{8}} + \frac{3}{\sqrt{2}} \quad \text{for} \quad n = 9,$$

$$ABC_2(G) \le ABC_2(S(n-5, 2, 0)) = (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} > (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3}{\sqrt{2}} \quad \text{for} \quad 10 \le n \le 15,$$

$$ABC_2(G) \le ABC_2(S(n-4, 1, 0)) = (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{2} + \sqrt{\frac{n-4}{n-3}} > (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3}{\sqrt{2}} \quad \text{for} \quad n \ge 16.$$

Using the above results with (24), (25) and (26), we get the required result. This completes the proof.

4. Conclusion

Graovac et al.[1] define the ABC_2 index as a new version of the ABC index. In this paper we obtain the maximal unicyclic graphs with respect to new atom-bond connectivity index (ABC_2). Maximal new atom-bond connectivity index in the case of bicyclic graphs and minimal atom-bond connectivity index in the case of trees, unicyclic graphs and bicyclic graphs, remains an open problem. Moreover, some extremal graphs with respect to new ABC index are still unknown which include certain chemical structure such as fullerene, benzenoid hydrocarbons, etc. And finding the chemical application of this new ABC index is more attractive in the near future.

5. Acknowledgement

The authors would like to thank two anonymous referees for valuable comments and useful suggestions, which improved this work very much. K. Ch. D. thanks for support by the Faculty research Fund, Sungkyunkwan University, 2012 and Sungkyunkwan University BK21 Project, BK21 Math Modeling HRD Div. Sungkyunkwan University, Suwon, Republic of Korea. K. X. thanks for support of NNSF of China (No. 11201227).

6. References

1. A. Graovac, M. Ghorbani, *Acta Chim. Slov.* **2010**, *57*, 609–612.
2. S. J. Cyvin, I. Gutman, Kekulé Structures in Benzenoid Hydrocarbons, Lecture Notes in Chemistry, Vol. 46, Springer Verlag, Berlin, **1988**.
3. I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer Verlag, Berlin, **1986**.
4. N. Trinajstić, I. Gutman, *Croat. Chem. Acta,* **2002**, *75*, 329–356.
5. A. Graovac, I. Gutman, N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules, Springer Verlag, Berlin, **1977**.
6. R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley–VCH, Weinheim, **2000**.
7. M. Randić, *J. Am. Chem. Soc.* **1975**, *97*, 6609–6615.
8. E. Estrada, L. Torres, L. Rodríguez, I. Gutman, *Indian J. Chem.* **1998**, *37 A,* 849–855.
9. E. Estrada, *Chem. Phys. Lett.* **2008**, *463*, 422–425.
10. K. C. Das, *Discrete Appl. Math.* **2010**, *158*, 1181–1188.
11. K. C. Das, N. Trinajstić, *Chem. Phys. Lett.* **2010**, *497*, 149–151.
12. K. C. Das, I. Gutman, B. Furtula, *Chem. Phys. Lett.* **2011**, *511*, 452–454.
13. K. C. Das, I. Gutman, B. Furtula, *Filomat*, **2012,** *26*(4) 733–738.
14. G. H. Fath-Tabar, B. Vaez-Zadeh, A. R. Ashrafi, A. Graovac, *Discrete Applied Math.* **2011**, *159*, 1323–1330.
15. B. Furtula, A. Graovac, D. Vukičević, *Discrete Applied Math.* **2009**, *157*, 2828–2835.
16. I. Gutman, B. Furtula, M. Ivanović, *MATCH Commun. Math. Comput. Chem.* **2012**, *67*(2), 467–482.
17. R. Xing, B. Zhou, Z. Du, *Discrete Appl. Math.* **2010**, *157*, 1536–1545.
18. R. Xing, B. Zhou, F. Dong, *Discrete Applied Math.* **2011**, *159*, 1617–1630.
19. B. Zhou, R. Xing, *Z. Naturforsch.* **2011**, *66* (a), 61–66.
20. J. A. Bondy, U. S. R. Murty, Graph Theory with Applications, Macmillan Press, New York, **1976**.
21. T. Živković, N. Trinajstić, R. Randić, Molecular Physics **1975**, *30,* 517–532.
22. W. Liu, Scientia Sinica **1979**, *5,* 539–554.
23. I. Gutman, J. Serb. Chem. Soc. **2005**, *70,* 441–456.

Povzetek

Koncept »atom-vez« indeksa povezanosti (ABC) je bil pred kratkim vpeljan v kemijsko teorijo grafov. »Atom-vez« indeks povezanosti (ABC) grafa G je definiran kot

$$ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}},$$

kjer je $E(G)$ niz povezav in d_i stopnja vozlišča (točke) v_i od G. Graovac in soavtorji je definiral novo verzijo ABC indeksa kot

$$ABC_2(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{n_i + n_j - 2}{n_i n_j}},$$

kjer n_i predstavlja število vozlišč v G katerega razdalje do vozlišča v_i so manjše od tistih do drugega vozlišča v_j povezave $e = v_i\, v_j$, n_i pa je definiran analogno. V tem članku determiniramo maksimalne enociklične grafe glede na novi »atom-vez« indeks povezanosti (ABC_2).