Short communication

A New Version of Atom-Bond Connectivity Index

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This paper is dedicated to Professor Milan Randić on the occasion of his 80th birthday

Abstract

The atom-bond connectivity index is a recently introduced topological index defined as $ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$, where d_u denotes degree of vertex u. Here we define a new version of the *ABC* index as $ABC_2(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$, where n_u denotes the number of vertices of G whose distances to vertex u are smaller than those to other vertex v of the edge $e = uv$, and n_v is defined analogously. The goal of this paper is to study the ABC_2 index.

Keywords: Topological indices, *ABC* Index, ABC_2 Index.

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.[1–3] Chemical graph theory is a branch of mathematical chemistry which applies graph theory in mathematical modeling of chemical phenomena.[4] This theory has an important effect on the development of the chemical sciences.

A graph is a collection of points and lines connecting them. The points and lines of a graph are also called vertices and edges respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say »u and v are adjacent«. A connected graph is a graph such that there exists a path between all pairs of vertices. The distance $d(u,v) = d_G(u,v)$ between two vertices u and v is the length of the shortest path between u and v in G. A simple graph is an unweighted, undirected graph without loops or multiple edges.

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. According to the IUPAC terminology, a topological index is a numerical value associated with chemical constitution which can be then used for correlation of chemical structure with various physical and chemical properties, chemical reactivity and biological activity.[5–12]

Let Σ be the class of finite graphs. A topological index is a function *Top* from Σ into real numbers where for G and H being isomorphic: $Top(G) = Top(H)$. Obviously, the number of vertices and the number of edges are topological indices. The Wiener index is the first graph invariant reported (distance based) topological index and is defined as a half sum of the distances between all the pairs of vertices in a molecular graph.

Let G be a connected graph and $e = uv$ be an edge of G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u = n_u(e|G)$. Analogously, $n_v = n_v(e|G)$ is the number of vertices of G whose distance to the vertex v is smaller than to u.

The vertex Szeged index is another topological index which was introduced by Gutman.[10] It is defined by: $Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e)$. The edge Szeged index of G is a recently proposed topologic al index[11] defined as $Sz(G) = \sum_{e=uv \in E(G)} m_u(e) m_v(e)$. where $m_u = m_u(e|G)$ (and $m_v = m_v(e|G)$) denote the number of edges of G whose distances to the vertex u are smaller than those to v (the number of edges of G whose distances to the vertex v are smaller

than those to u). Motivated by the success of the vertex Szeged index, Khadikar *et al.*[12, 13] proposed a seemingly similar molecular structure descriptor that in what follows we call the edge-*PI* index. In analogy with definition of the vertex Szeged index, the edge-*PI* index is defined as $Pl(G) = \sum_e [m_u(e) + m_v(e)]$. Quite recently the vertex-version of the *PI* index was also considered.[14] It is defined as $Pl_v(G) = \sum_e [m_u(e \mid G) + n_v(e \mid G)]$The atom-bond connectivity index is a novel topological index and was defined by Estrada et. al.[15] as

$$ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u . d_v}},$$

where d_u stands for the degree of vertex u. Now we define a new version of the atom-bond connectivity index as

$$ABC_2(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u . n_v}}.$$

The goal of this paper is to study the ABC_2 index. Our notation is standard and mainly taken from standard books of chemical graph theory.[5]

All graphs considered in this paper are finite, undirected, simple and connected. For background materials, see references.[16–22]

2. Results and Discussions

In this section we first determine some bounds for $ABC_2(G)$ index. Next we introduce the notion of transitive and edge-transitive action on vertices of graph G. Finally, by using this concept and some Lemmas we compute the ABC_2 index of the hypercube graph.

An automorphism of the graph $G = (V, E)$ is a bijection σ on V which preserves the edge set E, i. e., if $e = uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Here the image of vertex u under σ is denoted by $\sigma(u)$. The set of all automorphisms of G under the composition of mappings forms a group which is denoted by $Aut(G)$. $Aut(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha \in Aut(G)$ = such that $\alpha(u) = v$. Similarly $G = (V, E)$ is called an edge-transitive graph if for any two edges $e_1 = uv$ and $e_2 = xy$ in E there is an element $\beta \in Aut(G)$ such that $\beta(e_1) = e_2$ where $\beta(e_1) = \beta(u)\beta(v)$.

Lemma 3. If G is edge transitive, then

$$ABC(G) = |E| \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}}, \text{ for any } e = uv \in E(G).$$

Lemma 4. If G is edge transitive, then

$$ABC_2(G) = |E| \sqrt{\frac{n_u + n_v - 2}{n_u \cdot n_v}}, \text{ for any } e = uv \in E(G).$$

Example 5. Let S_n be the star graph with $n + 1$ vertices. It is easy to see that S_n is edge –transitive. Also, S_n is a tree and so by using Lemma 5 we have:

$$ABC_2(S_n) = n \times \sqrt{\frac{n-1}{n}} = \sqrt{n(n-1)}.$$

Fullerenes are molecules in the form of polyhedral closed cages made up entirely of n three-coordinated carbon atoms and having 12 pentagonal and (n/2 – 10) hexagonal faces, where n is an even number equal or greater than 20. Hence, the smallest fullerene, C_{20} ($n = 20$), has 12 pentagons. In the following example we compute the ABC_2 index of C_{20}.

Example 6. Consider the fullerene graph C_{20} shown in figure 1. It is easy to see C_{20} is edge-transitive and so by computing values of n_u and n_v, we have $n_u = n_v = 8$. Therefore: $|E| = 30$ and

$$ABC_2(C_{20}) = 30 \times \sqrt{\frac{14}{64}} = \frac{15}{8}\sqrt{14}.$$

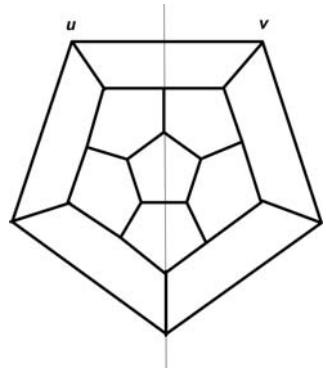

Figure 1: The graph of fullerene C_{20}.

The fullerene C_{20} is the only edge-transitive fullerene. So it is important to be able to compute ABC_2 index in the case where G is not an edge-transitive graph. One can apply then the following Lemma:

Lemma 1. Let $G = (V, E)$ be a graph. If $Aut(G)$ on E has orbits E_i, $1 \le i \le s$, where $e_i = u_i v_i$ is an edge of E_i, then:

$$ABC(G) = \sum_{i=1}^{s} |E_i| \sqrt{\frac{d_{u_i} + d_{v_i} - 2}{d_{u_i} \cdot d_{v_i}}}$$

and

$$ABC_2(G) = \sum_{i=1}^{s} |E_i| \sqrt{\frac{n_{u_i} + n_{v_i} - 2}{n_{u_i} \cdot n_{v_i}}}.$$

Proof. The values of n_u's for every $e = uv \in E_i$ are equal. So, it is enough to compute n_u and n_v for $e_i = uv$ ($1 \le i \le s$).

Example 2. Let P_n be the path on n vertices. P_n is not edge – transitive and by using Lemma 8 we have:

$$ABC_2(P_n) = \sqrt{n-2}\left[\frac{1}{\sqrt{n-1}} + \frac{1}{\sqrt{2(n-2)}} + \right.$$

$$\left. + \frac{1}{\sqrt{3(n-3)}} + \cdots + \frac{1}{\sqrt{n-1}}\right].$$

A hypercube is defined as follows. The vertex set of the hypercube H_n consists of all n-tuples $b_1b_2...b_n$ with $b_i \in \{0,1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Darafsheh[23] proved H_n is vertex and edge transitive. He also computed n_u and n_v for every edge $e = uv$ as $n_u = n_v = 2^{n-1}$. By using this result we have the following:

Theorem 7. Let H_n be the hypercube graph. Then,

$$ABC_2(H_n) = |E| \frac{\sqrt{2^n - 2}}{2^{n-1}} = n\sqrt{2^n - 2}.$$

Theorem 8. Let $G = (V, E)$ be a graph. Then $ABC_2(G) \leq Pl_v(G) - 2|E|$ and

$$ABC_2(G) \geq \sqrt{\frac{Pl_v(G) - 2|E|}{Sz(G)}}$$

Proof. By the definition of $ABC_2(G)$ index it is easy to see that $ABC_2(G) \leq \sum_{e=uv} \sqrt{n_u + n_v - 2} \leq \sum_{e=uv} n_u + n_v - 2 = Pl_v(G) - 2|E|$. This determines the upper bound. For the lower bound one can see that:

$$[ABC_2(G)]^2 \geq \sum_{e=uv} \frac{n_u + n_v - 2}{n_u . n_v} \geq \frac{\sum_{e=uv} n_u + n_v - 2}{\sum_{e=uv} n_u . n_v} =$$

$$= \frac{Pl_v(G) - 2|E|}{Sz(G)}.$$

Theorem 9. Let G be a bipartite graph on n vertices. Then we have:

$$\frac{2|E|}{n}\sqrt{n-2} \leq ABC_2(G) \leq |E|\sqrt{n-2}.$$

Proof. It is easy to see that for every bipartite graph on n vertices $n_u + n_v = n$. On the other hand $n_u, n_v \geq 1$. So,

$$ABC_2(G) \leq \sum_{e=uv} \sqrt{\frac{n-2}{1}} = |E|\sqrt{n-2}.$$

Also, for every edge $e = uv$, $n_u n_v \leq n^2 / 4$.

Corollary 10. Let T be a tree with n vertices. Then we have:

$$\frac{2(n-1)}{n}\sqrt{n-2} \leq ABC_2(T) \leq (n-1)\sqrt{n-2}.$$

Suppose G is an arbitrary graph. The distance matrix $M = [d_{ij}]$ of G is a $n \times n$ matrix in which d_{ij} is the length of the minimal path connecting vertices i and j, $i \neq j$, and zero for $i = j$. To compute the ABC_2 index of molecular graphs, we first draw the graph by HyperChem.[24] Then we apply TopoCluj software of Diudea and his team[25] to compute the distance matrices of the molecular graph under consideration. Using this method, we upload matrix M in our GAP program to compute the ABC_2 index. In what follows, we present our GAP program to compute ABC_2 index of any molecular graph.

3. Conclusions

By using the definition of the *ABC* index, we introduced here the ABC_2 index as a new version of the *ABC* index. Then we determined some bounds for this new topological index.

GAP Program for Computing the ABC_2 Index

```
f:=function(M)
    local l, v, ss, S, T, e, tt, FF, i,j, z, a, HH;
    l:=Length(M);v:=0;ss:=0;S:=[];T:=[];e:=[];tt:=0;FF:=[];
        for i in [1..l]do
            for j in[i+1..l] do
                if M[i][j]=1 then
                    Add(e,[i,j]);
                fi;
            od;
        od;
    for a in e do
        for i in [1..l] do
            if M[a[1]][i]>M[a[2]][i] then AddSet(S,i);
            fi;
            if M[a[1]][i]<M[a[2]][i] then
                AddSet(T,i);
            fi;
        od;
            ss:=ss+Sqrt((Length(S)+Length(T))/(Length(S)*Length(T)));
            z:=Union(S,T);
                for i in [1..Length(M[1])] do
                    Add(FF,i);
                od;
            HH:=Difference(FF,z);
        T:=[];S:=[];
    od;
    Print("ABC2 Index=",ss,"\n");
    return; end;
```

4. References

1. N. Trinajstić and I. Gutman, *Croat. Chem. Acta*, **2002,** *75*, 329–356.
2. I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer Verlag, Berlin, **1986**.
3. S. J. Cyvin and I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Lecture Notes in Chemistry, Vol 46, Springer Verlag, Berlin, **1988**.
4. A. Graovac, I. Gutman and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules,* Springer Verlag, Berlin, **1977**.
5. N. Trinajstić , *Chemical Graph Theory*, CRC Press, Boca Raton, FL, **1992**.
6. H. Wiener, *J. Am. Chem. Soc.,* **1947,** *69*, 17–20.
7. N. Raos and A. Miličević, *Arh. Hig. Rada Toksikol.*, **2009**, 60, 123–128;

8. A. Graovac, I. Gutman and D. Vukičević, Eds., *Mathematical Methods and Modelling for Students of Chemistry and Biology,* Hum naklada, Zagreb, **2003**.
9. H. Hosoya, *Disc. Appl. Math*., **1988,** *19*, 239–257.
10. I. Gutman, *Graph Theory Notes New York*, **1994,** *27*, 9–15.
11. I. Gutman and A. R. Ashrafi, *Croat. Chem. Acta*, **2008,** *81*, 263–266.
12. P. V. Khadikar, S. Karmarkar and V.K. Agrawal, *J. Chem. Inf. Comput. Sci.*, **2001,** *41*, 934–949.
13. P. V. Khadikar, P. P. Kale, N. V. Deshpande, S. Karmarkar and V.K. Agrawal, *J. Math. Chem.*, **2001,** *29*, 143–150.
14. M. H. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, *Disc. Appl. Math.*, **2008**, *156*, 1780–1789.
15. E. Estrada, L. Torres, L. Rodriguez and I. Gutman, *Indian J. Chem.,* **1998**, *37A*, 849-855.
16. K. Ch. Das, *Disc. Appl. Math.*, **2010**, *158*, 1181–1188.
17. A. R. Ashrafi, M. Ghorbani and M. Jalali, *J. Theor. Comput. Chem.*, **2008**, *7*, 221–231.
18. A. R. Ashrafi, M. Ghorbani and M. Jalali, *J. Theor. Comput. Chem.*, **2009**, *8*, 451–457.
19. A. R. Ashrafi, M. Jalali, M. Ghorbani and M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2008***, 60*, 905–916.
20. M. Ghorbani and M. Jalali, *MATCH Commun. Math. Comput. Chem.*, **2009**, *62*, 353–362.
21. A. R. Ashrafi and M. Ghorbani, *J. Serb. Chem. Soc*., **2010,** *75*, 1–8.
22. A. R. Ashrafi, M. Ghorbani and M. Jalali, *J. Theor. Comput. Chem*., **2008**, *7(2)*, 221–231.
23. M. R. Darafsheh, *Acta. Appl. Math*., **2009**, DOI 10. 1007/ s10440-009-9503-8 .
24. Hyper Chem package Release 7.5 for Windows, Hypercube Inc., 1115 NW 4th Street, Gainesville, Florida 32601, U. S. A. **2002**.
25. M. V. Diudea, O. Ursu and Cs. L. Nagy, *TOPOCLUJ*, Babes-Bolyai University, Cluj **2002**.

Povzetek

Pred kratkim vpeljani topološki indeks povezanosti za atomske vezi je definiran kot $ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$, kjer d_u predstavlja stopnjo vozla u. Tukaj definiramo novo verzijo *ABC* indeksa kot $ABC_2(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$, kjer n_u predstavlja število vozlov grafa G, katerih razdalja do vozla u je manjša od tiste do vozla v robu $e = uv$, medtem ko je n_v definiran analogno. Namen tega dela je študija ABC_2 indeksa.