On atom bond connectivity index of some molecular graphs

Mohanad A. Mohammed', K. A. Atan', A. M. Khalaf', M. R. Md. Said', and R. Hasni'

Citation: AIP Conference Proceedings **1739**, 020035 (2016); doi: 10.1063/1.4952515
View online: http://dx.doi.org/10.1063/1.4952515
View Table of Contents: http://aip.scitation.org/toc/apc/1739/1
Published by the American Institute of Physics

On Atom Bond Connectivity Index of Some Molecular Graphs

Mohanad A. Mohammed[1, 2, a)], K.A. Atan[1, b)], A.M. Khalaf[2, c)], M.R. Md. Said[1, d)] and R. Hasni[3, e)]

[1]*Institute for Mathematical Research, University Putra Malaysia 43400 Serdang, Selangor, Malaysia.*
[2]*Department of Mathematics Faculty of Computer Sciences and Mathematics, University Of Kufa, Najaf, Iraq.*
[3]*Department of Mathematics Faculty of Science and Technology University Malaysia Terengganu 21030 UMT Terengganu, Malaysia.*

[a)] Corresponding author: mohanadalim@gmail.com
[b)] kamel@upm.edu.my
[c)] abduljaleel.khalaf@uokufa.edu.iq
[d)] mrushdan@science.upm.edu.my
[e)] hroslan@umt.edu.my

Abstract. The atom-bond connectivity (ABC) index is one of the newly most studied degree based molecular structure descriptors, which have chemical applications. For a graph G, the ABC index can be defined as $ABC(G) = \sum_{uv\in E(G)} \sqrt{d_v + d_u - 2/d_v . d_u}$, where d_u, the degree of the vertex u is the number of edges with u as an end vertex denotes the degree of a vertex u in G. In this paper, we establish the general formulas for the atom bond connectivity index of molecular graphs of alkenes and cycloalkenes.

INTRODUCTION

Topological indices are beneficial instruments for modeling physical and chemical properties of molecules, for design of pharmacologically active compounds, for distinguishing environmentally hazardous materials, etc. [1]. There are many publications on the topological indices; see [2-8]. One of the best known is the Randić index introduced in 1975 by Randić [9], who has shown this index to reflect molecular branching. In order to take this into account but at the same time to keep the spirit of the Randić index, Ernesto Estrada et al. proposed a new index, nowadays known as the atom-bond connectivity (ABC) index, and it has many chemical applications [10]. This index is defined as follows: $ABC(G) = \sum_{uv\in E(G)} \sqrt{d_v + d_u - 2/d_v . d_u}$.

A critical re-examination ensures that the atom-bond connectivity index well denotes the heats of formation of alkanes (ΔH_f°). $\Delta H_f^{\circ} = -(a + b \times ABC)$ with $a = 65.98, b = 20.37$, denotes the heats of formation with an accuracy comparable to that of high-level and DFT(MP2,B3LYP) quantum chemical calculations. In the case of the ABC index, finding the tree for which this index is maximal was relatively easy [11], it is the star. The ABC indices for trees with second-maximal, third-maximal, and so forth were determined as in [12]. Chen and Guo, [13] have shown that by deleting an edge from any graph, the ABC index decreases. Thus the n-vertex trees with minimal ABC index are also the n-vertex connected graphs with minimal ABC index. But the problem of characterizing the n-vertex trees with minimal ABC index turned out to be much more difficult, and a complete solution of this problem is not known. For more results on ABC index see [14-21].In this paper we have two sections. In the first section, we present the general formula of atom bond connectivity index of class of chemical compounds and representing to Molecular graph as chemical trees. The second section supplies the general formula of ABC index of Cycloalkenes after representing as Unicyclic graph.

Innovations Through Mathematical and Statistical Research
AIP Conf. Proc. 1739, 020035-1–020035-7; doi: 10.1063/1.4952515
Published by AIP Publishing. 978-0-7354-1396-2/$30.00

PRELIMINARIES

A molecular graph can be defined as a connected graph with maximum vertex degree 4. It is a primary reason for representing graph theory in chemistry studies. Today, this space of mathematical chemistry is known as chemical graph theory [22]. A chemical tree is a tree which does not have vertex degree greater than 4. A vertex pendant that its degree equals one.

Many applications of trees are discovered in chemical studies. Some of which are applied to the classes of alkenes. An alkene is an unsaturated hydrocarbon that has at least one carbon–carbon double bond [23]. Alkenes contain two hydrogen atoms less than the corresponding alkane (with the same number of carbon atoms), with general formula C_nH_{2n}. The smallest alkene, ethylene (C_2H_4). We will establish the ABC index for Alkene, with only a Dobell bond between any two atoms of carbon, where the numbers of covalent bonds are 4 for Carbon and 1 for Hydrogen (see Fig. 1.).

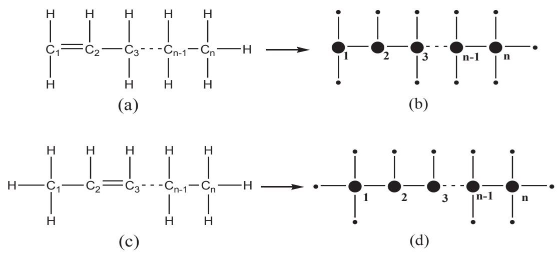


FIGURE 1. (a) and (c) Molecular structure of Alkenes (C_nH_{2n}); (b) and (d) Molecular graph associated with chemical compound of Alkenes (C_nH_{2n})

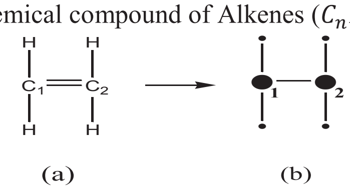


FIGURE 2. (a) Molecular structure of Alkenes (C_2H_4); (b) Molecular graph representing the Chemical compound of Alkenes (C_2H_4)

ATOM BOND CONNECTIVITY INDEX OF ALKENES

In this section, we set up the general formulas for the atom bond connectivity index of alkenes.

Example 1. Let G be the molecular graph associated with ethene (C_2H_4), it as a chemical compound of alkenes as in Fig. 2(b). The atom bond connectivity index of G is

$$ABC(G) = 4\sqrt{\frac{2}{3}} + \frac{2}{3} \cdot$$

Theorem 1. Let n be a positive integer and $n \geq 3$. Then the atom bond connectivity index of the graph G where G in Fig. 1 associated with C_nH_{2n} (Alkenes), is

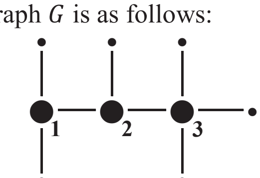
$$1 - ABC(G) = \frac{2}{3} + \sqrt{\frac{5}{12}} + 3\sqrt{\frac{2}{3}} + \frac{\sqrt{6}}{4}(n-3) + \frac{\sqrt{3}}{2}(2n-3) \quad if\ n \geq 3, \quad G = b \quad .$$

$$2 - ABC(G) = \frac{2}{3} + 2\sqrt{\frac{5}{12}} + 2\sqrt{\frac{2}{3}} + \frac{\sqrt{6}}{4}(n-4) + \frac{\sqrt{3}}{2}(2n-2) \ if\ n \geq 4, \quad G = d$$

Proof: We will prove this theorem by mathematical induction. There are two cases to be considered:

Case1. G is the molecular graph (b) as in Fig. 1.

Let $n = 3$ then G is associated with C_3H_6. The graph G is as follows:

G: 

Thus

$$ABC(G)=\sqrt{\frac{3+3-2}{3.3}}+\sqrt{\frac{3+4-2}{3.4}}+3\sqrt{\frac{3+1-2}{1.3}}+3\sqrt{\frac{4+1-2}{1.4}}=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+3\frac{\sqrt{3}}{2}$$

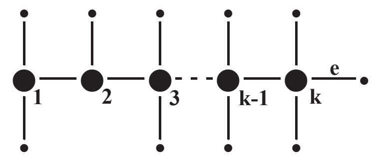
Hence it is true that

$ABC(G)=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+\frac{\sqrt{6}}{4}(n-3)+\frac{\sqrt{3}}{2}(2n-3)$, when G is the molecular graph (b) when $n=3$.

Suppose that the hypothesis is true for $n=k, k\geq 3$. That is the ABC index for the graph G associated in the graph C_kH_{2k} is given by:

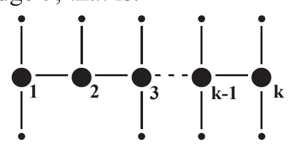
$$ABC(G)=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+\frac{\sqrt{6}}{4}(k-3)+\frac{\sqrt{3}}{2}(2k-3)$$

Construct the graph associated with $C_{k+1}H_{2k+2}$ as follows. The graph G associated with C_kH_{2k} has the form:

G: 

where C_i denotes the position of the Carbon vertex at the i^{th} position, and e is the edge that linking the vertex k of graph G with the vertex corresponding to the end Hydrogen vertex H.

Let G_1 be the graph got from G by removing the edge e, that is:

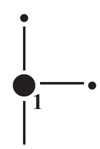
G_1: 

For the graph G_1,

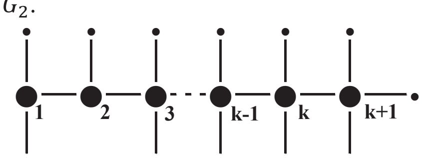
$$ABC(G_1)=ABC(G)-\sqrt{\frac{4+1-2}{4}}=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+\frac{\sqrt{6}}{4}(k-3)+\frac{\sqrt{3}}{2}(2k-3)-\frac{\sqrt{3}}{2}$$

$$=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+\frac{\sqrt{6}}{4}(k-3)+\frac{\sqrt{3}}{2}(2k-4)$$

Let G_2 be the graph

G_2: 

We construct the graph $\hat{G}$ by connecting the K^{th} vertex in G_1 with the vertex in G_2. We obtain the graph $\hat{G}$ as follows, where the K^{th} vertex is the vertex 1 from G_2.

$\hat{G}$: 

The $k+1^{th}$ vertex is adjacent to three other vertices in $\hat{G}$. Now $\hat{G}$, is the graph associated with the molecular structure of $C_{k+1}H_{2k+2}$.

Thus,

$$ABC(\hat{G})=ABC(G_1)+3\sqrt{\frac{4+1-2}{4}}+\sqrt{\frac{4+4-2}{16}}$$

$$=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+\frac{\sqrt{6}}{4}(k-3)+\frac{\sqrt{3}}{2}(2k-4)+3\frac{\sqrt{3}}{2}+\frac{\sqrt{6}}{4}$$

$$=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+\frac{\sqrt{6}}{4}(k-2)+\frac{\sqrt{3}}{2}(2k-1)$$

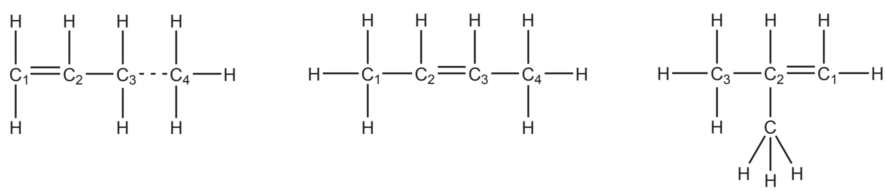
As a result the assertion is true when $n=k+1$.
Thus, as the assertion is true when $n=3$, and with the assumption that it is true for $n=k$ it is shown that it is true for $n=k+1$. Thus we have for all $n\geq 3$,

$ABC(G)=\frac{2}{3}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{2}{3}}+\frac{\sqrt{6}}{4}(n-3)+\frac{\sqrt{3}}{2}(2n-3)$, if G is the graph (b) in Fig. 1.

Case2. G is the molecular graph (d) as in Fig. 1. We prove this case by using the same argument as case 1. ▪

Isomerism of alkenes

All the alkenes with 4 or more carbon atoms in them show structural isomerism. Structural isomers have the same molecular formula but have different structural formula. This means that there are two or more different structural formula that we can draw for one molecular formula. For example, C_4H_8 could be either of these following two different molecules. These are called respectively 1-butene and 2-methylpropene (see Fig. 3).



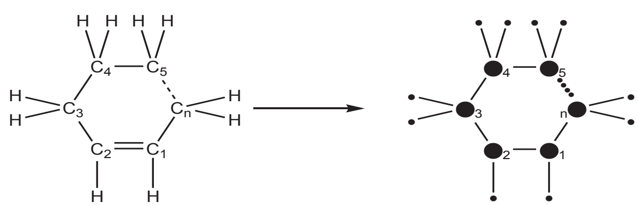
(1-butene) (2-butene) (2-methyl-1-propene)

FIGURE 3: Structural formula (C_4H_8) having the same molecular formula

Remark 1. The atom bond connectivity index of Isomers of Alkenes it is the same general formula in Theorem 1 because structural isomers have the same molecular formula but have different structural formula, this means Isomers of Alkenes have the same numbers of carbon and hydrogen atoms and the same number of edges with the same degree of vertices.

A cycloalkenes

Cycloalkenes (Also sometimes called a cycloolefin) is a kind of alkene hydrocarbon that has a closed ring of carbon atoms. The prefix cyclo- comes from ancient Greek and in this case means round. Whatever the ends of a carbon chain are linked together, that molecule is known as cyclic, and alkenes are no different from other carbon chains in that respect (see Fig. 4).



(a) (b)

FIGURE. 4. (*a*) Molecular structure of cycloalkenes C_n^H; (*b*) Molecular graph representing the chemical compound of cycloalkenes C_n^H.

ATOM BOND CONNECTIVITY INDEX OF CYCLOALKENES

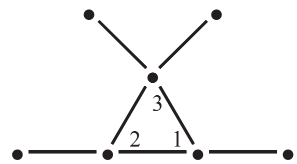
In this section, we construct the general formulas for the atom bond connectivity indices of graphs associated with cycloalkenes

Theorem 2. Let n be a positive integer and $n \geq 3$. The atom bond connectivity index of a graph G associated with C_n^H as in (b) of Fig. 4, is

$$ABC(G)=\frac{2}{3}+2\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2n-4)+\frac{\sqrt{6}}{4}(n-3).$$

Proof: We prove by induction.
Let G_n denote the graph associated with C_n^H.
Let $n=3$. Then, the graph G_3 associated with C_3H_4 is as follows:

G_3:



Thus

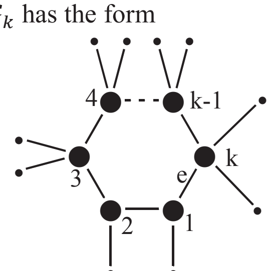
$$ABC(G_3)=\sqrt{\frac{3+3-2}{3.3}}+2\sqrt{\frac{3+4-2}{3.4}}+2\sqrt{\frac{1+3-2}{1.3}}+2\sqrt{\frac{1+4-2}{1.4}}$$
$$=\frac{2}{3}+2\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\sqrt{3}$$

Hence it is true that
$ABC(G_n)=\frac{2}{3}+2\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2n-4)+\frac{\sqrt{6}}{4}(n-3)$, when $n = 3$.
Suppose that the hypothesis is true for $n = k, (k \geq 3)$. That is the ABC index for G_k the graph associated with C_k^H is given by:

$$ABC(G_k)=\frac{2}{3}+2\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2k-4)+\frac{\sqrt{6}}{4}(k-3).$$

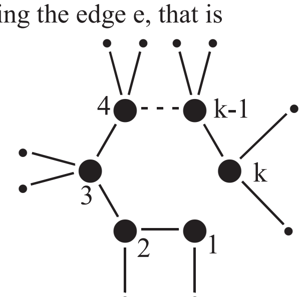
Construct the graph G_{k+1} as follows. The graph G_k has the form

G_k:



where i denotes the vertex of graph G_k at the i^{th} position, and e the edge connecting the vertex 1 with vertex k.
Let $\grave{G}$ be the graph obtained from C_n^H by removing the edge e, that is

$\grave{G}$:



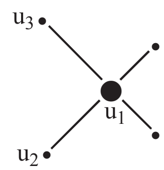
Therefore we will gain that,

$$ABC\left(\grave{G}\right)=ABC(G_k)-\sqrt{\frac{3+4-2}{12}}$$

$$=\frac{2}{3}+2\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2k-4)+\frac{\sqrt{6}}{4}(k-3)-\sqrt{\frac{5}{12}}$$
$$=\frac{2}{3}+\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2k-4)+\frac{\sqrt{6}}{4}(k-3)$$

Let F be the graph below:

F:



The vertex u_1 in F is adjacent to two vertices u_2, u_3 and two other pendant vertices.
Join $\grave{G}$ with F by letting $u_1 = k+1$, $u_2 = 1$ and $u_3 = k$. The vertices $u_1 = k+1$, $u3 = k$ of degree 4 and $u_2 = 1$ will have degree three as in Fig. 5. We get the graph G_{k+1} as follows.

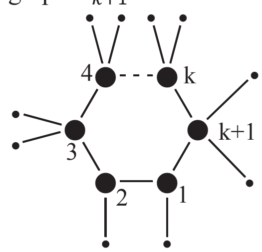


FIGURE 5. Graph of G_{k+1}.

Thus we will have,

$$ABC(G_{k+1}) = ABC(\grave{G})+\sqrt{\frac{3+4-2}{3.4}}+\sqrt{\frac{4+4-2}{4.4}}+2\sqrt{\frac{1+4-2}{1.4}}$$
$$=\frac{2}{3}+\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2k-4)+\frac{\sqrt{6}}{4}(k-3)+\sqrt{\frac{5}{12}}+\frac{\sqrt{6}}{4}+2\frac{\sqrt{3}}{2}$$
$$=\frac{2}{3}+2\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2k-2)+\frac{\sqrt{6}}{4}(k-2)$$

As a result our assertion is true when $n = k+1$.
Therefore, sum up it is true that.

$ABC(G)=\frac{2}{3}+2\sqrt{\frac{5}{12}}+2\sqrt{\frac{2}{3}}+\frac{\sqrt{3}}{2}(2n-4)+\frac{\sqrt{6}}{4}(n-3)$, for $n \geq 3$, where G is the graph associated with C_n^H as in (b) of Fig. 4. ▪

CONCLUSION

In conclusion, this study reveals four findings: first, we established the general formulas for classes of molecular graphs associated with some chemical compounds as Alkenes. Second, we have shown that Isomerism of Alkenes have the same general formulas of ABC index of Alkenes. Finally, we provided the general formulas to the cycloalkenes after represent it as molecular graphs.

REFERENCES

1. M. V. Diudea, I. Gutman and L. Jäntschi, Nova Science Pub Incorporated 2001. Nova, Huntington, 2001.
2. A. Behtoei, M. Jannesari and B. Taeri, Appl. Math. Lett. **22** (2009) 1571–1576.
3. K. C. Das, I. Gutman and B. Furtula, Survey on Geometric–Arithmetic indices of graphs, MATCH Commun. Math. Comput. Chem. **65** (2011) 595–644.
4. B. Liu and I. Gutman, MATCH Commun. Math. Comput. Chem. **58**, 147–154 (2007).
5. B. Liu and I. Gutman, MATCH Commun. Math. Comput. Chem. **62**, 143–154 (2009).

6. B. Liu and Z. You, MATCH Commun. Math. Comput. Chem. **65**, 581–593 (2011).
7. M. Zhang and B. Liu, MATCH Commun. Math. Comput. Chem. **64**, 433–442 (2010).
8. B. Zhou and N. Trinajstic, Chem. Phys. Lett. **455**, 120–123 (2008).
9. M. Randić and J. Am. Chem. Soc. **97**, 6609-6615 (1975).
10. E. Estrada and L. Torres, L. Rodríguez and I. Gutman, Indian J. Chem. A **37**, 849–855 (1998).
11. B. Furtula, A. Graovac and D. Vukičević, Discrete Appl. Math., **157**, 2828–2835 (2009).
12. B. Zhou and R. Xing, Z. Naturforsch. A, **66**, 61–66 (2011).
13. J. Chen and X. Guo, MATCH Commun. Math. Comput. Chem. **65**, 713–722 (2011).
14. J. S. Chen and X.-F. Guo, Appl. Math. A J. Chin. Univ **27**, 243–252 (2012).
15. J. Chen, J. Liu and X. Guo, Appl. Math. Lett. **25**, 1077–1081 (2012).
16. J. Chen, J. Liu and Q. Li, Discrete Dyn Nat Soc, vol. **2013**, Article ID 598517, 7 pages, (2013).
17. D. Dimitrov, Appl. Math. A J. Chin. Univ **224**, 663–670 (2013).
18. I. Gutman, B. Furtula and M. Ivanović, MATCH Commun. Math. Comput. Chem. **67**, 467–482 (2012).
19. I. Gutman and B. Furtula, MATCH Commun. Math. Comput. Chem. **68**, 131–136 (2012).
20. S. A. Hosseini, M. B. Ahmadi and I. Gutman, MATCH Commun. Math. Comput. Chem. **71**, 5–20 (2014).
21. W. Lin, X. Lin, T. Gao and X. Wu, MATCH Commun. Math. Comput. Chem. **69**, 549–557 (2013).
22. N. Trinajstić, CRC Press, Boca Raton, 1983 (second revised edn., 1992).
23. Wade, L.G., Organic Chemistry (6th ed.). (Pearson Prentice Hall 2006) p. 279.