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Some results on augmented Zagreb index of some trees and unicyclic graphs

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ABSTRACT. The augmented Zagreb index (AZI) of a graph G is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3,$$

where $E(G)$ and d_u denote set of edges of G and degree of the vertex u in G respectively. In this paper we establish some general results and bounds of AZI for certain unicyclic graphs and their corresponding chemical representation. We also obtain some results pertaining to AZI of certain trees.

1. INTRODUCTION

Let G be a simple connected graph with edge set $E(G)$ and vertex set $V(G)$ where $|E(G)| = m$ and $|V(G)| = n$ respectively. The degree of a vertex v in G is the number of immediate edges adjacent to v and denoted by d_v. Any vertex having degree one is termed as pendent vertex. A graph is said to be connected if there exists at least one path between any pair of vertices in G. Again any graph G having maximum vertex degree 4 is said to be a chemical or molecular graph which are associated with various chemical compounds and their structural formulae in chemistry. In a molecular graph, vertices and edges are represented by atoms and the chemical bonds between two atoms of their carbon-hydrogen skeleton respectively.

According to IUPAC definition, topological index or molecular descriptor is a numerical value associated with chemical constitution for correlation of chemical structure with various physio-chemical properties (viz. boiling point, enthalpy of vaporization, stability and so on) or biological activities [12]. These molecular descriptors of shape or structure of a molecule play a very important role in complex experiments for analyzing the properties and activities of molecules, specially in QSPR and QSAR investigations. Among these molecular descriptors, degree-based topological indices occupy its own place. These indices are also studied as graph invariant as these values are being preserved under graph automorphism. So far, a lot of topological indices have been introduced using different structural properties for their calculation viz. Estrada index of protien folding [2] or energy of a graph [6] is defined in terms of eigenvalues of the adjacency matrix of G; Wiener index [16] is based on distance between any two vertices of the graph; Randić index [14], Narumi-Katayama index [7], Atom-Bond Connectivity (ABC) index [3] etc., are based on degree of vertices whereas Hosoya Index [9], Zagreb coindices [10] etc., are calculated in terms of edges in its complement or non-incident edges of G. Another vertex-degree based graph invariant called augmented Zagreb index (AZI) and introduced by Furtula et

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al., [4] is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3,$$

which is proven to be a very helpful predictive measure in the study of heat of formation in heptanes and octanes. In a comparative study by Gutman and To$\tilde{s}$ovi$\tilde{c}$ [8], AZI emerged as more prominent index in case of normal boiling point and standard heat of formation of octane isomers. A sizeable number of research papers have been published with upper and lower bounds of ABC [1] [13], AZI [15] values for connected graphs, trees, unicyclic and bicyclic grpahs etc. and for almost all types of standard graphs with characterization of extremal cases.

In this paper, initially we obtain some bounds of AZI of n-vertex unicyclic graphs along with a few general formulae for certain unicyclic graphs and its chemical representation. Furthermore, we find some AZI results of certain kind of trees and hydrocarbons viz., alkanes, alkenes etc. The rest of the paper is organized as follows. In the next section we present AZI of certain unicyclic graphs and unicyclic chemical graphs. Then in section 3, we establish some result of AZI of certain trees.

2. AZI OF CERTAIN UNICYCLIC GRAPHS AND UNICYCLIC CHEMICAL GRAPHS

A graph $G(n; m)$ is said to be unicyclic if they have equal number of vertices and edges i.e., $n = m$ and it is denoted by U_n. The length of the cycle of such a unicyclic graph is called its girth. A unicyclic chemical graph U_n^* is a unicyclic graph such that degree of any vertex of it doesn't exceed 4.

Let us consider a unicyclic graph U_n^p obtained from attaching p pendent vertices to each vertex of the cycle of length n.

Theorem 2.1. [5] *Let G be a connected graph with $m \geq 2$ edges and minimum degree δ. Then*

$$AZI(G) \geq \frac{m\delta^6}{8(\delta - 1)^3},$$

with equality holds if and only if G is a δ-regular graph or every edge of G has at least one end vertex with degree two when $\delta = 2$.

Theorem 2.2. *Let U be a unicyclic connected graph of order n where $n \geq 2$ and minimum degree $\delta \geq 2$. Then*

$$AZI(G) \geq \frac{n\delta^6}{8(\delta - 1)^3},$$

equality holds iff $U = C_n$.

Proof. The bound is obvious from the above theorem and using the fact that in a unicyclic graph, $m = n$. Clearly for equality we must have $\delta = 2$ and for $U = C_n$, $\delta = 2$ and also $AZI(C_n) = 8n$. Hence the result. □

Now we present the following lemmas without proof.

Lemma 2.1. *Let $A_{ij} = (\frac{ij}{i+j-2})$, then*

i) A_{ij} is decreasing for $j \geq 2$,
ii) $A_{2j} = 2$ for $j \geq 2$,
iii) If $j \geq 3$ fixed, then A_{ij} is increasing for $i \geq 3$.

Lemma 2.2. [11] $A_{1\Delta} = \frac{\Delta}{\Delta - 1} \leq A_{1i} \leq A_{12} = A_{2j} = 2 < A_{33} = \frac{9}{4} \leq A_{kl} \leq A_{\Delta\Delta} = \frac{\Delta^2}{2\Delta - 2}$, *where $2 \leq i, j \leq \Delta$ and $3 \leq k \leq l \leq \Delta$.*

Let x_{ij} denotes the total number of edges in G joining vertices of degree i and j and also $\bar{ij} = A^3_{ij} = (\frac{ij}{i+j-2})^3$.

Theorem 2.3. *Let U^* be the unicyclic chemical graph of order n with p pendent vertices. Then*

$$AZI(U^*) \leq 8n,$$

and equality holds for $x_{13} = x_{14} = x_{33} = x_{34} = x_{44} = 0$.

Proof. From the above lemmas, we have

$$\begin{aligned} AZI(U^*) &= x_{12}\bar{12} + x_{13}\bar{13} + x_{14}\bar{14} + x_{22}\bar{22} + x_{23}\bar{23} + x_{24}\bar{24} + x_{33}\bar{33} + x_{34}\bar{34} + x_{44}\bar{44} \\ &= x_{13}\bar{13} + (p - x_{12} - x_{13})\bar{14} + 8(x_{12} + x_{22} + x_{23} + x_{24}) + x_{33}\bar{33} + x_{34}\bar{34} \\ &\quad +(n - p - x_{22} - x_{23} - x_{24} - x_{33} - x_{34})\bar{44} \\ &= p\bar{14} + (n-p)\bar{44} + (\bar{13} - \bar{14})x_{13} + (8 - \bar{14})x_{12} + (8 - \bar{44})x_{22} + (8 - \bar{44})x_{23} \\ &\quad +(8 - \bar{44})x_{24} + (\bar{33} - \bar{44})x_{33} + (\bar{34} - \bar{44})x_{34} \end{aligned}$$

As $\bar{13} - \bar{14} > 0$, $8 - \bar{14} > 0$, and $\bar{34} - \bar{44} < 0$, $\bar{33} - \bar{44} < 0$, we have

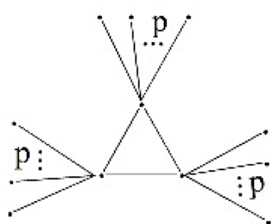
$$\begin{aligned} AZI(U^*) &\leq p\bar{14} + (n-p)\bar{44} + (\bar{13} - \bar{14})x_{13} + (8 - \bar{14})x_{12} + (8 - \bar{44})x_{22} + x_{23} + x_{24}) \\ &\leq p\bar{14} + (n-p)\bar{44} + (8 - \bar{14})x_{13} + (8 - \bar{14})x_{12} + (8 - \bar{44})x_{22} + x_{23} + x_{24}) \\ &\leq p\bar{14} + (n-p)\bar{44} + (8 - \bar{14})p + (8 - \bar{44})(n-p) \\ &= 8n. \end{aligned}$$

Therefore $AZI(U^*) \leq 8n$ with equality holds for $x_{13} = x_{14} = x_{33} = x_{34} = x_{44} = 0$. □

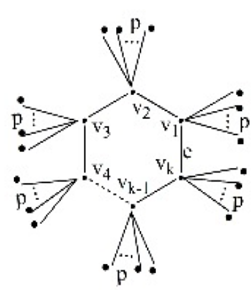
Theorem 2.4. *For positive integers n and p where $n \geq 3$ and $p \geq 1$, the augmented Zagreb index of U^p_n is given by*

$$AZI(U^p_n) = np\left(\frac{p+2}{p+1}\right)^3 + \frac{n}{8}\frac{(p+2)^6}{(p+1)^3}.$$

Proof. We prove this theorem by method of induction on n, the number of vertices. The result is clearly true for $n = 3$ and $p \geq 1$. Now let us assume that proposed hypothesis is hold for $n = k (k \geq 3)$ and $p \geq 1$. Graphically U^p_3 and U^p_k can be represented as follows:



(a) Fig: U^p_3

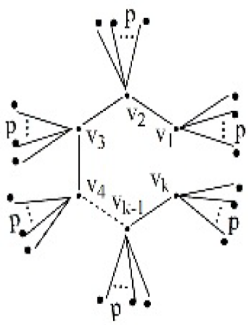


(b) Fig: U^p_k

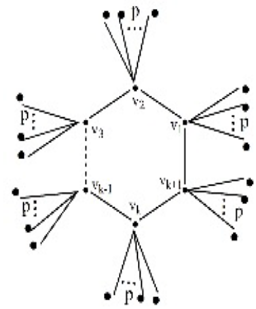
Let v_i denotes vertex at i-th position of the cycle of U^p_k and e be the edge incident on vertex v_k and v_1. Furthermore, let G_1 be the corresponding graph obtained from U^p_k by deleting the particular edge e. Thus we get

$$\begin{aligned} AZI(G_1) &= AZI(U^p_k) - \left(\tfrac{(p+2)(p+2)}{(p+2)+(p+2)-2}\right)^3 \\ &= kp\left(\tfrac{p+2}{p+1}\right)^3 + \tfrac{(k-1)}{8}\tfrac{(p+2)^6}{(p+1)^3}. \end{aligned}$$

Now let S be the graph in which u_1 is adjacent to u_2 and u_3 together with p pendent vertices. So, to construct U^p_{k+1} let us join G and S in a way such that $u_1 = v_{k+1}$, $u_2 = v_1$ and $u_3 = v_k$ having each of them degree $p+2$ as follows: Thus we have



(c) Fig: Graph G_1



(d) Fig: $G \cup S = U^p_{k+1}$

$$\begin{aligned} AZI(U^p_{k+1}) &= AZI(G_1) + 2\left(\tfrac{(p+2)(p+2)}{(p+2)+(p+2)-2}\right)^3 + p\left(\tfrac{1.(p+2)}{1+(p+2)-2}\right)^3 \\ &= kp\left(\tfrac{p+2}{p+1}\right)^3 + \tfrac{(k-1)}{8}\tfrac{(p+2)^6}{(p+1)^3} \\ &= (k+1)p\left(\tfrac{p+2}{p+1}\right)^3 + \tfrac{(k+1)}{8}\tfrac{(p+2)^6}{(p+1)^3}. \end{aligned}$$

Therefore our assertion holds for $n = k+1$ and $p \geq 1$. And hence the theorem. □

In the above theorem if we put $p = 2$, then we have $AZI(U^{*2}_n) = \frac{640n}{27}$. So for $p = 2$, the corresponding chemical compound of the unicyclic chemical graph U^{*2}_n are cycloalkanes having chemical formula C_nH_{2n}. An alkyl substituent or branches of alkyl are alkanes having one hydrogen atom less than it. An acyclic alkyl group has the general formula $C_nH_{2n+1}(n \geq 1)$.

If we replace the hydrogen atoms in cycloalkanes by alkyl group or branches of alkyl, it results a new class of unicyclic chemical graph denoted by U^{*alkyl}_n where n is signifies the total number of carbon atoms. Here we obtain another results of AZI associated with unicyclic chemical graph U^{*alkyl}_n.

Theorem 2.5. *For any positive integer n where $n \geq 4$, the augmented Zagreb index of U^{*alkyl}_n is*

$$AZI(U^{*alkyl}_n) = 2n\left(\frac{64}{27}\right) + n\frac{512}{27}.$$

Proof. For $n = 4$ it is easy to verify that the result is true. Let us consider that the result s true for $n = k(k \geq 4)$. Now in U^{*alkyl}_k , let c_i denotes carbon atom of the cycle of length m in i-th position and e be the edge joining the end vertices of the cycle c_m and c_1. Also let G_1 be the corresponding graph after deleting the edge e from U^{*alkyl}_k . Thus we have,

$$\begin{aligned} AZI(G_1) &= AZI(U^{*alkyl}_k) - \left(\tfrac{4.4}{4+4-2}\right)^3 \\ &= 2k\left(\tfrac{64}{27}\right) + (k-1)\tfrac{512}{27}. \end{aligned}$$

To construct U^{*alkyl}_{k+1}, let us introduce another graph S having vertex u_1 connected to u_2 and u_3 and two other pendent vertices of hydrogen atoms such that $u_1 = c_{k+1}$, $u_2 = c_1$ and $u_3 = c_m$ with each of degree 4. Hence we get

$$\begin{aligned} AZI(U^{*alkyl}_{k+1}) &= AZI(G_1) + 2\left(\tfrac{4.4}{4+4-2}\right)^3 + 2\left(\tfrac{1.4}{1+4-2}\right)^3 \\ &= 2(k+1)\left(\tfrac{64}{27}\right) + (k+1)\tfrac{512}{27}. \end{aligned}$$

Thus our assertion is true for $n = k+1$, and hence the result. □

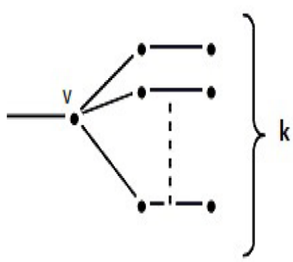
3. AZI OF CERTAIN TREES

A graph with no cycle is called acyclic. An undirected graph with vertices n in which there is exactly one connected path between any two vertices is called a tree and it is denoted by T_n. Briefly, a tree is a connected acyclic graph.

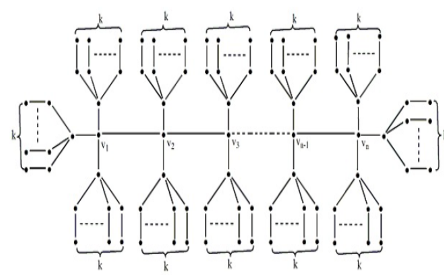
Let B_k be a branch of tree obtain from attaching k paths of length 2 to a particular vertex v so that it has degree $k+1$ in T_n. Let us construct another tree $T_n^{B_k}$ by joining the branch B_k three times to the terminal vertex of path P_n and two times in the remaining vertices both opposite to each other.

Theorem 3.6. *For positive integers n and k where $n \geq 1$, $k \geq 1$, the augmented Zagreb index of $T_n^{B_k}$ is*

$$AZI(T_n^{B_k}) = 32k(n+1) + 128(n+1)\left(\frac{k+1}{k+3}\right)^3 + (n-1)\frac{512}{27}.$$



(e) Fig: The branches of B_k



(f) Fig: The tree $T_n^{B_k}$

Proof. In $T_n^{B_k}$, there are $2n+2$ branches of B_k in which each Bk again have $2k$ edges having k edges with terminal vertex of degree 1 and degree 2 and remaining k edges with degree 2 and degree $k+1$. Secondly, there is another $2n+2$ edges with each edge having end vertex of degree 4 and degree $k+1$. Furthermore in P_n, the number of edges is equal to $n-1$ having each of them of degree 4. Thus we have,

$$\begin{aligned} AZI(T_n^{B_k}) &= (2n+2)k\left(\tfrac{1.2}{1+2-2}\right)^3 + (2n+2)k\left(\tfrac{2.(k+1)}{2+(k+1)-2}\right)^3 + (2n+2)\left(\tfrac{4.(k+1)}{4+(k+1)-2}\right)^3 \\ &\quad + (n-1)\left(\tfrac{4.4}{4+4-2}\right)^3 \\ &= 32k(n+1) + 128(n+1)\left(\tfrac{k+1}{k+3}\right)^3 + (n-1)\tfrac{512}{27}. \end{aligned}$$

Hence the theorem. □

Molecular structures of certain hydrocarbons are closely resemble to trees in graph theory. For example, alkanes, alkenes etc. Alkanes are organic compounds having structural formula C_nH_{2n+2} $(n \geq 1)$ and consisting of carbon and hydrogen atoms without any double bonds. Similarly alkenes are saturated hydrocarbons with structural formula C_nH_{2n} $(n \geq 2)$ with two hydrogen atoms less than alkane. Here we will establish some AZI results of these hydrocarbons.

Theorem 3.7. *For any positive integer $n(n \geq 1)$, the Augmented Zagreb index of C_nH_{2n+2} (alkane) is given by*

$$AZI(C_nH_{2n+2}) = (2n+1)\frac{64}{27} + \frac{512}{27}(n-1).$$

Proof. We can prove this result by method of induction on n. Clearly the result is true for $n = 1$. Now suppose the statement is true for $n = k(k \geq 1)$, Therefore AZI associated with C_kH_{2k+2}, is $AZI(C_kH_{2k+2}) = (2k+1)\frac{64}{27} + \frac{512}{27}(k-1)$.

Let us construct $C_{k+1}H_{2(k+1)+2}$ in the following ways: Let c_i denotes the vertex of carbon atom at i-th position of C_kH_{2k+2} and e be the edge incident on k-th carbon and corresponding end hydrogen vertex. Let G_1 be the graph yielded from C_kH_{2k+2} by deleting the edge e. Therefore,

$$\begin{aligned} AZI(G_1) &= AZI(C_kH_{2k+2}) - \left(\tfrac{1.4}{1+4-2}\right)^3 \\ &= 2k\tfrac{64}{27} + \tfrac{512}{27}(k-1) \end{aligned}$$

Now connecting k-th vertex of G_1 with the center of $K_{1,3}$, we get the graph structure associated with alkane $C_{k+1}H_{2k+4}$, where

$$\begin{aligned} AZI(C_{k+1}H_{2k+4}) &= AZI(G_1) + 3\left(\tfrac{1.4}{1+4-2}\right)^3 + \left(\tfrac{4.4}{4+4-2}\right)^3 \\ &= 2k\tfrac{64}{27} + \tfrac{512}{27}(k-1) + 3\left(\tfrac{64}{27}\right) + \tfrac{512}{27} \\ &= [2(k+1)+1]\tfrac{64}{27} + \tfrac{512}{27}[(k+1)-1]. \end{aligned}$$

Thus our assertion is true for $n = k+1$, and hence the theorem. □

Similarly for alkenes we can propose the following theorem, which can be proved mutatis mutandis.

Theorem 3.8. *For any positive integer $n(n \geq 2)$, the augmented Zagreb index of C_nH_{2n} (alkene having double bond in first position) is*

$$AZI(C_nH_{2n}) = \begin{cases} 4\left(\frac{3}{2}\right)^3 + \left(\frac{9}{4}\right)^3 & \text{if } n = 2 \\ 3\left(\frac{3}{2}\right)^3 + \left(\frac{9}{4}\right)^3 + \left(\frac{12}{5}\right)^3 + (n-3)\left(\frac{512}{27}\right) + (2n+1)\left(\frac{64}{27}\right) & \text{if } n \geq 3 \end{cases}$$

4. Conclusion

Augmented Zagreb index is found to be an important predictor of various physical and chemical properties of a molecule. But the study of this index as a graph invariant receives limited attention. In this paper we study augmented Zagreb index of certain tress and unicyclic graphs. We establish some bounds of AZI for certain unicyclic graphs and their corresponding chemical representation, especially for a new class of unicyclic chemical graph which can be obtained by replacing the hydrogen atoms in cycloalkanes by alkyl group or branches of alkyl.

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REFERENCES

[1] Das, K. Ch., Gutman, I. and Furtula, B., *On atom-bond connectivity index*, Chem. Phys. Lett., **511** (2011), No. 4-6, 452–454

[2] Estrada, E., *Characterization of 3D molecular structure*, Chem. Phys. Lett., **319** (2000), 713–718

[3] Estrada, L., Rodríguez, L., Torres, L. and Gutman., I., *An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes*, Indian J. Chem., **37** (1998), No. 10, 849–855

[4] Furtula, B., Graovac, A. and Vukičević, D., *Augmented Zagreb index*, J. Math. Chem., **48** (2010), No. 2, 370–380

[5] Gan, L., Hou, H. and Liu, B., *Some results on atom-bond connectivity index of graphs*, Discr. Appl. Math., **66** (2011), No. 2, 669–680

[6] Gutman, I., *The energy of a graph*, Ber. Math.-Statist. Sekt. Forschungsz. Graz, **103** (1978), 1–22

[7] Gutman, I., *Degree-based topological indices*, Croat. Chem. Acta., **86** (2013), 351–361

[8] Gutman, I., et al., *Testing the quality of molecular structure descriptors: vertex degree-based topological indices*, J. Serb. Chem. Soc., **78** (2013), 805–810

[9] Hosoya, M., *Topological index: A newly proposed quantity characterising the topological nature of structural isomers of saturated hydrocarbons*, Bull. Chem. Soc, **44** (1971), 2332–2339

[10] Hua, H. and Zhang, S., *Relations between Zagreb coindices and some distance-based topological indices*, MATCH Commun. Math. Comput. Chem., **68** (2012), 199–208

[11] Huang, Y., Liu, B. and Gan, L., *Augmented Zagreb Index of Connected Graphs*, MATCH Commun. Math. Comput. Chem., **67** (2012), No. 2, 483–494

[12] Jagadeesh, R., Rajesh Kanna, M. R. and Indumathi, R. S., *Some results on topological indices of graphene*, Nanomaterials and Nanotechnology, **6** (2016), 1–6

[13] Mohammed, M. A., Atan, K. A., Khalaf, A. M. and Hasni, R., *On the atom bond connectivity index of certain trees and unicyclic graphs*, 7^{th} International Conference on Research and Educations of Mathematics, 2015

[14] Randić, M., *On characterization of molecular branching*, J. Am. Chem. Soc., **97** (1975), 6609–6615

[15] Wang, D., Huang, Y. and Liu, B., *Bounds on augmented Zagreb index*, MATCH Commun. Math. Comput. Chem., **68** (2012), No. 1, 209–216

[16] Wiener, H., *Relation of the physical properties of the isomeric alkanes to molecular structure. Surface tension, specific dispersion and critical solution temperature in aniline*, J. Phys. Chem., **52** (1948), 1082-1089

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