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Study of Topological Properties of Molecular Structure of Aztec Diamond

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Abstract: Chemical graph theory is a branch of mathematics which combines graph theory and chemistry. A numerical quantity that gives information related to be topology of graph. our objective is to compute the degree based topological indices foe the molecular structure of aztec diamond. In the degree based topological indices, we compute first K-banhatti index, second K-banhatti index, Modified first K-banhatti index, Modified second K-banhatti index, First K-hyper banhatti index, second K-hyper banhatti index, First hyper revan indices, second hyper Revan indices. These Topological indices are calculated by direct method.

MSC: 05C92.

Keywords: Topological indices, Banhatti indices, Aztec diamond.

1. Introduction

There was a creation of useful tools by Chemists like topological indices. Usage of molecular graph is mainly to model molecular compounds. Molecular represents the structure graph. Graph as a compound's formula, top point of which connects to the compound's atoms. And edges connect to the compound's edges. Chemiosmosis is a sub field of study that assembled to the chemistry, mathematics and information science. It explores the quantitative body-activity and connection between QSAR and QSPR develops is being used to forecast compound features and biological exercise.

Molecule graph is relevant to graph that is made of molecule. Topological indices, Polynomials, sequences, and matrices is being used to point out objects. The vertices and edges of any graph in mathematics are introduced by atoms and chemical bonds. A molecular graph is that kind of graph that presents a molecule's structure and relevancy and depiction is considered to be as a topological depiction of molecules. There are some significant topological markers that must be kept in mind. Topological indexes like far off topological indexes and degree-based topological indexes are used most of the time. In these parts, remoteness is very important. Units that depend strongly on topological pointers are responsible for a crucial task. There are uncountable features in a lot of fields. There is a possibility of usage of diagrams.for more information about Topological indices and polynomial of graph see [1–10].

Suppose D be a simple connected graph. Space between f and g in $d(f, g)$, level of a node f in D in $d(f)$, edge e in the middle of nodes f and g in $e = fg$, the degree of an edge e by $d(e)$ (situation $d(e) = d(f) + d(g) - 2$), and the highest and lowest

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degree of the graph with $\Delta(D)$ and $\delta(D)$.

An Indian mathematician has introduced some of Banhatti's most important first and second K Banhatti indicators, the first and second K hyper Banhatti index, the first and second K Banhatti index and the K Banhatti harmonic index for 2016. Chemical graph degree and grade-based topological indicators have been a hot topic for research over the past decade. Many mathematicians have calculated these variables of various chemical graphs to study its chemical properties of living organisms. Topological indices are defined as [11–15]:

(1). First K-Banhatti index:

$$B_1(D) = \sum_{f e \epsilon E(D)} [d(f) + d(e)]$$

(2). Second K-Banhatti index:

$$B_2(D) = \sum_{f e \epsilon E(D)} [d(f) \times d(e)]$$

(3). Modified first K-Banhatti index:

$$mB_1(D) = \sum_{f e \epsilon E(D)} \frac{1}{d(f) + d(e)}$$

(4). Modified second K-Banhatti index:

$$mB_2(D) = \sum_{f e \epsilon E(D)} \frac{1}{d(f) \times d(e)}$$

(5). First K-hyper Banhatti index:

$$HB_1(D) = \sum_{f e \epsilon E(D)} [d(f) + d(e)]^2$$

(6). Second K-hyper Banhatti index:

$$HB_2(D) = \sum_{f e \epsilon E(D)} [d(f) \times d(e)]^2$$

(7). First-hyper Revan indices:

$$HR_1(D) = \sum_{f g \epsilon E(D)} [r_D(f) \times r_D(g)]^2$$

(8). Second-hyper Revan indices:

$$HR_2(D) = \sum_{f g \epsilon E(D)} [r_D(f) r_D(g)]^2$$

2. The Molecular Structures of Subdivided Aztec Diamonds

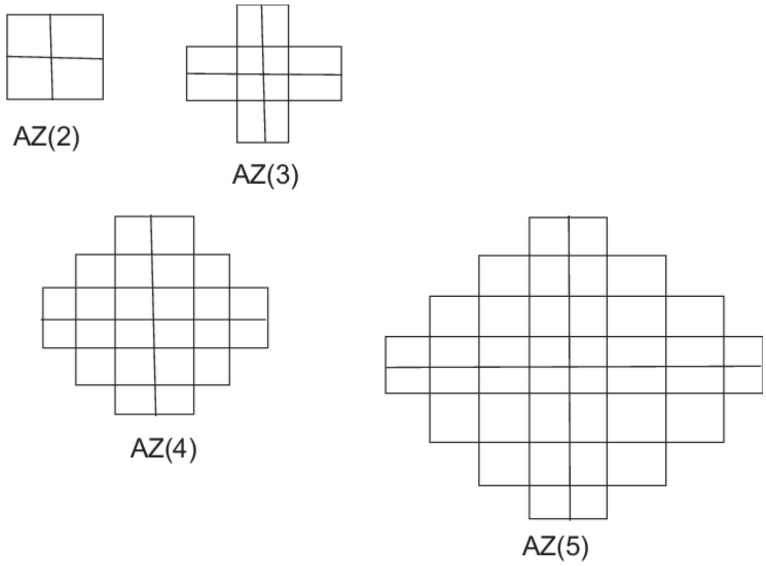

Figure 1. SAZ_4 **(Aztec diamond)**

In the figure above various sizes of Aztec diamonds divided into sections. We describe here two important things called nodes and edges for the Graph shown in image and displayed with D. In the following theories, various formulas of the above-mentioned indicators aztec diamond split with parts SAZ_n calculated. Let d_f into degree node also belongs to $T(D)$ and d_g to edge level and to $E(D)$ and $e = |F(D)|$ is a cardinal edge of D. SAZ_a is based on the end of each edge.
In this way, depending on the degrees of vertices at the end of $F(D)$ elements, set $F(D)$ of SAZ_a may also be divided into three sub-sets of F_1, F_2, and F_3. Suppose $fg \epsilon F_1$, if $d(f) = d(g) = 2$, then F_1 hold $8a$ edges. If $fg \epsilon F_2$, then $d(f) = 2$ and $d(g) = 3$, then by counting, we see that F_2 carry edges of 12. The set F_3 carry $8a^2 + 8a - 12$ edges fg, where $d(f) = 2$ and $d(g) = 4$. The below box provides details of the segmentation of SAZ_a for $a \geq 1$ depending on the degrees.

(d_f, d_g)	$NumberofedgesE(D)$	d(e)
(2,2)	8a	2
(2,3)	12	3
(2,4)	$8a^2 + 8a - 12$	4

Table 1. **The separation of the edges of graph D is created from the level of the vertices ending at all edges**

Theorem 2.1. *Let $D = SAZ_4$ be the graph of Aztec diamond. The degree based topological indies of D are the following:*

(1). $B_1[D] = 112a^2 + 176a - 48$

(2). $B_2[D] = 192a^2 + 256a - 108$

(3). $m_1^B[D] = \frac{7}{3}a^2 + \frac{25}{3}a + \frac{9}{10}$

(4). $m_2^B[D] = \frac{3}{2}a^2 + \frac{11}{2}a + \frac{13}{12}$

(5). $HB_1[D] = 800a^2 + 1056a - 468$

(6). $HB_2[D] = 2112a^2 + 2368a - 2436$

(7). $HR_1[D] = 288a^2 + 800a + 156$

(8). $HR_2[D] = 512a^2 + 2560a + 960$

Proof.

(1). **First K-Banhatti index**

$$B_1[D] = 8a[(2+2)+(2+2)] + (12)[(2+3)+(3+2)] + (8a^2+8a-12)[(2+4)+(4+4)]$$
$$B_1[D] = 64a + 120 + 112a^2 + 112a - 168$$
$$B_1[D] = 112a^2 + 176a - 48.$$

(2). **Second K-Banhatti index**

$$B_2[D] = 8a[(2\times 2)+(2\times 2)] + (12)[(2\times 3)+(3\times 3) + (8a^2+8a-12)[(2\times 4)+(4\times 4)]$$
$$B_2[D] = 64a + 180a + 192a^2 + 192a - 288$$
$$B_2[D] = 192a^2 + 256a - 108$$

(3). **Modified first K-Banhatti index**

$$m_1^B[D] = 8a[\frac{1}{2+2} + \frac{1}{2+2}] + (12)[\frac{1}{2+3} + \frac{1}{3+3}] + (8a^2+8a-12)[\frac{1}{2+4} + \frac{1}{4+4}]$$
$$m_1^B[D] = (8a)\frac{3}{4} + (2)\frac{11}{5} + (8a^2+8a-12)\frac{7}{24}$$
$$m_1^B[D] = \frac{7}{3}a^2 + \frac{25}{3}a + \frac{9}{10}$$

(4). **Modified second K-Banhatti index**

$$m_2^B[D] = (8a)[\frac{1}{4} + \frac{1}{4}] + (12)[\frac{1}{6} + \frac{1}{9}] + (8a^2+8a-12)[\frac{1}{8} + \frac{1}{16}]$$
$$m_2^B[D] = (4a) + \frac{10}{3}a + (8a^2+8a-12)\frac{3}{16}$$
$$m_2^B[D] = \frac{3}{2}a^2 + \frac{11}{2}a + \frac{13}{12}$$

(5). **First K-hyper Banhatti index**

$$HB_1[D] = (8a)[(2+2)^2 + (2+2)^2] + (12)[(2+3)^2 + (3+3)^2] + (8a^2+8a-12)[(2+4)^2 + (4+4)^2]$$
$$HB_1[D] = 8a[32] + 12[61] + (8a^2+8a-12)[100]$$
$$HB_1[D] = 800a^2 + 1056a - 468$$

(6). **Second K-hyper Banhatti index**

$$HB_2[D] = 8a[16+16] + 12[36+81] + (8a^2+8a-12)[64+256]$$
$$HB_2[D] = 8a[32] + 12[117] + (8a^2+8a-12)[320]$$
$$HB_2[D] = 2112a^2 + 2368a - 2436$$

(7). **First-hyper Revan indices**

$$HR_1[D] = 8a[4+4]^2 + (12)[4+3]^2 + (8a^2+8a-12)[4+2]^2$$
$$HR_1[D] = 8a[8]^2 + (12)[7]^2 + (8a^2+8a-12)[6]^2$$
$$HR_1[D] = 288a^2 + 800a + 156$$

(8). **Second-hyper Revan indices**

$$HR_2[D] = 8a[4\times 4]^2 + (12)[4\times 3]^2 + (8a^2+8a-12)[4\times 2]^2$$
$$HR_2[D] = 8a[16]^2 + (12)[12]^2 + (8a^2+8a-12)[8]^2$$
$$HR_2[D] = 512a^2 + 2560a + 960$$

□

2.1. Graph Analysis

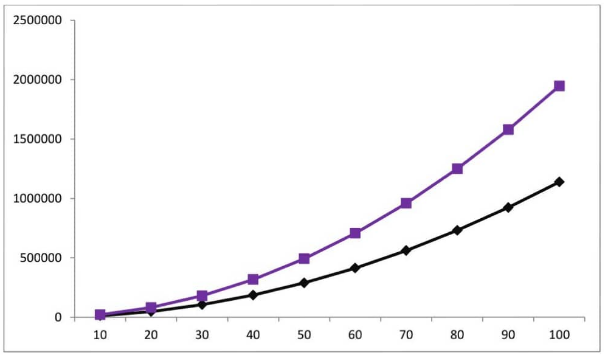

Figure 2. **Relating $B_1[D]$ and $B_2[D]$ indices**

In figure 2, 1st K-Banhatti index who's notation B_1 is shown by black color. 2nd K-Banahatti index who's notation B_2 is shown by purple color. By Observing graph we easily identify that unit cell in B_1 index is smaller then B_2 index.

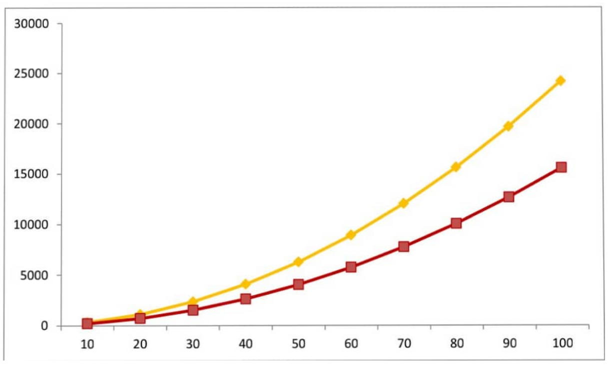

Figure 3. **Relating $m_1^B[D]$ and $m_2^B[D]$ indices**

In figure 3, modified K-banhatti indices who's notation $m_1^B[D]$ is shown by orange color. $m_2^B[D]$ is shown by dark Red color. In the graph we clearly watching that the unit cell of $m_2^B[D]$ are smaller then the $m_1^B[D]$.

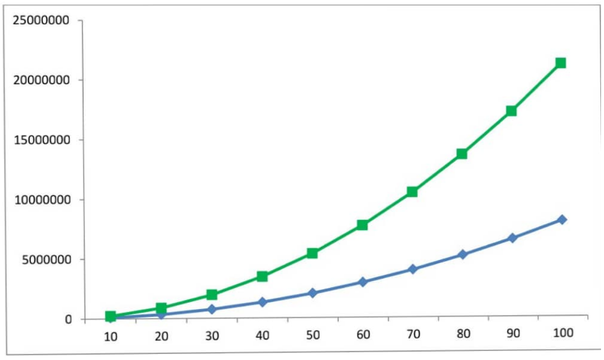

Figure 4. **Relating $HB_1[D]$ and $HB_2[D]$ indices**

In figure 4, K-hyper banhatti indices who's notation $HB_1[D]$ is shown by blue color. $HB_2[D]$ is shown by Green color. In the graph we clearly watching that the number of unit cell of $HB_1[D]$ are smaller then the $HB_2[D]$.

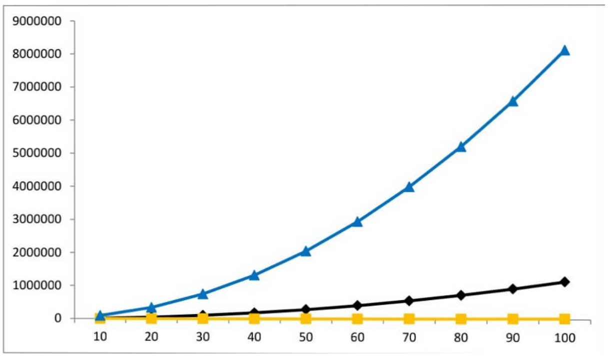

Figure 5. **Relating $B_1[D]$, $m_1^B[D]$ and $HB_1[D]$ indices**

In figure 5, shown 1^{st} K-Banhatti index, modified K-banhatti indices $m_1^B[D]$ and K-hyper banhatti index $HB_1[D]$.

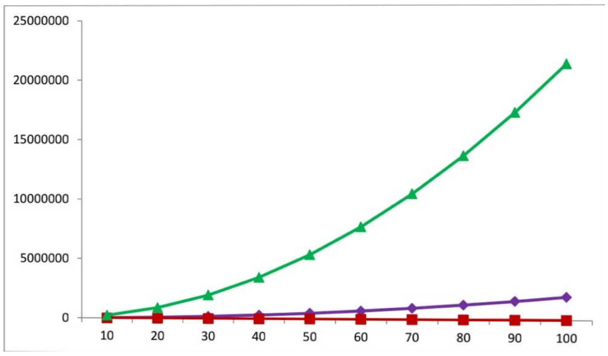

Figure 6. **Relating $B_2[D]$, $m_2^B[D]$ and $HB_2[D]$ indices**

In figure 6, shown 2^{st} K-Banhatti index, modified K-banhatti indices $m_2^B[D]$ and K-hyper banhatti index $HB_2[D]$.

3. Conclusion

Due to the rapid development of chemistry a large number of compounds are being developed on a daily basis so there is a need for research to test the properties of new chemical compounds. But developing countries could not afford the right equipment, human resources and reagents due to lack of funding. Topological indicators support us to reduce the number of experiments. Because they are based on the composition of the compound cells and are easily computed. The results listed in this work have a brilliant performance in chemistry. In this article we computed the topological indices likely banhatti and revan indices of Aztec diamond.

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