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Computation of Zagreb indices and forgotten index of Aztec Diamond

H. S. Ramanes and R. B. Jummannaver

Department of Mathematics, Karnatak University,

Dharwad - 580 003, Karnataka, India

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An Aztec diamond of order k is the region obtained from four staircase shapes of height k by gluing them together along the straight edges. It can therefore be defined as the union of unit squares in the plane whose edges lie on the lines of a square grid and whose centers (x, y) satisfy $|x-\frac{1}{2}|+|y-\frac{1}{2}|\leq k$. We obtain the explicit expressions for Zagreb indices, forgotten index of Aztec diamond and of their line garaphs and subdivision graphs.

Mathematics Subject Classification:05C12, 05C90

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1 Introduction

In chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This can be modeled by a graph taking vertices as atoms and edges as covalent bonds. Topological indices are the numerical quantities of a graph which are invariant under graph isomorphism. The exact transfer of chemical formula (or molecular graph) into numerical format has been a major task in Quantitative structure-activity (QSAR)/ structure-property (QSPR). There are many methods to quantify the molecular structures, in which topological index is the most popular since it can be obtained directly from molecular structures and rapidly computed for large numbers of molecules[15]. Lot of research has been done on topological indices of different graph families so far, and is of much importance due to their chemical significance.

Let G be a connected graph of order n and size m. Let $V(G)$ be the vertex set and $E(G)$ be the edge set of G. The edge joining the vertices u and v is denoted by uv. The *degree* of a vertex u is the number of edges incident to it and is denoted by $d(u)$. The *subdivision graph* $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length 2, or equivalently, by inserting an additional vertex into each edge of G. The *line graph* of a graph G, denoted by $L(G)$ is the graph whose vertices has one to one correspondence with the edges of G and two vertices in $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G.For a graph theoretic terminology, we refer the books [1, 9].

The first and second *Zagreb indices* of a graph G are defined as [8]

$$M_1(G) = \sum_{uv \in E(G)} \left[d(u) + d(v)\right] \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

The Zagreb indices were used in the structure property model [7, 16]. Recent results on the Zagreb indices can be found in [2, 5, 6, 10].

Fortula and Gutman [4] introduced forgotten index also called as F-index and is defined as

$$F(G) = \sum_{u \in V(G)} \left[d(u)^3\right] = \sum_{uv \in E(G)} d\left[(u)^2 + d(v)^2\right]$$

Recent results of forgotten index on drugs structures can be found in [17, 18]

Certain degree based and counting related topological indices of aztec diamond has obtained in [13]. In this paper we obtain the explicit expressions for Zagreb indices, forgotten index of Aztec diamond and of their line garaphs and subdivision graphs.

The Aztec diamond of order k, denoted by $AZ(k)$, is defined as the union of all the unit squares with integral corners (x, y) satisfying $|x| + |y| \leq k+1$. A domino is simply a 1-by-2 or 2-by-1 rectangles with integral corners. The number of squares in the Aztec diamond of order k are $2k(k+1)$ .May previous studies of aztec diamond appears in [12, 3, 11, 13].

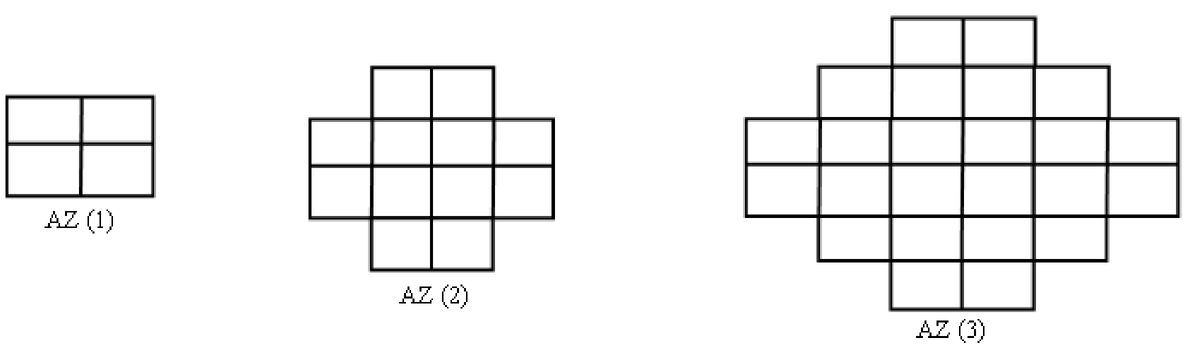

Figure 1: Aztec diamond of different dimensions

2 Computation of Zagreb indices and forgotten index of Aztech diamond *AZ(k)*

Theorem 2.1 *Let* $AZ(k)$ *be the graph of aztec diamond then we obtain*

$$M_1(AZ(k)) = 32k^2 + 48k - 12$$

$$F(AZ(k)) = 128k^2 + 160k - 84$$

Proof. Partition the vertex set of $AZ(k)$ into three subsets as $V_1 = \{u \mid d(u) = 2\}, V_2 = \{u \mid d(u) = 3\}$ and $V_3 = \{u \mid d(u) = 4\}$. By means structure analysis we have $|V_1| = 4k$, $|V_2| = 4$, $|V_3| = 2k^2 + 2k - 3$

Therefore, using the definition of First Zagreb index, we obtain

$$M_1(AZ(k)) = \sum_{u \in V(AZ(k))} (d(u))^2$$

$$= \sum_{u \in V_1} (d(u))^2 + \sum_{u \in V_2} (d(u))^2 + \sum_{u \in V_3} (d(u))^2$$

$$= (4k)(4) + (4)(9) + (2k^2 + 2k - 3)(16)$$

$$= 32k^2 + 48k - 12.$$

By using the definition of Forgotten index, we obtain

$$F(AZ(k)) = \sum_{u \in V(AZ(k))} (d(u))^3$$

$$= \sum_{u \in V_1} (d(u))^3 + \sum_{u \in V_2} (d(u))^3 + \sum_{u \in V_3} (d(u))^3$$

$$= (4k)(8) + (4)(27) + (2k^2 + 2k - 3)(64)$$

$$= 128k^2 + 160k - 84.$$

Theorem 2.2 *Let* $AZ(k)$ *be the graph of aztec diamond then we obtain*

$$M_2(AZ(k)) = 64k^2 + 64k - 32$$

Proof. Partition the edge set of $(AZ(k))$ into three subsets as $E_1 = \{uv \mid d(u) = 2 \text{ and } d(v) = 3\}$, $E_2 = \{uv \mid d(u) = 2 \text{ and } d(v) = 4\}$, $E_3 = \{uv \mid d(u) = 3 \text{ and } d(u) = 4\}$ and $E_4 = \{uv \mid d(u) = 4 = d(v)\}$. By means structure analysis we have $|E_1| = 8$, $|E_2| = 8k - 8$, $|E_3| = 4$ and $E_4 = 4k^2 - 4$

Therefore, using the definition of Second Zagreb index, we obtain

$$M_2(AZ(k)) = \sum_{uv \in E(AZ(k))} (d(u)d(v))$$

$$= \sum_{u \in E_1} (d(u)d(v)) + \sum_{u \in E_2} (d(u)d(v)) + \sum_{u \in E_3} (d(u)d(v)) + \sum_{u \in E_4} (d(u)d(v))$$

$$= (8)(6) + (8n - 8)(8) + (4)(12) + (4k^2 - 4)(16)$$

$$= 64k^2 + 64k - 32.$$

3 Computation of Zagreb indices and forgotten index of subdivision graph of Aztec diamond S[*AZ*(*k*)]

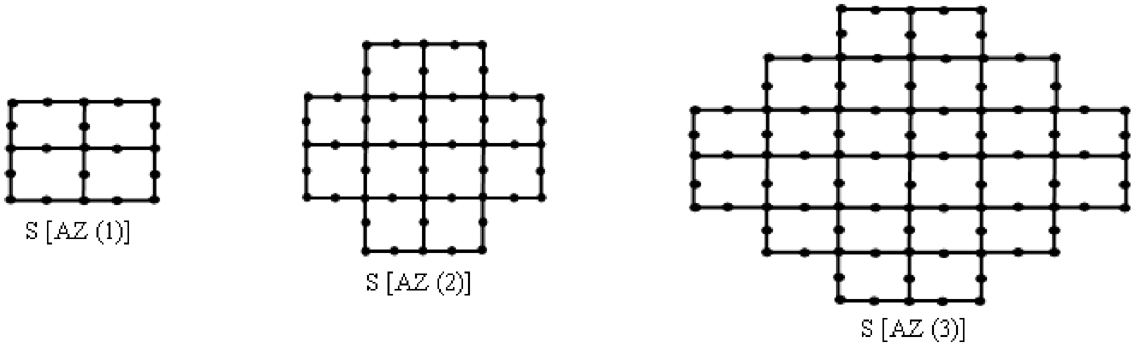

Figure 2: subdivision graph of Aztec diamond of different dimensions

Theorem 3.1 *Let* $S[AZ(k)]$ *be the subdivision graph of aztec diamond then we obtain*

$$M_1[S(AZ(k))] = 48k^2 + 80k - 12$$

$$F[S(AZ(k))] = 160k^2 + 224k - 84$$

Proof. Partition the vertex set of $S[(AZ(k))]$ into three subsets as $V_1 = \{u \mid d(u) = 2\}$, $V_2 = \{u \mid d(u) = 3\}$ and $V_3 = \{u \mid d(u) = 4\}$. By means structure analysis we have $|V_1| = 4k^2 + 12k$, $|V_2| = 4$, $|V_3| = 2k^2 + 2k - 3$

Therefore, using the definition of First Zagreb index, we obtain

$$M_1[S(AZ(k))] = \sum_{u \in V[S(AZ(k))]} (d(u))^2$$

$$= \sum_{u \in V_1} (d(u))^2 + \sum_{u \in V_2} (d(u))^2 + \sum_{u \in V_3} (d(u))^2$$

$$= (4k^2 + 12k)(4) + (4)(9) + (2k^2 + 2k - 3)(16)$$

$$= 48k^2 + 80k - 12.$$

By using the definition of Forgotten index, we obtain

$$F[S(AZ(n))] = \sum_{u \in V[S(AZ(k))]} (d(u))^3$$

$$= \sum_{u \in V_1} (d(u))^3 + \sum_{u \in V_2} (d(u))^3 + \sum_{u \in V_3} (d(u))^3$$

$$= (4k^2 + 12k)(8) + (4)(27) + (2k^2 + 2k - 3)(64)$$

$$= 160k^2 + 224k - 84.$$

Theorem 3.2 *Let* $S(AZ(k))$ *be the subdivison graph of aztec diamond then we obtain*

$$M_2[S(AZ(k))] = 64k^2 + 96k - 24$$

Proof. Partition the edge set of $S(AZ(k))$ into three subsets as $E_1 = \{uv \mid d(u) = 2 = d(v)\}$, $E_2 = \{uv \mid d(u) = 2 \ and \ d(v) = 3\}$ and $E_3 = \{uv \mid d(u) = 2 \ and \ d(v) = 4\}$. By means structure analysis we have $|E_1| = 8k$, $|E_2| = 12$ and $E_3 = 8k^2 + 8k - 12$

Therefore, using the definition of Second Zagreb index, we obtain

$$M_2[S(AZ(k))] = \sum_{uv \in E[S(AZ(k))]} (d(u)d(v))$$

$$= \sum_{u \in E_1} (d(u)d(v)) + \sum_{u \in E_2} (d(u)d(v)) + \sum_{u \in E_3} (d(u)d(v))$$

$$= (8k)(4) + (12)(6) + (8k^2 + 8k - 12)(8)$$

$$= 64k^2 + 96k - 24.$$

4 Computation of Zagreb indices and forgotten index of line graph of Aztec diamond L[*AZ*(*k*)]

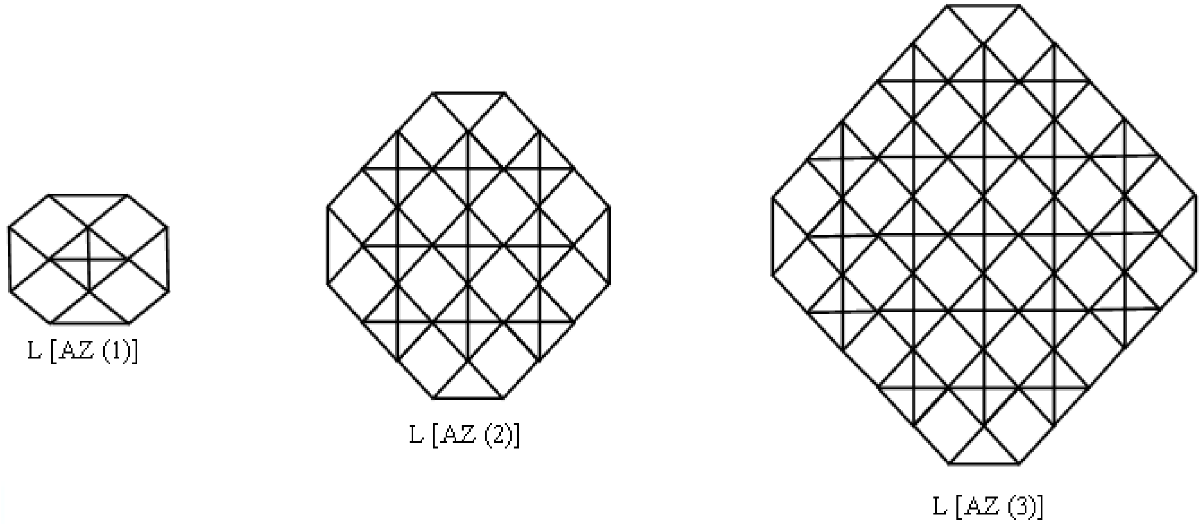

Figure 3: line graph of Aztec diamond of different dimensions

Theorem 4.1 *Let* $L[AZ(k)]$ *be the line graph of aztec diamond then we obtain*

$$M_1[L(AZ(k))] = 144k^2 + 128k - 100.$$

$$F[L(AZ(k))] = 864k^2 + 512k - 660.$$

Proof. Partition the vertex set of $L[(AZ(k))]$ into two subsets as $V_1 = \{u \mid d(u) = 3\}$, $V_2 = \{u \mid d(u) = 4\}$, $V_3 = \{u \mid d(u) = 5\}$ and $V_4 = \{u \mid d(u) = 6\}$. By means structure analysis we have $|V_1| = 8$, $|V_2| = 8k - 8$, $|V_3| = 4$ and $|V_4| = 4k^2 - 4$

Therefore, using the definition of First Zagreb index, we obtain

$$M_1[L(AZ(k))] = \sum_{u \in V[L(AZ(k))]} (d(u))^2$$

$$= \sum_{u \in V_1} (d(u))^2 + \sum_{u \in V_2} (d(u))^2 + \sum_{u \in V_3} (d(u))^2 + \sum_{u \in V_4} (d(u))^2$$

$$= (8)(9) + (8k-8)(16) + (4)(25) + (4k^2-4)(36)$$

$$= 144k^2 + 128k - 100.$$

By using the definition of Forgotten index, we obtain

$$F[L(AZ(k))] = \sum_{u \in V[S(AZ(k))]} (d(u))^3$$

$$= \sum_{u \in V_1} (d(u))^3 + \sum_{u \in V_2} (d(u))^3 + \sum_{u \in V_3} (d(u))^3 + \sum_{u \in V_4} (d(u))^3$$

$$= (8)(27) + (8k-8)(64) + (4)(125) + (4k^2-4)(216)$$

$$= 864k^2 + 512k - 660.$$

Conclusion: Topological indices such as Zagreb and forgitten indices of Aztec diamond graphs and of their subdivision and line graphs are obtained. The second Zagreb index of $L(AZ(k))$ is not so easy. One can try the bound for it and extremities.

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