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DEGREE BASED TOPOLOGICAL INDICES OF SANIDIC POLYAMIDES

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ABSTRACT

Sanidic polyamides are special polymers with many applications in textile and clothing industries. In this paper, we calculate several degree based topological graph indices of the sanidic polyamides as these values helps to determine several chemical and physicochemical properties of these polyamides.

1. INTRODUCTION

Polyamides are polymers containing repeating amides in the form of "-CO-NH-" linkages. The names of the types of polyamides are derived according to the number of carbon atoms in their molecule structures. Some of the naturally occurring polyamides are silk, wool and proteins. Polyamides are classified into two categories. Aliphatic polyamides, known as nylons, and aromatic polyamides, known as aramids.

Polyamides find applications in several fields ranging from the textile to the automotive industry. They are used in making medical instruments and clothing, electrical appliances, and in many more areas. Polyamide fibers are used in a wide

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range of applications due to their excellent mechanical properties and good adhesion property to other materials like rubber. These fibers are used in women's hosiery and in all the stretch fabrics such as blouses, lingerie, and swimwear. They are also used in several house furnishings such as upholstery and curtains. This type of fibers has mostly been used in some technical textile derivatives like vehicle tires, parachutes, nets and tents. The main factors for preferring polyamide fibers for a wide range of military applications are high strength, elasticity, toughness, and abrasion resistance of them compared with other equivalent materials. In general, polyester has gained considerable significant market share compared to polyamides because of its easy-care characteristics, [**7**].

In this work, we study on the sanidic polyamide which is one of the aromatic polyamides briefly called aramids, see Fig. 1. In [**2**], a series of fully aromatic polyesters, polyamides and polyimides having n-alkoxy side chains for $2 \leq n \leq 18$ have been investigated for their applications in optical microscopy, X-ray analysis and DSC. All members of these series have a rigid backbone and exhibit a decreasing melting range with increasing length of the side chains. This characteristic is very similar to the Wiener index which helps to determine the boiling temperatures of the isomers of alkanes where the longer chains have lower boiling temperature. The polyester with short side chains ($2 \leq n \leq 6$) form nematic melts. Some of aramid applications include the hot-air filtration fabrics, optical-fiber cables, jet-engine enclosures, heat-protective clothings, helmets, loudspeaker diaphragms, and reinforced-thermoplastic pipes all having a lot of areas of application. Although the aramids are non-conductive, they are sensitive to UV. They provide good resistance to organic solvents and abrasion which is the main reason to study with them.

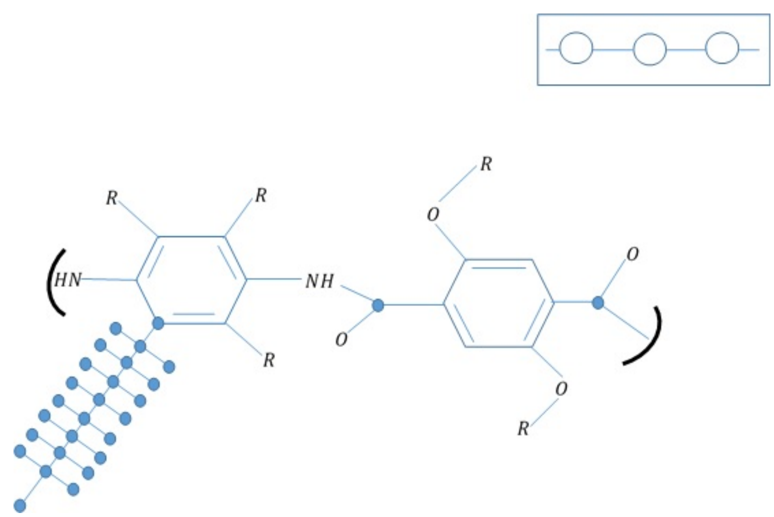

Figure 1: Sanidic Polyamide where $R = C_8H_{17}$.

Topological graph indices are defined and used in many areas to study several properties of different objects such as atoms and molecules. A large number of topological graph indices have been defined and studied by many mathematicians and chemists as most graphs are generated from molecules by replacing atoms with vertices and bonds with edges. They are defined as topological graph invariants measuring several physical, chemical, pharmacological, pharmaceutical, biological etc. properties of graphs which are modelling real life situations. They can mainly be grouped into three classes according to the way they are defined: by vertex degrees, by matrices or by distances.

Let $G = (V, E)$ be a simple graph with $\mid V(G) \mid = n$ vertices and $\mid E(G) \mid = m$ edges. That is, no loops nor multiple edges are allowed. For a vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$ or d_v.

Two of the most important topological graph indices are called the first and second Zagreb indices denoted by $M_1(G)$ and $M_2(G)$, respectively:

$$(1) \qquad M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

They were defined in 1972 by Gutman and Trinajstic, [**8**], and are referred to due to their uses in QSAR and QSPR studies in chemical studies. In [**3**], some results on the first Zagreb index together with some other indices are given. For some graph operations, these indices are calculated in [**4**].

The F-index, also called as forgotten index, of a graph G is denoted by $F(G)$ or $M_3(G)$ and is defined as the sum of the cubes of the degrees of the vertices of the graph. The total π-electron energy depends on the degree based sums $M_1(G)$ and $F(G) = \sum_{u \in V(G)} d_G^3(u)$. They were first appeared in the study of structure-dependency of total π-electron energy in 1972, [**8**]. The first index was later named as the first Zagreb index and the second sum has never been further studied until the last few years. As a result, recently, this sum was named as the forgotten index or the F-index briefly by Furtula and Gutman, [**6**], and it was shown to have an exceptional applicative potential.

The hyper-Zagreb index was defined as a variety of the classical Zagreb indices as

$$HM(G) = \sum_{(uv \in E} (d_u + d_v)^2,$$

see e.g. [**6**].

Inspired by the study of heat formation for heptanes and octanes in [**5**], Furtula et. al. proposed an index, called the augmented Zagreb index, which gives a better prediction power. It is defined by

$$AZI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v - 2}.$$

The harmonic index was introduced by Zhang [**11**]. It is shown that it correlates well with Π-electron energy of benzenoid hydrocarbons and defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

Reformulated first, second and third Zagreb indices for a graph G are defined by

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v},$$

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v},$$

$$ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v).$$

Milicevic et. al., [**10**], reformulated the Zagreb indices in terms of the edge degrees instead of the vertex-degrees as

$$RM_1(G) = \sum_{uv \in E(G)} d(e)^2,$$

$$RM_2(G) = \sum_{e,e' \in E(G)} d(e)d(e')$$

where e, e' are pairs of adjacent edges of the graph G.

Aram and Dehgardi, [**1**], introduced the concept of reformulated F-index as

$$RF(G) = \sum_{uv \in E(G)} d(uv)^3.$$

Kulli, [**9**], introduced the first and second Banhatti indices with the intention of taking into account the contributions of pairs of incident elements, not only the vertices or edges. They are defined as

$$B_1(G) = \sum_{u,e} [d_G(u) + d(e)],$$

$$B_2(G) = \sum_{u,e} d_G(u) d(e).$$

2. TOPOLOGICAL INDICES OF SANIDIC POLYAMIDES

Now we will determine some well-known topological indices of sanidic polyamides G^*.

Lemma 1. *The first and second Zagreb indices of G^* are $M_1(G^*) = 1016n$ and $M_2(G^*) = 1318n$.*

Proof. We partition the set of edges of G^* into edges according to their types $E_{(d_u,d_v)}$ where uv is an edge. In G^*, we get edges of type $E_{(1,3)}$, $E_{(1,4)}$, $E_{(2,3)}$, $E_{(2,4)}$, $E_{(3,3)}$, $E_{(3,4)}$ and $E_{(4,4)}$. The number of edges of these types are 4, 102, 6, 2, 14, 4 and 42, respectively.

We know that $M_1(G) = \sum_{uv\in E(G)}(d_u + d_v)$, i.e.,

$$\begin{aligned} M_1(G^*) &= \mid E_{(1,3)} \mid (1+3)+ \mid E_{(1,4)} \mid (1+4)+ \mid E_{(2,3)} \mid (2+3) \\ &+ \mid E_{(2,4)} \mid (2+4)+ \mid E_{(3,3)} \mid (3+3+ \mid E_{(3,4)} \mid (3+4)) \\ &+ \mid E_{(4,4)} \mid (4+4) \\ &= 4(1+3) + 102(1+4) + 6(2+3) + 2(2+4) + 14(3+3) \\ &+ 4(3+4) + 42(4+4) \\ &= 1016. \end{aligned}$$

For n unit, we have the general result as $M_1(G^*) = 1016n$ by the additivity property.

As $M_2(G) = \sum_{uv\in E(G)} d_u d_v$, we get the result for $M_2(G^*)$ by similar calculations to $M_1(G^*)$.

□

Lemma 2. *The third Zagreb index (forgotten index) of G^* is $F(G^*) = 3588n$.*

Proof. We know that $F(G) = \sum_{u\in V(G)} {d_u}^3$, i.e.,

$$\begin{aligned} F(G^*) &= \sum_{u\in V(G^*)} {d_u}^3 = 1^3 \cdot 106 + 2^3 \cdot 4 + 3^3 \cdot 14 + 4^3 \cdot 48 \\ &= 3588. \end{aligned}$$

For n unit, we get $F(G^*) = 3588n$. □

Lemma 3. *The hyper Zagreb index of G^* is $HM(G^*) = 6220n$.*

Proof. We know that $HM(G) = \sum_{uv\in E(G)}(d_u + d_v)^2$, i.e.,

$$\begin{aligned} HM(G^*) &= \mid E_{(1,3)} \mid (1+3)^2 + \mid E_{(1,4)} \mid (1+4)^2 + \mid E_{(2,3)} \mid (2+3)^2 \\ &+ \mid E_{(2,4)} \mid (2+4)^2 + \mid E_{(3,3)} \mid (3+3)^2 + \mid E_{(3,4)} \mid (3+43)^2 \\ &+ \mid E_{(4,4)} \mid (4+4)^2 \\ &= 4(1+3)^2 + 102(1+4)^2 + 6(2+3)^2 \\ &+ 2(2+4)^2 + 14(3+3)^2 + 4(3+4)^2 + 42(4+4)^2 \\ &= 6220. \end{aligned}$$

For n unit, we similarly get $HM(G^*) = 6220n$. □

Lemma 4. *The augmented Zagreb index of G^* is $AZI(G^*) = 2462,07 \cdot n$.*

Proof. We know that $AZI(G) = \sum_{uv\in E(G)}(\frac{d_u \cdot d_v}{d_u+d_v-2})^3$, i.e.,

$$\begin{aligned} AZI(G^*) &= \mid E_{(1,3)} \mid (\frac{1\cdot 3}{1+3-2})^3 + \mid E_{(1,4)} \mid (\frac{1\cdot 4}{1+4-2})^3 + \mid E_{(2,3)} \mid (\frac{2\cdot 3}{2+3-2})^3 \\ &+ \mid E_{(2,4)} \mid (\frac{2\cdot 4}{2+4-2})^3 + \mid E_{(3,3)} \mid (\frac{3\cdot 3}{3+3-2})^3 \\ &+ \mid E_{(3,4)} \mid (\frac{3\cdot 4}{3+4-2})^3 + \mid E_{(4,4)} \mid (\frac{4\cdot 4}{4+4-2})^3 \\ &= 4(\frac{3}{8}) + 102(\frac{64}{27}) + 48 + 16 + 14\cdot(\frac{721}{64}) + 4\cdot(\frac{1728}{125}) + 42\cdot(\frac{512}{27}) \\ &= 2462,07 \end{aligned}$$

giving the result for n unit. □

The following results can similarly be obtained by counting the edges and using the formulae of the given indices:

Lemma 5. *The harmonic index of G^* is $H(G^*) = 62,177 \cdot n$.*

Proof. We know that $H(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v}$, i.e.,

$$\begin{aligned} H(G^*) &= \mid E_{(1,3)} \mid \frac{2}{1+3} + \mid E_{(1,4)} \mid \frac{2}{1+4} + \mid E_{(2,3)} \mid \frac{2}{2+3} \\ &+ + \mid E_{(2,4)} \mid \frac{2}{2+4} + \mid E_{(3,3)} \mid \frac{2}{3+3} + \mid E_{(3,4)} \mid \frac{2}{3+4} + \mid E_{(4,4)} \mid \frac{2}{4+4} \\ &= 36,177. \end{aligned}$$

For n unit, we conclude that $H(G^*) = (62,177)n$. □

Lemma 6. *The Re-defined version of Zagreb indices of G^* are $ReZG_1(G^*) = 171,99 \cdot n$, $ReZG_2(G^*) = 206,327 \cdot n$, $ReZG_3(G^*) = 8832n$.*

Proof. We know that $ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v}$, i.e.,

$$\begin{aligned} ReZG_1(G^*) &= \mid E_{(1,3)} \mid \frac{1+3}{1 \cdot 3} + \mid E_{(1,4)} \mid \frac{1+4}{1 \cdot 4} + \mid E_{(2,3)} \mid \frac{2+3}{2 \cdot 3} \\ &+ \mid E_{2,4)} \mid \frac{2+4}{2 \cdot 4} + \mid E_{(3,3)} \mid \frac{3+3}{3 \cdot 3} + \mid E_{(3,4)} \mid \frac{3+4}{3 \cdot 4} + \mid E_{(4,4)} \mid \frac{4+4}{4 \cdot 4} \\ &= 171,99. \end{aligned}$$

For n unit, we find that $ReZG_1(G^*) = 171,99 \cdot n$.

As $ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v}$ and $ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v)$, by using the similar methods we get the results for G^*. □

Lemma 7. *The Reformulated Zagreb indices of G^* are $RM_1(G^*) = 2856n$, $RM_2(G^*) = 5856n$.*

Proof. In G^* the degrees of the edges $d(uv)$ where uv is an edge are 2, 3, 4, 5 and 6. The number of these edge degrees of G^* are $\mid d(uv) = 2 \mid = 4, \mid d(uv) = 3 \mid = 108, \mid d(uv) = 4 \mid = 16, \mid d(uv) = 5 \mid = 4$ and $\mid d(uv) = 6 \mid = 42$.

We know that $RM_1(G) = \sum_{uv \in E(G)} d(uv)^2$, i.e.,

$$\begin{aligned} RM_1(G^*) &= \mid d(uv) = 2 \mid \cdot 2^2 + \mid d(uv) = 3 \mid \cdot 3^2 + \mid d(uv) = 4 \mid \cdot 4^2 \\ &+ \mid d(uv) = 5 \mid \cdot 5^2 + \mid d(uv) = 6 \mid \cdot 6^2 \\ &= 4 \cdot 2^2 + 108 \cdot 3^2 + 16 \cdot 4^2 + 4 \cdot 5^2 + 42 \cdot 6^2 = 2856. \end{aligned}$$

For n unit, $RM_1(G^*) = 2856n$.

For calculating $RM_2(G^*)$, we partition the incident edges of G^* according to product of their edge degrees $d(e) \cdot d(e')$ where $e, e' \in E$ and $e\ e'$. In G^*, we get $d(2) \cdot d(4), d(3) \cdot d(3), d(3) \cdot d(4), d(3) \cdot d(5), d(3) \cdot d(6), d(4) \cdot d(4), d(4) \cdot d(5), d(4) \cdot d(6), d(4) \cdot d(6)$ and $d(6) \cdot d(6)$. The number of these type of products are 7, 64, 9, 8, 174, 15, 8, 2, 4 and 36, respectively.

We know that $RM_2(G) = \sum_{e,e' \in E(G)} d(e)d(e')$, i.e.,

$$\begin{aligned} RM_2(G^*) &= \mid d(2) \cdot d(4) \mid \cdot 2 \cdot 4 + \mid d(3) \cdot d(3) \mid \cdot 3 \cdot 3 + \mid d(3) \cdot d(4) \mid \cdot 3 \cdot 4 \\ &+ \mid d(3) \cdot d(5) \mid \cdot 3 \cdot 5 + \mid d(3) \cdot d(6) \mid \cdot 3 \cdot 6 + \mid d(4) \cdot d(4) \mid \cdot 4 \cdot 4 \\ &+ \mid d(4) \cdot d(5) \mid \cdot 4 \cdot 5 + \mid d(4) \cdot d(6) \mid \cdot 4 \cdot 6 + \mid d(5) \cdot d(6) \mid \cdot 5 \cdot 6 \\ &+ \mid d(6) \cdot d(6) \mid \cdot 6 \cdot 6 \\ &= 5856. \end{aligned}$$

For n unit, $RM_2(G^*) = 5856n$.

□

Lemma 8. *The reformulated F-index of G^* is $RF(G^*) = 16616n$.*

Proof. Appyling the formula $RF(G) = \sum_{uv \in E(G)} d(uv)^3$ to the proof of $RM_1(G^*)$, we get the result. □

Lemma 9. *The Banhatti indices of G^* are $B_1(G^*) = 2352n$, $B_2(G^*) = 4192n$.*

Proof. We know that $B_1(G) = \sum_{u,e} d_G(u) + d(e)$, i.e.,

$$\begin{aligned} B_1(G^*) &= 4[(2+1)+(2+3)] + 102[(3+1)+(3+4)] + 6[(3+2)+(3+3)] \\ &+ 16[(4+3)+(4+3)] + 4[(5+3)+(5+4)] + 42[(6+4)+(6+4)] \\ &= 2352. \end{aligned}$$

For n unit, $B_1(G^*) = 2352n$.

We know that $B_2(G) = \sum_{u,e} d_G(u) \cdot d(e)$, so by similar methods to the proof of $B_1(G^*)$, we get the desired result. □

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