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ANGULAR GEOMETRIC INDICES

Mehmet Şerif Aldemir, Süleyman Ediz, Kerem Yamaç

ABSTRACT

Topological indices (TIs) are important tools for analyzing the nature of biological and chemical networks. There are five types of TIs: Degree based TIs, distance based TIs, eigenvalue based TIs, matching based TIs and mixed TIs. Degree based TIs are defined by using classical degree concept in graph theory. The Zagreb and Randić TIs are the most used TIs in literature. Angular geometric graph, geometric degree and angle degree notions have been defined recently in graph theory. The angles between the atoms (vertices) and bonds (edges) are important in biology and chemistry but are not important in graph theory. In this respect, angular geometric graphs, in which the angles within this graph are important and unalterable, represent more realistic model for biological and chemical networks and molecular structures. In this study, we firstly defined angular geometric Zagreb and angular geometric Randić TIs by using geometric degree notion. We compare these novel TIs with their classical degree based counterparts TIs for the prediction of some chemical properties of octanes. It is shown that the newly defined angular geometric indices do not give a higher correlation coefficients than their classical counterparts and not suitable for QSPR researches.

1. INTRODUCTION

Chemical graph theory is considered to be the intersection of graph theory and chemistry. Topological indices constitute a significant part of the chemical

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graph theory. A topological index is a derived numeric value of a graph. The value of a topological index depends on how accurately model physical and chemical properties of molecules. Topological indices (TIs) are important tools for analyzing the nature of biological and chemical networks. There are five types of TIs: Degree based TIs, distance based TIs, eigenvalue based TIs, matching based TIs and mixed TIs. Degree based TIs are defined by using classical degree concept in graph theory. The Zagreb and Randić TIs are the most used TIs in literature [**1, 2, 3**]. Angular geometric graph, geometric degree and angular degree notions have been defined recently in graph theory [**4**]. The author in [**4**] investigated the geometric degrees of the Cartesian product of two paths and a path with a cycle. The angles between the atoms (vertices) and bonds (edges) are important in biology and chemistry but are not important in graph theory. In this respect, angular geometric graphs, in which the angles within this graph are important and unalterable, represent more realistic model for biological and chemical networks and molecular structures. In this study, we firstly defined angular geometric Zagreb and angular geometric Randić TIs by using geometric degree notion. We compare these novel TIs with their classical degree based counterparts TIs for the prediction of some chemical properties of octanes.

2. ANGULAR GEOMETRIC INDICES

We consider only connected graphs throughout this paper. For undefined terminology, we referred to the reference [**5**]. Let G be a graph with the vertex set $V(G)$, the edge set $E(G)$ and $v \in V(G)$. The degree of a vertex $v \in V(G)$, $deg(v)$, equals the number of edges incident to v that is the cardinality of the set $N(v) = \{u | uv \in E(G)\}$. P_n and C_n showed the path and cycle, respectively.
The first Zagreb and the second Zagreb index of the graph G are defined as:

(1) $$M_1 = M_1(G) = \sum_{v \in V(G)} d_v^2$$

and

(2) $$M_2 = M_2(G) = \sum_{uv \in E(G)} d_u \, d_v$$

respectively. In 1972, the quantities M_1 and M_2 were found to occur within certain approximate expressions for the total π-electron energy [**2**]. For details of the mathematical theory and chemical applications of the Zagreb indices, see the surveys [**6, 7**]. Randić is defined as;

(3) $$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Definition 1. *[**4**] An angular geometric graph denoted as AGG is a graph in which given angles between vertices and edges can not be changed. If the angles are not* *given spesifically in an angular geometric graph, all the angles are considered to be equal.*

Definition 2. *[4] Let AGG be an angular geometric graph and $v \in AGG$. The sum of the sines of the all angles of the vertex v is called the angular degree of v and denoted as $ang(v)$.*

Definition 3. *[4] Let AGG be an angular geometric graph and $v \in AGG$. The sum of the degree of the vertex v and the angular degree of the vertex v is called the geometric degree of v and denoted as $geom(v)$. That is $geom(v) = deg(v) + ang(v)$.*

Definition 4. *The first and second angular geometric Zagreb indices, GM_1 and GM_2, of an angular geometric graph defined as;*

$$GM_1 = GM_1(AAG) = \sum_{v \in V(AAG)} geom(v)^2 \tag{4}$$

and

$$GM_2 = GM_2(AAG) = \sum_{uv \in E(AAG)} geom(u)\, geom(v) \tag{5}$$

Definition 5. *Angular geometric Randić index of an angular geometric graph defined as;*

$$GR = GR(AAG) = \sum_{uv \in E(AAG)} \frac{1}{\sqrt{geom(u)geom(v)}}. \tag{6}$$

3. RESULTS AND DISCUSSION

In this section we compare the novel angular geometric indices with the well-known the classical corresponding indices by using strong correlation coefficients acquired from the chemical graphs of octane isomers. We get the experimental results at the www.moleculardescriptors.eu (see Table 1). The following physicochemical features have been modeled: Entropy (E), Acentric factor (AF), Enthalpy of vaporization (HV), Standard enthalpy of vaporization (SEV). We select those physicochemical properties of octane isomers for which give reasonably good correlations. Also we find the the Zagreb and Randić indices of octane isomers values at the www.moleculardescriptors.eu (see Table 2). We also calculate and show the novel angular geometric indices of octane isomers values in Table 2. Correlation analysis of the indices are given in Table 4.

It can be seen from the Table 3 that the newly defined angular geometric indices did not give a higher correlation coefficients than their classical counterparts.

Table 1: Some physicochemical properties of octane isomers.

Molecule	E	AF	HV	SEV
n-octane	111.70	0.39790	73.19	9.915
2-methyl-heptane	109.80	0.37792	70.30	9.484
3-methyl-heptane	111.30	0.37100	71.30	9.521
4-methyl-heptane	109.30	0.37150	70.91	9.483
3-ethyl-hexane	109.40	0.36247	71.70	9.476
2,2-dimethyl-hexane	103.40	0.33943	67.70	8.915
2,3-dimethyl-hexane	108.00	0.34825	70.20	9.272
2,4-dimethyl-hexane	107.00	0.34422	68.50	9.029
2,5-dimethyl-hexane	105.70	0.35683	68.60	9.051
3,3-dimethyl-hexane	104.70	0.32260	68.50	8.973
3,4-dimethyl-hexane	106.60	0.34035	70.20	9.316
2-methyl-3-ethyl-pentane	106.10	0.33243	69.70	9.209
3-methyl-3-ethyl-pentane	101.50	0.30690	69.30	9.081
2,2,3-trimethyl-pentane	101.30	0.30082	67.30	8.826
2,2,4-trimethyl-pentane	104.10	0.30537	64.87	8.402
2,3,3-trimethyl-pentane	102.10	0.29318	68.10	8.897
2,3,4-trimethyl-pentane	102.40	0.31742	68.37	9.014
2,2,3,3-tetramethylbutane	93.06	0.25529	66.20	8.410

Table 2: Topological indices of octane isomers.

Molecule	M_1	M_2	R	GM_1	GM_2	GR
n-octane	26	24	3.914	56	51	2.821
2-methyl-heptane	28	26	3.770	70.338	57.990	2.666
3-methyl-heptane	28	27	3.808	70.338	63.186	2.732
4-methyl-heptane	28	27	3.808	70.338	63.186	2.732
3-ethyl-hexane	28	28	3.846	73.338	68.382	2.220
2,2-dimethyl-hexane	32	30	3.561	95	69	1.642
2,3-dimethyl-hexane	30	30	3.681	84.676	76.926	2.601
2,4-dimethyl-hexane	30	29	3.664	84.676	70.176	2.577
2,5-dimethyl-hexane	30	28	3.626	84.676	64.980	2.511
3,3-dimethyl-hexane	32	32	3.621	95	79	2.603
3,4-dimethyl-hexane	30	31	3.719	84.676	82.123	2.666
2-methyl-3-ethyl-pentane	30	31	3.719	84.676	82.123	2.666
3-methyl-3-ethyl-pentane	32	34	3.682	95	89	2.697
2,2,3-trimethyl-pentane	34	35	3.481	109.338	94.176	2.454
2,2,4-trimethyl-pentane	34	32	3.417	109.338	75.990	2.354
2,3,3-trimethyl-pentane	34	36	3.504	109.338	93.382	2.483
2,3,4-trimethyl-pentane	32	33	3.553	99.015	90.667	2.470
2,2,3,3-tetramethylbutane	38	40	3.250	134	112	2.246

4. CONCLUSIONS

Table 3: Correlation coefficients.

Index	E	AF	HV	SEV
M_1	-0.9543	-0.9731	-0.8860	-0.9361
M_2	-0.9410	-0.9864	-0.7281	-0.8118
R	0.9063	0.9043	0.9359	0.9580
GM_1	-0.9509	-0.9745	-0.8926	-0.9408
GM_2	-0.9005	-0.9468	-0.6308	-0.7241
GR	0.4371	0.3402	0.501	0.5103

We proposed novel angular geometric indices based on geometric degree concept which has been defined very recently in graph theory. It has been shown that these novel indices can not be used as predictive means in QSAR researches. Predictive power of these indices have been tested on by using some physicochemical properties of octanes. Acquired results show that these novel indices are not convenient to predict physico-chemical properties of octanes.

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Mehmet Şerif Aldemir
Faculty of Science, Van Yüzüncü Yıl University, Van, Turkey
msaldemir@yyu.edu.tr

Süleyman Ediz
Faculty of Education, Van Yüzüncü Yıl University, Van, Turkey
suleymanediz@yyu.edu.tr

Kerem Yamaç
Faculty of Education, Van Yüzüncü Yıl University, Van, Turkey
keremyamac@yahoo.com

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VE-DEGREES IN SOME GRAPH PRODUCTS

Süleyman Ediz, Bünyamin Şahin

ABSTRACT

Let G be a graph and v be a vertex of G. The *ve*-degree of the vertex v defined as the number of different edges incident to the vertices of the open neighborhood of v. In this study we investigate the *ve*-degrees in Cartesian, direct and strong products of two graphs.

1. INTRODUCTION

We consider only connected and simple graphs throughout this paper. Let G be a graph with the vertex set $V(G)$, the edge set $E(G)$ and $v \in V(G)$. The degree of a vertex $v \in V(G)$, $deg(v)$, equals the number of edges incident to v that is the cardinality of the set $N(v) = \{u|uv \in E(G)\}$. This set is named as "the open neighborhood of v". For the vertex v, n_v denotes the number of triangles which contain the vertex v. Let A and B be two non-empty sets. Then the Cartesian product of these sets is the set $A\Box B = \{(a,b)|a \in A \,\text{and}\, b \in B\}$. The Cartesian, direct and strong products of two graphs G and H have the vertex set $V(G)\Box V(H)$. The edge set of the Cartesian product of G and H is $E(G\Box H)= \{(a,b)(c,d)|a = c$ and $bd \in E(H)$ or $b = d$ and $ac \in E(G)\}$. The edge set of the direct product of G and H is $E(G \times H) = \{(a,b)(c,d)|ac \in E(G) \,\text{and}\, bd \in E(H)\}$. And the edge set of the strong product of G and H is $E(GH)= \{(a,b)(c,d)|a = c$ and $bd \in E(H)$ or $b = d$ and $ac \in E(G)$ or $ac \in E(G)$ and $bd \in E(H)\}$. Note that $E(GH) = E(G\Box H) \cup E(G \times H)$ and $E(G\Box H) \cap E(G \times H) = \emptyset$. The following Lemma 1 gives the degrees in above mentioned graph products.

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Lemma 1. *Let G and H be two graphs. Then;*
(a) $deg_{G\Box H}(a,b) = deg(a) + deg(b)$,
(b) $deg_{G\times H}(a,b) = deg(a)deg(b)$,
(c) $deg_{GH}(a,b) = deg(a) + deg(b) + deg(a)deg(b)$.

Very recently Chellali *et al* have published very seminal study about the novel two degree concepts: *ve*-degrees and *ev*-degrees in graph theory [**1**]. The authors defined these novel degree concepts in relation to the vertex-edge domination and the edge-vertex domination parameters[**2, 3, 4**]. And also, the authors defined the *ve*-regularity, the *ev*-regularity and investigated basic mathematical properties of *ev* and *ve* regularities of graphs [**1**]. The *ev*-degree and *ve*-degree topological indices have been defined and their basic mathematical properties have been investigated in [**5, 6**]. In this paper we investigate the *ve*-degrees in Cartesian, direct and strong product of two graphs.

2. THE VE-DEGREES IN GRAPH PRODUCTS

We firstly give some basic facts related to *ve*-degrees.

Definition 2. *[**1**] Let G be a connected graph and $v \in V(G)$. The ve-degree of the vertex v, $deg_{ve}(v)$, equals the number of different edges that incident to any vertex from the closed (or open) neighborhood of v.*

Definition 3. *[**1**] Let G be a connected graph and $e = uv \in E(G)$. The ev-degree of the edge e, $deg_{ev}(e)$, equals the number of vertices of the union of the closed (or open) neighborhoods of u and v.*

Lemma 4. *[**5**] Let G be a connected graph and $v \in V(G)$, then;*

$$deg_{ve}(v) = \sum_{u\in N(v)} deg(u) - n_v$$

where n_v denotes the number of triangles contain the vertex v.

And now, we begin to compute the *ve*-degrees in Cartesian product of two graphs.

Lemma 5. *Let G and H be two graphs. Then both G and H contain no triangle if and only if $G\Box H$ contains no triangle*

Proof. Let accept that G and H be two triangle-free graphs and $G\Box H$ contains a triangle, say $(a,u)(b,u)(c,u)$. Then absolutely abc must be a triangle in G. This is a contradiction. The same argument holds for the supposition that $(v,a)(v,b)(v,c)$ a triangle in $G\Box H$. The other part of the proof comes from the fact that if $G\Box H$ contains a triangle then either G or H must be contain a triangle. □

Lemma 6. *Let G and H be two connected graphs and $(a,b) \in G\Box H$. Then;*

$$n_{(a,b)} = n_a + n_b$$

Proof. Let auv be one of the triangle which contains the vertex a in G. Then $(a,b)(u,b)(v,b)$ must be a triangle in $G\Box H$ from the definition of Cartesian product of graphs. Similarly let brt be one of the triangle which contains the vertex b in H. Then $(a,b)(a,r)(a,t)$ must be a triangle in $G\Box H$. The same argument holds for the all triangles which contain the vertex a and the vertex b in G and H, respectively. From the Lemma 5 the desired result acquired. □

Proposition 7. *Let $(a,b) \in V(G\Box H)$. Then;*

$$\sum_{(c,d)\in N((a,b))} deg(c,d) = 2deg(a)deg(b) + deg_{ve}a + deg_{ve}b + n_a + n_b.$$

Proof. Let $N(a) = \{v_1, v_2, ..., v_n\}$ and $N(b) = \{u_1, u_2, ..., u_m\}$. From the definition of the Cartesian product of graphs, we can write that;

$$\sum_{(c,d)\in N((a,b))} deg(c,d) = \sum_{(a=c),d\in N(b)} deg(a,d) + \sum_{(b=d),c\in N(a)} deg(c,b)$$

$= deg(a,u_1) + deg(a,u_2) + ... + deg(a,u_m) + deg(b,v_1) + deg(b,v_2) + ... + deg(b,v_n)$
$= deg(a)deg(b) + \sum_{d\in N(b)} deg(d) + deg(b)deg(a) + \sum_{c\in N(a)} deg(c)$.
From the Lemma 4 we know that $\sum_{u\in N(v)} deg(u) = deg_{ve}(v) + n_v$. Therefore, from the last equality we get that;
$= 2deg(a)deg(b) + deg_{ve}a + deg_{ve}b + n_a + n_b$. □

Corollary 8. *Let $(a,b) \in V(G\Box H)$. Then;*

$$deg_{ve}(a,b) = deg_{ve}a + deg_{ve}b + 2deg(a)deg(b).$$

Proof. The proof comes from the Lemma 4, Lemma 6 and Proposition 7. □

And now we can investigate the ve-degrees in direct(tensor, kronocker) product of two arbitrary graphs. We know that the direct product of two graphs is connected as far as at least one of the two graphs contains an odd cycle. But here, we focus degree not connectivity.

Lemma 9. *Let G and H be two connected simple graphs. If both G and H contain triangles then $G \times H$ contains triangles.*

Proof. Clearly if both G and H contain no triangle then $G \times H$ must not contain no triangle. Let accept that G contain a triangle and H contain no triangle. Then we can said from the definition of the direct product of graphs that $G \times H$ contains no triangle. Let accept that both G and H contain exactly one triangle, say uvw and brt respectively. Then $(ub)(vr)(wt)$ and $(ub)(vt)(wr)$ are the corresponding triangles in $G \times H$. □

Lemma 10. *Let G and H be two connected graphs and $(a,b) \in G \times H$. Then;*

$$n_{(a,b)} = 2n_a n_b$$

Proof. Let $n_a = k$ and $n_b = l$ for the positive natural numbers $k, l > 0$. And let $u_1v_1w_1$, $u_2v_2w_2$, ..., $u_kv_kw_k$ be the triangles in G and $b_1r_1t_1$, $b_2r_2t_2$, ..., $b_lr_lt_l$ be the triangles in H. Then the pairs of triangles $(u_1b_1)(v_1r_1)(w_1t_1)$ and $(u_1b_1)(v_1t_1)(w_1r_1)$, $(u_1b_2)(v_1r_2)(w_1t_2)$ and $(u_1b_2)(v_1t_2)(w_1r_2)$,..., $(u_1b_l)(v_1r_l)(w_1t_l)$ and $(u_1b_l)(v_1t_l)(w_1r_l)$ are corresponding triangles of the triangle $u_1v_1w_1$. That is exactly there are $2l$ triangles in $G \times H$ for the the triangle $u_1v_1w_1$. The same argument holds for the other triangles of G. Therefore, there are exactly $2kl$ triangles in $G \times H$. □

Proposition 11. *Let $(a,b) \in V(G \times H)$. Then;*

$$\sum_{(c,d)\in N((a,b))} deg(c,d) = (deg_{ve}a + n_a)(deg_{ve}b + n_b)$$

Proof. Let $N(a) = \{v_1, v_2, ..., v_n\}$ and $N(b) = \{u_1, u_2, ..., u_m\}$. From the definition of the direct product of graphs, we can write that;

$$\sum_{(c,d)\in N((a,b))} deg(c,d) = \sum_{(c,d)\in N((a,b))} deg(c)deg(d)$$

$= (deg(v_1) + deg(v_2) + ... + deg(v_n))(deg(u_1) + deg(u_2) + ... + deg(u_m))$
From the Lemma 4 we know that $\sum_{u\in N(v)} deg(u) = deg_{ve}(v) + n_v$. Therefore, from the last equality we get that;
$= (deg_{ve}(a) + n_a)(deg_{ve}b + n_b)$. □

Corollary 12. *Let $(a,b) \in V(G \times H)$. Then;*

$$deg_{ve}(a,b) = (deg_{ve}a + n_a)(deg_{ve}b + n_b) - 2n_a n_b$$

Proof. The proof comes from the Lemma 4, Lemma 10 and Proposition 11. □

We begin to investigate *ve*-degrees in strong product of two graphs.

Lemma 13. *Let G and H be two connected graphs and $(a,b) \in GH$. Then;*

$$n_{(a,b)} = n_a(1 + |E(H)|) + n_b(1 + |E(G)|) + 2n_a n_b + 2deg(a)deg(b)$$

Proof. The triangles belong to $G \square H$ and $G \times H$ are in the GH. There are new two kind of triangles in GH. The first group consists of two Cartesian (product) edges and one direct (product) edge. And the second group consists of one Cartesian (product) edge and two direct (product) edges.
(a) *2 Cartesian 1 direct triangles*: Let $(a,b) \in GH$, $N(a) = \{v_1, v_2, ..., v_n\}$ and $N(b) = \{u_1, u_2, ..., u_m\}$. There are m four cycles such as; ab, au_1, v_1b, v_1u_1, ab, au_2, v_1b, v_1u_2,..., ab, au_m, v_1b, v_1u_m for the Cartesian product of the edges av_1 and bu_i for the $1 \leq i \leq m$. And the same argument holds for Cartesian product of all the

edges av_i and bu_j. Therefore, there are $nm = deg(a)deg(b)$ four cycles in $G\Box H$ including the vertex (a, b). Note that every four cycle consists of only the Cartesian product edges in GH has two triangles with two cartesian edges and one direct edges. For example there are two triangles, namely ab, v_1u_1, v_1b and ab, au_1, v_1b in the four cycle ab, au_1, v_1b, v_1u_1 in GH. Thus, there are $2deg(a)deg(b) = 2nm$ triangles with two Cartesian edges and one direct edge in GH including the vertex (a, b).

(b) *1 Cartesian 2 direct triangles*: Let $(a, b) \in GH$. If $n_a = n_b = 0$ then there is no any triangle with two direct edge and one Cartesian edge in GH. Let accept that $n_a = 1$, av_1v_2 be triangle in G and bu_1 be an edge of H. Note that the triangle ab, v_1u_1, v_2u_1 is the only triangle, which consists of two direct edge and one Cartesian edge in GH, contains the vertex (a, b). Therefore, there are $|E(H)|$ triangle, which consists of two direct edge and one Cartesian edge in GH, contains the vertex (a, b). Clearly if $n_a = k \geq 1$ then there are $k|E(H)|$ triangle, which consists of two direct edge and one Cartesian edge in GH, contain the vertex (a, b). The same argument of the vertex a holds for the vertex b. Thus, the proof is completed from these facts and Lemma 6 and Lemma 10. □

Proposition 14. *Let $(a, b) \in V(GH)$. Then;*
$\sum_{(c,d)\in N((a,b))} deg(c, d) = 2deg(a)deg(b) + deg_{ve}a + deg_{ve}b + (deg_{ve}a + n_a)(deg_{ve}b + n_b) + n_a + n_b$

Proof. We know that $E(GH) = E(G\Box H) \cup E(G \times H)$. From this and Propositions 7 and 11, we get the desired result. □

Corollary 15. *Let $(a, b) \in V(GH)$. Then;*
$deg_{ve}(a, b) = deg_{ve}a + deg_{ve}b + (deg_{ve}a + n_a)(deg_{ve}b + n_b) - 2n_an_b - n_a|E(H)| - n_b|E(G)|$

Proof. The proof comes from the Lemma 4, Lemma 13 and Proposition 14. □

3. CONCLUSION

There are many open problems related to *ve*-degrees for further studies. It can be interesting to compute the exact values of *ve*-degrees in some other graph operations.

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Süleyman Ediz
Faculty of Education, Van Yüzüncü Yıl University, Van, Turkey
suleymanediz@yyu.edu.tr

Bünyamin Şahin
Faculty of Science, Selçuk University, Konya, Turkey
shnbnymn25@gmail.com

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DEGREE BASED TOPOLOGICAL INDICES OF SANIDIC POLYAMIDES

Aysun YURTTAS

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.

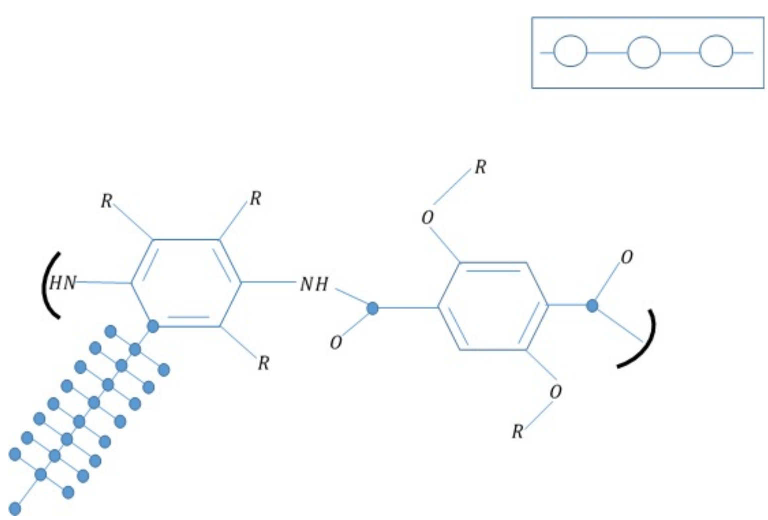

Figure 1: Sanidic Polyamide where $R = C_8H_{17}$.

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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Aysun YURTTAS
Faculty of Arts and Science
Department of Mathematics
Bursa Uludag University
16059 Bursa, TURKEY
ayurttas@uludag.edu.tr