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ANGULAR GEOMETRIC INDICES

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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:

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

and

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

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;

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

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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