QSPR Analysis of Degree-Based Topological Indices with physical properties of Benzenoid Hydrocarbons

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Abstract Benzenoid hydrocarbons are condensed polycyclic unsaturated fully conjugated hydrocarbons composed exclusively of six membered rings. Benzenoid system may be represented by different kinds of graphs. Each hexagon of a benzenoid or coronoid system may be represented by a single vertex. In this paper, we find the values of six important degree-based topological indices of molecular graph of benzenoid hydrocarbons. Further, we show that these parameters are highly correlated with physical properties of benzenoid hydrocarbons.

Keywords: Degree-based topological indices, Benzenoid hydrocarbons.

1. Introduction

Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u . The edge connecting the vertices u and v is denoted by uv [6].

Chemical graph theory is the branch of mathematical chemistry. It is concerned with handling chemical graphs that represent chemical system. Hence chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. It has found to be a useful tool in QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) [8, 10, and 13]. Numerous studies have been made relating to the above mentioned fields by using what are called topological indices. In 1975, Randic [11] proposed a topological index that has become one of the most widely used in both QSAR and QSPR studies.

It has remarked that mathematics is a more effective tool in the natural sciences than might be reasonably expected. Much of the current panorama of chemical theory has been created on foundations that are essentially graph-theoretical in nature. Chemical graphs are now being used for much different purpose in all the major branches in chemistry [1]. Recent studies have shown that the revived resonance theory successfully gives not only quantitative predictions on π -electronic properties of benzenoid hydrocarbons [17]. Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds. Some physical properties, such as the boiling point, are related to the geometric structure of the compound.

Benzenoid hydrocarbons are conveniently represented through benzenoid graphs made up of hexagons in whereas only two types of vertices appear, that is, vertices with degree 2 and vertices with degree 3 [2, 12]. This generates only three types of edges in benzenoids, that is, 22, 23 and 33 edges where the numerals are the degrees of vertices making up a given edge.

2. Selected Degree Based Topological Indices

We consider the following most studied degree based topological indices for QSPR study.

Randic Index: Historically, the first vertex-degree-based structure descriptors were the graph invariants that now a days are called Zagreb indices however, initially these were intended to be used for a completely different purpose and these were included among topological indices much later. The first genuine degree-based topological index was put-forward in 1975 by Milan Randic in his seminar paper “on characterization of molecular branching [11]” his index was defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}} \quad (1)$$

Harmonic Index: In the 1980s, Siemion Fajtlowicz [18] created computer program for automatic generation of conjectures in graph theory. Then he examined the possible relations between countless graph invariants, among which there was a vertex-degree-based quantity.

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)} \quad (2)$$

Geometric-Arithmetic Index: Another recently conceived vertex-degree based topological index utilizes the difference between the Geometric and Arithmetic means and is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} \quad (3)$$

Where of course, $\sqrt{d_G(u)d_G(v)}$ and $\frac{2}{d_G(u) + d_G(v)}$ are the Geometric and Arithmetic means respectively of the degrees of the end vertices of an edge. Recall that the former is always less than or equal to the later. The index was invented by Vukicevic [5] and was named “Geometric-Arithmetic index”.

Arithmetic-Geometric (AG_I) Index: Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u , then AG_I index [29, 32] of G is defined as

$$AG_I(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) \cdot d_G(v)}} \quad (4)$$

Where, AG_I index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v , where $d_G(u)$ (or $d_G(v)$) denote the degree of the vertex u (or v).

SK Index: The SK index [29, 32] of a graph $G = (V, E)$ is defined as

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2} \quad (5)$$

Where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G .

Sum Connectivity Index: The so called “sum connectivity index” is a recent invention by Bo Zhou and Nenad Trinajstić [3]. They noticed that in the definition of Randić’s branching index, there is no a prior reason for using the product $d_G(u) \times d_G(v)$ of vertex degrees, and this term may be replaced by the sum $d_G(u) + d_G(v)$. If so, then instead of Randić Index, one gets

$$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}} \quad (6)$$

For recent work on degree-based topological indices, we refer the interested reader to the articles [7, 19, 24, 28, 30, 31 and 33].

3. Data Sources and Analytical Method

Energy of benzenoid hydrocarbons are taken from [4, 9]. Eight physicochemical properties of benzenoid hydrocarbons have been selected on the availability of a suitable body of data: boiling point (BP), critical temperature (CT), critical pressure (CP), critical volume (CV), GE , $LogP$, MR , *Henry’s law*. The values are compiled in Table 2.

Fig.1. Molecular Graphs of benzenoid hydrocarbons

Table 1. The topological indices (Randic Index, Harmonic Index, GA Index, AG_1 Index, SK Index, and Sum Connectivity Index) values of benzenoid hydrocarbons.

S.NO.	Compound Name	R(G)	H(G)	GA(G)	AG_1 (G)	SK(G)	SCI(G)
1	Benzene	3	3	6	6	12	3
2	Naphthalene	4.9663	4.9333	10.9191	11.09	25	5.1971
3	Anthracene	6.9326	6.8666	15.8383	16.19	38	7.3942
4	Phenanthrene	6.9494	6.8999	15.8787	16.19	38	7.4080
5	Tetracene	8.8989	8.7999	20.7575	21.29	51	9.5913
6	Benzo[c]phenanthrene	8.9326	8.8666	20.8383	21.29	51	9.6189
7	Benzo[a]anthrene	8.9158	8.8333	20.7979	21.29	51	9.6051
8	Chrysene	8.9326	8.8666	20.8383	21.29	51	9.6189
9	Triphenylene	8.9494	8.8999	20.8787	21.14	51	9.6327
10	Pyrene	7.9326	7.8666	18.8383	18.17	44.5	8.6189
11	Pentacene	10.8653	10.7333	25.6767	26.39	64	11.7884
12	Benzo[a]tetracene	10.8821	10.7666	25.7171	26.39	64	11.8022
13	Dibenzo[a,h]anthracene	10.8989	10.7999	25.7575	26.39	64	11.8160
14	Dibenzo[a,j]anthracene	10.8989	10.7999	25.7575	26.39	64	11.8160
15	Pentaphene	10.8821	10.7666	25.7171	26.39	64	11.8022
16	Benzo[g]chrysene	10.9326	10.8666	25.8383	26.19	64	11.8436
17	Benzo[c]chrysene	10.9158	10.8333	25.7979	26.39	64	11.8298
18	Picene	10.9158	10.8333	25.7979	26.39	64	11.8298
19	Benzo[b]chrysene	10.8989	10.7999	25.7575	26.39	64	11.8160
20	Dibenzo[a,c]anthracene	10.9158	10.8333	25.7979	26.24	64	11.8298
21	Perylene	9.9326	9.8666	23.8383	24.19	60	10.8436
22	Benzo[e]pyrene	9.9326	9.8666	23.8383	24.19	60	10.8436
23	Benzo[a]pyrene	9.9158	9.8333	27.7979	24.24	60	10.8298
24	Benzo[ghi]perylene	10.9158	10.8333	26.7979	27.24	69	12.0546
25	Hexacene	12.8316	12.6666	30.5959	31.29	77	13.9855
26	Coronene	11.8989	11.7999	29.7575	30.29	78	13.2655

Table 2. The physical and chemical properties (*BP*, *CT*, *CP*, *CV*, *GE*, *LogP*, *MR*, *Henry's Law*) of benzenoid hydrocarbons.

S.N O.	Compound Name	<i>bp</i> °C	<i>CT</i>	<i>CP</i>	<i>CV</i>	<i>GE</i>	<i>Log</i> <i>P</i>	<i>MR</i>	<i>Henry</i> <i>'s</i> <i>Law</i>
1	Benzene	80.10	323.79	47.69	263.5	121.68	2.03	25.28	0.66
2	Naphthalene	218	484.95	38.97	409.5	252.38	3.03	42.45	1.67
3	Anthracene	340	586.11	32.43	555.5	383.08	4.03	59.62	2.68
4	Phenanthrene	340	586.11	32.43	555.5	383.08	4.03	59.62	2.68
5	Tetracene	432.0 2	650.8	27.41	701.5	513.78	5.9	76.79	3.69
6	Benzo[c]phenanthrene	436.7	650.8	27.41	701.5	513.78	5.03	76.79	3.69
7	Benzo[a]anthrene	438	650.8	27.41	701.5	513.78	5.03	76.79	3.69
8	Chrysene	448	650.8	27.41	701.5	513.78	5.03	76.79	3.69
9	Triphenylene	438	650.8	27.41	701.5	513.78	5.03	76.79	3.69
10	Pyrene	404	625.65	30.73	619.5	491.18	5.08	68.36	3.47
11	Pentacene	524.6	714.53	23.47	847.5	644.48	6.02	93.96	4.7
12	Benzo[a]tetracene	547.5	714.53	23.47	847.5	644.48	6.02	93.96	4.7
13	Dibenzo[a,h]anthracene	524	714.53	23.47	847.5	644.48	6.02	93.96	4.7
14	Dibenzo[a,j]anthracene	524.7	714.53	23.47	847.5	644.48	6.02	93.96	4.7
15	Pentaphene	547.5	714.53	23.47	847.5	644.48	6.02	93.96	4.7
16	Benzo[g]chrysene	525	714.53	23.47	847.5	644.48	6.02	93.96	4.7
17	Benzo[c]chrysene	524.7	714.53	23.47	847.5	644.48	6.02	93.96	4.7
18	Picene	520	714.53	23.47	847.5	644.48	6.02	93.96	4.7
19	Benzo[b]chrysene	524.7	714.53	23.47	847.5	644.48	6.02	93.96	4.7
20	Dibenzo[a,c]anthracene	518	714.53	23.47	847.5	644.48	6.02	93.96	4.7
21	Perylene	400	689.17	26.08	765.5	621.88	5.34	85.53	4.48
22	Benzo[e]pyrene	467.5	689.17	26.08	765.5	621.88	5.34	85.53	4.48
23	Benzo[a]pyrene	495	689.17	26.08	765.5	621.88	5.34	85.53	4.48
24	Benzo[ghi]perylene	500	728.06	24.85	829.5	729.98	5.66	94.28	5.27
25	Hexacene	604	779.67	20.33	993.5	775.18	7.02	111.13	5.71
26	Coronene	525	767.68	23.7	893.5	838.08	5.98	103.02	6.06

Table 3. Correlation of topological indices with physicochemical properties of benzenoid hydrocarbons.

	<i>bp</i> °C	<i>CT</i>	<i>CP</i>	<i>CV</i>	<i>GE</i>	<i>LogP</i>	<i>MR</i>	<i>Henry's Law</i>
<i>RI</i>	0.975	0.979	-0.977	0.999	0.980	0.972	1	0.985
<i>HI</i>	0.975	0.979	-0.977	0.999	0.980	0.972	1	0.985
<i>GA</i>	0.961	0.970	-0.957	0.982	0.985	0.948	0.987	0.987
<i>AG₁</i>	0.967	0.977	-0.969	0.995	0.988	0.962	0.998	0.991
<i>SK</i>	0.955	0.975	-0.957	0.987	0.996	0.950	0.994	0.998
<i>SCI</i>	0.972	0.979	-0.973	0.997	0.986	0.969	1	0.990

4. Results and Discussion

Table 3, the correlation coefficient of topological indices with physicochemical properties of benzenoid hydrocarbons are found to be good.

4.1. Regression Models:

We have tested the following linear regression model

$$P = A + B (TI) \quad (7)$$

Where, P = Physical property, TI = topological index.

Using (7), we have obtained the following different linear models for each degree-based topological index, which are listed below.

1. Randic Index ($R(G)$) :

$$bp = 0.9431 + 0.0189 R(G) \quad (8)$$

$$CT = -5.6908 + 0.0229 R(G) \quad (9)$$

$$CP = 19.529 - 0.3693 R(G) \quad (10)$$

$$CV = -0.5996 + 0.0136 R(G) \quad (11)$$

$$GE = 1.6679 + 0.0138 R(G) \quad (12)$$

$$LogP = -1.0664 + 1.9883 R(G) \quad (13)$$

$$MR = 0.0979 + 0.1149 R(G) \quad (14)$$

$$Henry's\ law = 2.0762 + 1.8196 R(G) \quad (15)$$

2. Harmonic Index ($H(G)$) :

$$bp = 0.9714 + 0.0187 H(G) \quad (16)$$

$$CT = -5.5878 + 0.0226 H(G) \quad (17)$$

$$CP = 19.326 - 0.3648 H(G) \quad (18)$$

$$CV = -0.5552 + 0.0135 H(G) \quad (19)$$

$$GE = 1.6793 + 0.0137 H (G) \quad (20)$$

$$\text{LogP} = -1.009 + 1.9624 H (G) \quad (21)$$

$$MR = 0.1325 + 0.1135 H (G) \quad (22)$$

$$\text{Henry's law} = 2.0833 + 1.7982 H (G) \quad (23)$$

3. Geometric-arithmetic Index (GA(G)) :

$$bp = 0.781 + 0.0482 GA (G) \quad (24)$$

$$CT = -16.364 + 0.0586 GA (G) \quad (25)$$

$$CP = 47.994 - 0.9357 GA (G) \quad (26)$$

$$CV = -3.0828 + 0.0346 GA (G) \quad (27)$$

$$GE = 2.2327 + 0.0359 GA (G) \quad (28)$$

$$\text{LogP} = -4.0452 + 5.0108 GA (G) \quad (29)$$

$$MR = -1.4126 + 0.2932 GA (G) \quad (30)$$

$$\text{Henry's law} = 3.3398 + 4.7156 GA (G) \quad (31)$$

4. AG₁ Index (AG₁ (G)) :

$$bp = 0.5954 + 0.0492 AG_1 (G) \quad (32)$$

$$CT = -16.959 + 0.0599 AG_1 (G) \quad (33)$$

$$CP = 48.96 - 0.9613 AG_1 (G) \quad (34)$$

$$CV = -3.5531 + 0.0356 AG_1 (G) \quad (35)$$

$$GE = 2.1308 + 0.0366 AG_1 (G) \quad (36)$$

$$\text{LogP} = -4.5821 + 5.1622 AG_1 (G) \quad (37)$$

$$MR = -1.7856 + 0.301 AG_1 (G) \quad (38)$$

$$\text{Henry's law} = 3.2362 + 4.8071 AG_1 (G) \quad (39)$$

5. SK Index (SK (G)) :

$$bp = -1.8424 + 0.127 SK (G) \quad (40)$$

$$CT = -48.149 + 0.1516 SK (G) \quad (41)$$

$$CP = 122.9 - 2.4803 SK (G) \quad (42)$$

$$CV = -12.87 + 0.0923 SK (G) \quad (43)$$

$$GE = 0.9974 + 0.0963 SK (G) \quad (44)$$

$$\text{LogP} = -15.208 + 13.314 SK (G) \quad (45)$$

$$MR = -8.4873 + 0.7823 SK (G) \quad (46)$$

$$\text{Henry's law} = 3.9951 + 12.631 SK (G) \quad (47)$$

6. Sum connectivity Index (SCI (G)) :

$$bp = 0.7035 + 0.0212 SCI (G) \quad (48)$$

$$CT = -6.8131 + 0.0258 SCI (G) \quad (49)$$

$$CP = 21.532 + 0.4139 SCI (G) \quad (50)$$

$$CV = -1.0492 + 0.0153 SCI (G) \quad (51)$$

$$GE = 1.4258 + 0.0157 SCI (G) \quad (52)$$

$$\text{LogP} = -1.5481 + 2.2281 SCI (G) \quad (53)$$

$$MR = -0.2823 + 0.1292 SCI (G) \quad (54)$$

$$\text{Henry's law} = 1.8954 + 2.0581 SCI (G) \quad (55)$$

Table 4. Statistical parameters for the linear QSPR model for $R(G)$.

Physical Properties	N	a	b	r	R^2	S	F
Boiling point	26	0.9431	0.0189	0.975	0.951	0.490	470.31
Critical temperature	26	-5.6908	0.0229	0.979	0.958	0.458	542.78
Critical Pressure	26	19.529	-0.3693	-0.977	-0.954	0.475	502.1
Critical volume	26	-0.5996	0.0136	0.999	0.998	0.098	1.225
GE	26	1.6679	0.0138	0.980	0.961	0.442	583.65
LogP	26	-1.0664	1.9883	0.972	0.946	0.518	418.37
MR	26	0.0979	0.1149	1	1	0.019	3.061
Henry's law	26	2.0762	1.8196	0.985	0.975	0.385	776.62

Table 5. Statistical parameters for the linear QSPR model for $H(G)$.

Physical Properties	N	a	b	R	R^2	S	F
Boiling point	26	0.9714	0.0187	0.975	0.950	0.489	459.89
Critical temperature	26	-5.5878	0.0226	0.979	0.958	0.451	544.33
Critical Pressure	26	19.326	-0.3648	-0.977	0.954	0.470	500.56
Critical volume	26	-0.5552	0.0135	0.999	0.998	0.107	1.005
GE	26	1.6793	0.0137	0.980	0.961	0.432	596.17
LogP	26	-1.009	1.9624	0.972	0.944	0.520	404.85
MR	26	0.1325	0.1135	1	1	0.358	9.011
Henry's law	26	2.0833	1.7982	0.985	0.971	0.376	794.96

Table 6. Statistical parameters for the linear QSPR model for $GA(G)$.

Physical Properties	N	a	b	r	R^2	S	F
Boiling point	26	0.781	0.0482	0.961	0.924	1.589	290.56
Critical temperature	26	-16.364	0.0586	0.970	0.941	1.393	385.51
Critical Pressure	26	47.994	-0.9357	-0.957	0.916	1.664	263.11
Critical volume	26	-3.0828	0.0346	0.982	0.964	1.092	641.53
GE	26	2.2327	0.0359	0.985	0.969	1.006	760.35
LogP	26	-4.0452	5.0108	0.948	0.898	1.834	212.13
MR	26	-1.4126	0.2932	0.987	0.974	0.928	897.84
Henry's law	26	3.3398	4.7156	0.987	0.974	0.921	911.29

Table 7. Statistical parameters for the linear QSPR model for $AG_l(G)$.

Physical Properties	N	a	B	R	R^2	S	F
Boiling point	26	0.5954	0.0492	0.967	0.935	1.493	343.10
Critical temperature	26	-16.959	0.0599	0.977	0.955	1.239	508.97
Critical Pressure	26	48.96	-0.9613	-0.969	0.939	1.440	370.84
Critical volume	26	-3.5531	0.0356	0.995	0.990	0.570	2.496
GE	26	2.1308	0.0366	0.988	0.976	0.907	970.65
LogP	26	-4.5821	5.1622	0.962	0.926	1.592	299.04
MR	26	-1.7856	0.301	0.998	0.997	0.329	7.530
Henry's law	26	3.2362	4.8071	0.991	0.983	0.761	1.389

Table 8. Statistical parameters for the linear QSPR model for $SK(G)$.

Physical Properties	N	a	b	R	R ²	S	F
Boiling point	26	-1.8424	0.127	0.955	0.911	4.545	246.25
Critical temperature	26	-48.149	0.1561	0.975	0.950	3.412	455.56
Critical Pressure	26	122.9	-2.4803	-0.957	0.917	4.400	264.41
Critical volume	26	-12.87	0.0923	0.987	0.975	2.412	935.79
GE	26	0.9974	0.0963	0.996	0.991	1.420	2.744
LogP	26	-15.208	13.314	0.950	0.903	4.753	233.18
MR	26	-8.4873	0.7823	0.994	0.987	1.722	1.859
Henry's law	26	3.9951	12.631	0.998	0.995	1.056	4.983

Table 9. Statistical parameters for the linear QSPR model for $SCI(G)$.

Physical Properties	N	a	b	r	R ²	S	F
Boiling point	26	0.7035	0.0212	0.972	0.944	0.593	403.29
Critical temperature	26	-6.8131	0.0258	0.979	0.959	0.506	563
Critical Pressure	26	21.532	0.4139	-0.973	0.947	0.577	427.27
Critical volume	26	-1.0492	0.0153	0.997	0.994	0.190	4.106
GE	26	1.4258	0.0157	0.986	0.972	0.417	840.38
LogP	26	-1.5481	2.2281	0.969	0.938	0.623	363.73
MR	26	-0.2823	0.1292	1	0.999	0.074	2.721
Henry's law	26	1.8954	2.0581	0.990	0.980	0.352	1.185

By inspection of the data in Tables 4 to 9, it is possible to draw a number of conclusions for the given topological indices like invariants.

The QSPR study of Randic index reveals that $R(G)$ can be useful in predicting the boiling point, critical temperature, critical pressure, critical volume, GE, LogP, MR, Henry's law of benzenoid hydrocarbons also from Table 4, one can easily verify that Randic index shows good correlation with all physical properties of benzenoid hydrocarbons. We can see that the correlation coefficient value of $R(G)$ with physical properties of benzenoid hydrocarbons lies between 0.972 to 1. Further, the correlation coefficient value of Randic index is very high for the MR of benzenoid hydrocarbons with $r = 1$. Thus the QSPR study reveals that the Randic index is an useful tool in predicting the physical properties of benzenoid hydrocarbons.

The harmonic index did not attract anybody's attention, especially, not of chemists. No chemical applications of the harmonic index were reported so far, but knowing the present situation in the mathematical chemistry we here explore the chemical applications of harmonic index. Table 5, one can easily verify that Harmonic index shows good correlation with all physical properties of benzenoid hydrocarbons. Further, we can see that the correlation coefficient value of $H(G)$ with physical properties of benzenoid hydrocarbons lies between 0.972 to 1. Further, the correlation coefficient value of Harmonic index is very high for the MR of benzenoid hydrocarbons with $r = 1$. Thus the QSPR study reveals that the Harmonic index is a useful tool in predicting the physical properties of benzenoid hydrocarbons.

The QSPR study of Geometric-Arithmetic index reveals that $GA(G)$ can be useful in predicting the boiling point, critical temperature, critical pressure, critical volume, GE, LogP, MR, Henry's law of benzenoid hydrocarbons also from Table 6, one can easily verify that Geometric-Arithmetic index shows good correlation with all physical properties of benzenoid hydrocarbons. We can see that the correlation coefficient value of $GA(G)$ with physical properties of benzenoid hydrocarbons lies between 0.961 to 0.987. Further, the correlation coefficient value of Geometric-Arithmetic index is very high for the Henry's law of benzenoid hydrocarbons with $r = 0.987 \square 1$. Thus the QSPR study reveals that the Geometric-Arithmetic index is a useful tool in predicting the physical properties of benzenoid hydrocarbons.

Motivated by Geometric-Arithmetic index. Here we introduced a new topological index namely, Arithmetic-Geometric (AG_1) index. The QSPR study of Arithmetic-Geometric (AG_1) index reveals that $AG_1(G)$ can be useful in predicting the boiling point, critical temperature, critical pressure, critical volume, GE, LogP, MR, Henry's law of benzenoid hydrocarbons also from Table 7, one can easily verify that Arithmetic-Geometric (AG_1) index shows good correlation with all physical properties of benzenoid hydrocarbons. Further, we can see that the correlation coefficient value of $AG_1(G)$ with physical properties of benzenoid hydrocarbons lies between 0.962 to 0.998. Further, the correlation coefficient value of Arithmetic-Geometric (AG_1) index is very high for the MR of benzenoid hydrocarbons with $r = 0.998 \square 1$. Thus the QSPR study reveals that the Arithmetic-Geometric (AG_1) index is an useful tool in predicting the physical properties of benzenoid hydrocarbons.

Motivated by Harmonic index. Here we introduced a new topological index namely, SK index. The QSPR study of SK index reveals that the predicting power of SK index for the physical properties of benzenoid hydrocarbons is equally good as Arithmetic-Geometric

(AG₁) index. Table 8 the correlation coefficient value lies between 0.950 to 0.998. Surprisingly, we could that the correlation of SK index with Henry's law of benzenoid hydrocarbons is very high with correlation coefficient $r = 0.998 \approx 1$. Thus SK index found to be useful tool in predicting the physical properties of benzenoid hydrocarbons.

The QSPR study in Table 9 reveals that the predicting power of sum-connectivity index is very high compared to other degree-based topological indices. The correlation coefficient value lies between 0.969 to 1. Further, the correlation coefficient value of sum-connectivity index is very high for the MR of benzenoid hydrocarbons with $r = 1$. Thus the QSPR study reveals that the sum-connectivity index is an useful tool in predicting the physical properties of benzenoid hydrocarbons.

From practical point of view, topological indices for which the absolute values of correlation coefficient are less than 0.8 can be characterized as useless. Thus, the QSPR study of the six degree-based topological indices with physical properties of 26 benzenoid hydrocarbons helps us to characterize useful topological indices with absolute value of correlation coefficient lies between 0.950 to 1.

Fig.2. Correlation of Randic index with physicochemical properties of benzenoid hydrocarbons. **Fig.3.** Correlation of Harmonic index with physicochemical properties of benzenoid hydrocarbons.

Fig.4. Correlation of Geometric-Arithmetic index with physicochemical properties of benzenoid hydrocarbons.

Fig.5. Correlation of AG_1 index with physicochemical properties of benzenoid hydrocarbons.

Fig.6. Correlation of SK index with physicochemical properties of benzenoid hydrocarbons.

Fig.7. Correlation of Sum-Connectivity index with physicochemical properties of benzenoid hydrocarbons.

References

- [1] B. Bonchere , D. H. Rouvray , Chemical graph theory introduction and Fundamentals, Gordon and Breach Science Publishers, S. A. O. Favaron , M. Maheo, J.F. Scale, Some eigenvalue properties in graphs(conjectures of Graffiti - II), Discrete Math., 111, (1993), 197-220.
- [2] B. Lucic, N. Trinajstic, Bo Zhou, Comparison between the sum-connectivity index and product-connectivity index for benzenoid hydrocarbons, Chemical Physics Letters, 475 (2009), 146-148.
- [3] B. Zhou, N. Trinajstic, Sum-connectivity index, J. Math. Chem. 46, (2009), 1252.
- [4] C. A. Coulson, A. Streitwieser, Dictionary of π -Electron Calculations, Freeman, San Francisco, 1965.
- [5] D.Vukicevic, B.Furtula, Topological index based on the ratios of geometrical and arithmetical mean of end-vertex degrees of edges, J. Math. Chem. 26, (2009), 1369-1376.
- [6] F. Harary, Graph theory, Addison-Wesely, Reading mass (1969).
- [7] I. Gutman, Degree-based topological indices, Croat. Chem. Acta, 86, (2013), 251-361.
- [8] J. Devillers , A. T. Balban , Topological indices and related descriptors in QSAR and QSPR, Gordon and Breach Science Publishers, Amsterdam, Netherland, (1999).
- [9] J.R. Dias, Handbook of Polycyclic Hydrocarbons. Part A: Benzenoid Hydrocarbons, Elsevier, Amsterdam, 1987.
- [10] M. Randic, on characterization of molecular branching, J. Am. Chem.Soc. 97, (1975), 6609-6615.
- [11] M. Randic, on history of the Randic index and emerging hostility toward chemical graph theory, MATCH Commun. Math. Comput. Chem., 59, (2008), 5-124.
- [12] M. Randic, Quantitative Structure-Property Relationship: boiling point and planar benzenoids, New. J. Chem. 20,(1996),1001-1009.
- [13] M. Thakur, A. Thakur, P. V. Khadikar, QSAR study of benzene sulphonamide carbonic anhydrase inhibitors: Topological approach using Balban index, Bioorg. Med. Chem. 12(4), (2004), 789-793.
- [14] M.V.Diudea, I. Gutman, J.Lorentz, Molecular Topology, Babes-Bolyai University, Romania 2001.
- [15] Minati Kuanar, Saroj K Kuanar, Bijay K Mishra, Correlation of line graph parameters with physical properties of octane isomers, Indian Journal of Chemistry, 38A, (1999),525-528.
- [16] N.Trinajstic, Chemical Graph theory, CRC Press, Boca Raton (1992).
- [17] Noriko Ohkami, Haruo Hosoya, Topological dependency of the aromatic sextets in polycyclic benzenoid hydrocarbons. Recursive relation of the sextet polynomial,Theoret. Chem. Acta (Berl), 64, (1983), 153-170.
- [18] S. Fajtlowicz, Harmonic Index, Congr. Number. 60, (1987), 187.
- [19] S.M. Hosamani, Deepa. M.Perigidad, ShrutiY. Jamagoud Yallavva B. Maled and Sharada Gavade , QSPR Analysis of Certain Degree Based Topological Indices, Journal of Statistics Applications and Probability,2016(in press).
- [20] S.M. Hosamani, I.Gutman, Zagreb indices of transformation graphs and total transformation graphs, Appl.Math.Comput. 247, (2014), 1156-1160.
- [21] S.M. Hosamani, M.Krzywkowski, on the difference of Zagreb coindices of graph operations, Gulf Journal of Mathematics, 4(3), (2016), 36-41.

- [22] S.M. Hosamani, S.H. Malaghan, I.N. Cangul, The first geometric-arithmetic index of graph operations, *Advances and Applications in Mathematical Sciences*, 14(6), (2015), 155-163.
- [23] S.M.Hosamani, Computing Sanskrit index of certain nanostructures, *J.Appl. Math. Comput.*1-9, (2016).
- [24] S.M.Hosamani, Correlation of Domination Parameters with physico- chemical properties of Octane isomers, *Applied Mathematics and Nonlinear Sciences*, 1(2), (2016). 345-352.
- [25] Simge Öztunç, Ali Mutlu and Necdet Bildik, Computing Hypercrossed Complex Pairings in Digital Images, *Abstract and Applied Analysis*, 2013.
- [26] Simge Öztunç, Necdet Bildik and Ali Mutlu, The Construction of Simplicial Groups in Digital Images, *Journal of Inequalities and Applications*, 143,(2013), 1-13.
- [27] Simge Öztunç, Sultan İhtiyar, Properties of Soft Homotopy in Digital Images, *American Institute of Physics*, 1798, 020120 (2017), 1-9.
- [28] V.S Shigehalli, R.Kanabur, Degree Based Topological Indices of n-Heptane Isomers, *Jamal Academic Research Journal: An Interdisciplinary Special Issue* (2016), 235-238.
- [29] V.S. Shigehalli, R. Kanabur , New Version of Degree-Based Topological Indices of Certain nanotube, *Journal of Mathematical Nano science*, 6(1-2), (2016), 29-39.
- [30] V.S. Shigehalli, R. Kanabur , Arithmetic-Geometric indices of Path Graph, *Journal of Computer and Mathematical sciences*, 6(1), (2015), 19-24.
- [31] V.S. Shigehalli, R. Kanabur, Arithmetic-Geometric indices of some class of Graph, *Journal of Computer and Mathematical sciences*, 6(4),(2015), 194-199.
- [32] V.S. Shigehalli, R. Kanabur, Computation of New Degree-Based Topological Indices of Graphene, *Journal of Mathematics*, 2016.
- [33] V.S. Shigehalli, R.Kanabur, Correlation between the Arithmetic-Geometric Indices of n-heptane Alkane Isomers, *IOSR Journal of Mathematics(IOSR-JM)*,12(2) Ver.IV, (2016), 36-39.