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A Study Of Reverse Topological Indices And Their Importance In Chemical Sciences*

Gowtham Kelkere Jayanna†

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Abstract

The main objective of this paper is to find out how reverse topological indices can help in the studies of QSPR. We have defined new reverse topological indices named, reverse harmonic index, reverse randić index and reverse sombor index studied for the same. Further, we tested their predictive ability of some physiochemical properties of polycyclic aromatic hydrocarbons. Using this, we predicted boiling point(BP), entropy(S), acentric factor(ω), octanol-water partition coefficient $log\ P$, enthalpy of formation (RI) and Kovats retention index of benzenoid hydrocarbons(ΔH_f).

1 Introduction

The chemical graph theory is a new branch of mathematical chemistry, that combines graph theory and chemistry. The main idea of this new branch is to understand the structural properties of a molecular graph. Let $G = (V, E)$ be the molecular graph which is a finite, simple, and connected graph consisting of atoms as vertices and bonds of atoms as edges. Here the set $V(G)$ is called the vertex set, and $E(G)$ is called the edge set of G. The number of edges incident to the vertex, $v \in V(G)$ is known as the degree of a vertex v, and it is usually denoted by, $d_G(v)$. A topological index is a unique numerical quantity obtained from a molecular graph that characterizes its topology, and it can be easily computed for any chemical species with the help of simple mathematical tools. Nowadays, topological indices are more frequently used in $QSPR/QSAR$ studies. With the help of topological indices, it is proven that several physicochemical properties of molecules are to be well correlated, so with the good predictive ability, they are to be chosen to develop $QSAR$ models, and are found in [1, 2, 3, 4, 5]. There are many topological indices [6, 7] that help us to study physical, chemical reactivities, and biological properties. In [8] Wiener, introduced the concept of the topological index while working on boiling point. In this paper, we use the reverse vertex degree concept to find the boiling point, entropy, acentric factor, octanol-water partition coefficient, enthalpy of formation, and Kovats retention index of benzenoid hydrocarbons. Before moving to the sole of the paper, let us know some definition. In [9] Kulli introduced the concept of reverse vertex degree c_{v_i} of the vertex v_i, defined as $c_{v_i} = \Delta(G) - d_G(v_i) + 1$, where $\Delta(G)$ is the maximum degree of vertex among the vertices of a graph. Further studies of reverse topological indices are in [10, 11, 12, 13, 14, 15, 16].

The first and second reverse Zagreb indices are defined as follows:

$$CM_1(G) = \sum_{uv \in E(G)} (c_u + c_v) \quad \text{and} \quad CM_2(G) = \sum_{uv \in E(G)} (c_u \cdot c_v).$$

Now, the first and second reverse hyper-Zagreb indices are given by

$$HCM_1(G) = \sum_{uv \in E(G)} (c_u + c_v)^2 \quad \text{and} \quad HCM_2(G) = \sum_{uv \in E(G)} (c_u \cdot c_v)^2.$$

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†Department of Mathematics, University College of Science, Tumkur University, Tumakuru, Karnataka State, India

Benzenoid hydrocarbons	BP	S(Cal/mol K)	ω	$log\ P$	RI	ΔH_f (KJ/mol)
Naphthalene	218	79.38	0.302	3.3	200	150.6
Phenanthrene	338	93.79	0.394	4.46	300	209.1
Anthrancene	340.05	92.43	0.402	4.45	301.69	218.3
Chrysene	431	106.86	0.46	5.81	400	267.7
Tetraphene	425	108.22	0.46	5.76	398.5	276.9
Triphenylene	429	104.66	0.46	5.49	400	258.5
Naphthacene	440	105.47	0.46	5.76	408.3	286.1
Benzo[a]pyrene	496	111.85	-	6.13	453.44	279.9
Benzo[e]pyrene	493	110.46	-	6.44	450.73	289.1
Perylene	497	109.1	0.49	6.25	456.22	279.9
Anthanthrene	547	114.1	-	7.04	503.89	310.5
Benzo[ghi]perylene	542	114.1	-	6.63	501.32	301.3
Dibinz[a,h]anthracene	536	119.87	-	6.75	495.45	335.5
Dibinz[a,j]anthracene	531	119.87	-	6.54	489.8	335.5
Picene	519	119.87	0.54	7.11	500	326.3
Coronene	590	116.36	0.54	7.64	549.67	322.7
Benzo[c]phenanthrene	448	113.61	-	5.7	391.12	280.5
Pyrene	404	96.06	0.41	4.88	351.22	230.5
Dibenzo[a,e]pyrene	592	124.89	-	7.28	551.53	338.5
Dibenzo[a,h]pyrene	596	123.5	-	7.28	559.9	347.7
Dibenzo[a,i]pyrene	594	123.5	-	7.28	556.47	347.7
Dibenzo[a,l]pyrene	595	131.69	-	7.71	553	351.2

Table 1: Experimental values of some physiochemical properties of benzenoid hydrocarbons.

The F and F_1 reverse index of a molecular graph G is defined as

$$FC(G) = \sum_{uv \in E(G)} (c_u^2 + c_v^2) \quad \text{and} \quad FC_1(G) = \sum_{u \in V(G)} c_u^3.$$

The reverse Geometric-arithmetic index is defined as follows:

$$CGA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{c_u \cdot c_v}}{(c_u + c_v)}.$$

We introduce the idea of reverse Harmonic index($CH(G)$), reverse Randić index ($CR(G)$) and reverse Sombor index ($CS(G)$) as follow, respectively,

$$\begin{aligned} CH(G) &= \sum_{uv \in E(G)} \frac{2}{(c_u + c_v)}, \\ CR(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{c_u \cdot c_v}}, \\ CSO(G) &= \sum_{uv \in E(G)} \sqrt{c_u^2 + c_v^2}. \end{aligned}$$

RTI	BP	S	ω	$log\ P$	RI	ΔH_f
CM1	0.992221518	0.968990959	0.992299136	0.986560525	0.996551188	0.982671556
CM2	0.960465085	0.968990959	0.986891199	0.962069781	0.967876191	0.977833202
HCM1	0.954839185	0.970375662	0.948930967	0.958035132	0.961814338	0.967558131
HCM2	0.824384434	0.917909261	0.859261782	0.828853722	0.837268629	0.889165359
FC	0.966303297	0.94710966	0.974604429	0.975145476	0.972403138	0.964471977
FC1	0.940779108	0.939780619	0.973903107	0.956344393	0.950912101	0.961499564
CSO	0.983000629	0.956911613	0.992220158	0.971049755	0.98556331	0.964267301
CGA	0.932099249	0.86366657	0.971804543	0.941668348	0.93373525	0.861516205
CH	0.942692212	0.892029703	0.944656676	0.937838152	0.929634871	0.88230487
CR	0.956873944	0.87873695	0.946096514	0.957573391	0.95367325	0.891274414

Table 2: Correlation coefficients (R) between some physicochemical properties of benzenoid hydrocarbons and some well-known reverse vertex degree-based topological indices(RTI).

2 Methodology

Let $G = (V, E)$ be a graph with vertex and edge set as $V(G)$, and $E(G)$ respectively. In this paper, we use reverse edge partition to compute reverse vertex degree-based topological indices. The reverse edge partition depends on the reverse vertex degree of the end vertices of edges. With the help of Microsoft excel data analysis tools, we have done the regression analysis.

3 Results and Discussion

3.1 Chemical Significance of Some Well-Known and Newly Defined Reverse Vertex Degree-Based Topological Indices

In this section, we study the predictive potential of some physicochemical properties of polycyclic aromatic hydrocarbons for some well-known and newly defined reverse vertex degree-based topological indices with the help of a data set of 22 benzenoid hydrocarbons. Those data are collected from the given sources [17, 18, 19, 20, 21, 22, 23, 24, 25, 26] and $https://pubchem.ncbi.nlm.nih.gov$. The experimental data of some physicochemical properties of benzenoid hydrocarbons are shown in Table 1. The reverse topological indices of benzenoid hydrocarbons are computed and shown in Table 3. With the help of some well-known reverse vertex degree-based topological indices and newly defined reverse vertex degree-based topological indices we found, the correlation coefficient(R) for boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) of some benzenoid hydrocarbons. And are shown in the Table 2.Throughout this paper, we use symbols, N for the population, S_e for standard error of the estimate, F for F-values, and SF for significance F.

3.2 The Linear Regression Models for the First Reverse Zagreb Index(CM_1)

With help of data in the Table 1 and 3, in this subsection, the linear regression model for the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) are obtained.

$$
\begin{aligned}
BP &= -59.3696(\pm 15.420) + 7.5842(\pm 0.2127)CM_1,\\
N &= 22,\quad S_e = 12.6145,\quad F = 1270.6170,\quad SF = 1.4171 \times 10^{-19},\\
S &= -45.034(\pm 3.8137) + 0.9229(\pm 0.0526)CM_1,\\
N &= 22,\quad S_e = 3.11986,\quad F = 307.5653,\quad SF = 1.3053, \times 10^{-13},
\end{aligned}
$$

Benzenoid hydrocarbons	CM1	CM2	HCM1	HCM2	FC	FC1	CSO	CGA	CH	CR
Naphthalene	38	33	136	113	70	66	27.329	10.7712	6.6666	6.8284
Phenanthrene	52	43	178	139	98	84	37.458	15.6	10.5	10.7426
Anthrancene	52	42	144	130	92	84	37.6875	15.5424	10.3333	10.6568
Chrysene	66	53	220	165	114	102	47.587	20.5424	14.3333	14.6568
Tetraphene	66	52	218	156	114	102	47.8165	20.428	14.1666	14.571
Triphenylene	66	54	210	162	114	102	47.3575	20.6568	14.5	14.7426
Naphthacene	66	51	211	147	114	102	48.046	20.3137	14	14.4852
Benzo[a]pyrene	72	55	230	159	120	104	59.0591	23.428	17.1666	17.571
Benzo[e]pyrene	72	56	232	168	120	104	51.8296	23.5424	17.3333	17.6568
Perylene	72	56	232	168	120	104	51.8296	23.5427	17.3333	17.6568
Anthanthrene	78	57	240	153	126	106	56.5313	26.3137	20	20.4852
Benzo[ghi]perylene	78	58	242	162	126	106	56.3018	26.428	20.1666	20.571
Dibinz[a,h]anthracene	80	62	260	182	136	120	57.9455	25.3137	17	17.4852
Dibinz[a,j]anthracene	80	62	260	182	136	120	57.9455	17.7712	18	18.4852
Picene	80	63	262	191	136	120	57.716	25.428	18.1666	18.571
Coronene	84	60	252	152	152	132	60.7739	29.3137	23	23.4852
Benzo[c]phenanthrene	66	53	220	165	114	102	47.587	20.5424	18.3333	14.6568
Pyrene	58	45	188	133	98	86	41.9301	18.5424	13.3333	13.6568
Dibenzo[a,e]pyrene	86	66	274	194	142	122	61.9586	28.428	21.1666	20.071
Dibenzo[a,h]pyrene	86	62	260	182	136	120	62.1881	25.3137	17	17.4852
Dibenzo[a,i]pyrene	86	65	272	185	142	122	62.1881	28.3137	21	21.4852
Dibenzo[a,l]pyrene	86	66	272	185	142	122	61.9586	28.3137	21	21.4852

Table 3: Reverse topological indices of benzenoid hydrocarbons.

$$\begin{aligned}
\omega &= 0.1182(\pm 0.01394) + 0.00516(\pm 0.002)CM_1,\\
N &= 11, \quad S_e = 0.0089, \quad F = 577.6087, \quad SF = 1.7866, \times 10^{-9},\\
\log P &= -0.0672(\pm 0.2345) + 0.087(\pm 0.0032)CM_1,\\
N &= 22, \quad S_e = 0.1918, \quad F = 729.1105, \quad SF = 3.2822, \times 10^{-17},\\
RI &= -85.3297(\pm 10.0127) + 7.42(\pm 0.1381)CM_1,\\
N &= 22, \quad S_e = 8.1909, \quad F = 2884.558, \quad SF = 4.235 \times 10^{-25},\\
\Delta H_f &= 7.4541(\pm 12.0325) + 3.9363(\pm 0.1660)CM_1,\\
N &= 22, \quad S_e = 9.8432, \quad F = 562.1296, \quad SF = 4.1019 \times 10^{-16}.
\end{aligned}$$

3.3 The Linear Regression Models for the Second Reverse Zagreb Index(CM_2)

Now, we obtained the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for second Zagreb index(CM_2).

$$\begin{aligned}
BP &= -133.534(\pm 40.3379) + 11.1522(\pm 0.7228)CM_2,\\
N &= 22, \quad S_e = 28.2113, \quad F = 238.0418, \quad SF = 1.4298 \times 10^{-12},\\
S &= 32.6036(\pm 3.5356) + 1.4187(\pm 0.0633)CM_2,\\
N &= 22, \quad S_e = 2.4724, \quad F = 501.5608, \quad SF = 1.2329, \times 10^{-15},\\
\omega &= 0.0578(\pm 0.0215) + 0.0077(\pm 0.0004)CM_2,
\end{aligned}$$

$$N = 11, \quad S_e = 0.0116, \quad F = 336.5457, \quad SF = 1.9421, \times 10^{-8},$$
$$\log P = -0.97416(\pm 0.4579) + 0.1294(\pm 0.0082)CM_2,$$
$$N = 22, \quad S_e = 0.3202, \quad F = 240.7387, \quad SF = 9.5107, \times 10^{-13},$$
$$RI = -159.899(\pm 35.4865) + 10.9473(\pm 0.6358)CM_2,$$
$$N = 22, \quad S_e = 24.8182, \quad F = 296.3772, \quad SF = 1.8497, \times 10^{-13},$$
$$\Delta H_f = -39.9744(\pm 15.8990) + 5.9501(\pm 0.2841)CM_2,$$
$$N = 22, \quad S_e = 11.1193, \quad F = 436.1813, \quad SF = 4.7280 \times 10^{-15}.$$

3.4 The Linear Regression Models for the Second Reverse Zagreb Index(HCM_1)

Here, we obtained the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the second reverse Zagreb index(HCM_1).

$$BP = -72.5482(\pm 39.1076) + 2.4330(\pm 0.1692)HCM_1,$$
$$N = 22, \quad S_e = 30.1085, \quad F = 206.5464, \quad SF = 5.2832 \times 10^{-12},$$
$$S = 40.6891(\pm 3.9621) + 0.3080(\pm 0.0171)HCM_1,$$
$$N = 22, \quad S_e = 3.0504, \quad F = 322.6355, \quad SF = 8.3141 \times 10^{-14},$$
$$\omega = 0.1155(\pm 0.0378) + 0.0001(\pm 0.0001)HCM_1,$$
$$N = 11, \quad S_e = 0.0228, \quad F = 81.4249, \quad SF = 8.3572 \times 10^{-6},$$
$$\log P = -0.2771(\pm 0.4371) + 0.0282(\pm 0.0018)HCM_1,$$
$$N = 22, \quad S_e = 0.3365, \quad F = 223.4017, \quad SF = 2.5699 \times 10^{-12},$$
$$RI = -99.8116(\pm 35.0918) + 2.3874(\pm 0.1519)HCM_1,$$
$$N = 22, \quad S_e = 27.0172, \quad F = 246.9757, \quad SF = 1.0160 \times 10^{-12},$$
$$\Delta H_f = -6.0524(\pm 17.4267) + 1.2920(\pm 0.0754)HCM_1,$$
$$N = 22, \quad S_e = 13.4168, \quad F = 293.3261, \quad SF = 2.0385 \times 10^{-13}.$$

3.5 The Linear Regression Models for the Second Reverse Zagreb Index(HCM_2)

In this section, we obtained the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the second Zagreb index (HCM_2).

$$BP = -142.115(\pm 96.5774) + 3.8420(\pm 0.5898)HCM_2,$$
$$N = 22, \quad S_e = 57.3579, \quad F = 42.423, \quad SF = 2.3865 \times 10^{-16},$$
$$S = 24.3248(\pm 8.4353) + 0.5380(\pm 0.0515)HCM_2,$$
$$N = 22, \quad S_e = 5.0099, \quad F = 107.0304, \quad SF = 1.7815 \times 10^{-9},$$
$$\omega = 0.0333(\pm 0.0828) + 0.0027(\pm 0.0005)HCM_2,$$
$$N = 11, \quad S_e = 0.0369, \quad F = 25.3947, \quad SF = 0.7 \times 10^{-3},$$
$$\log P = -1.1008(\pm 1.1059) + 0.0447(\pm 0.0067)HCM_2,$$
$$N = 22, \quad S_e = 0.6568, \quad F = 43.8974, \quad SF = 1.8809 \times 10^{-6},$$
$$RI = -173.131(\pm 90.8793) + 3.8010(\pm 0.5550)HCM_2,$$
$$N = 22, \quad S_e = 53.9738, \quad F = 46.8638, \quad SF = 1.1789 \times 10^{-6},$$
$$\Delta H_f = -64.3353(\pm 40.9156) + 2.1716(\pm 0.2499)HCM_2,$$

$$N = 22, \quad S_e = 24.3000, \quad F = 75.5178, \quad SF = 3.1723 \times 10^{-8}.$$

3.6 The Linear Regression Models for the F Reverse Index(FC)

We obtained the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the F reverse index(FC).

$$\begin{aligned}
BP &= -111.212(\pm 35.7616) + 4.9014(\pm 0.2919)FC,\\
N &= 22, \quad S_e = 26.0839, \quad F = 281.8506, \quad SF = 2.9639 \times 10^{-13},\\
S &= 39.4634(\pm 5.5551) + 0.5985(\pm 0.0453)FC,\\
N &= 22, \quad S_e = 4.0518, \quad F = 174.2063, \quad SF = 2.4832 \times 10^{-11},\\
\omega &= 0.1082(\pm 0.0264) + 0.0030(\pm 0.0002)FC,\\
N &= 11, \quad S_e = 0.0162, \quad F = 170.4752, \quad SF = 3.7407 \times 10^{-8},\\
\log P &= -0.7665(\pm 0.3566) + 0.0573(\pm 0.0029)FC,\\
N &= 22, \quad S_e = 0.2601, \quad F = 387.4042, \quad SF = 1.4654 \times 10^{-14},\\
RI &= -137.176(\pm 31.5743) + 4.8047(\pm 0.2577)FC,\\
N &= 22, \quad S_e = 23.0297, \quad F = 347.43, \quad SF = 4.1264 \times 10^{-14},\\
\Delta H_f &= -21.8554(\pm 19.2348) + 2.5637(\pm 0.1570)FC,\\
N &= 22, \quad S_e = 14.0295, \quad F = 266.5584, \quad SF = 4.9935 \times 10^{-13}.
\end{aligned}$$

3.7 The Linear Regression Models for the F_1 Reverse Index(FC_1)

We obtained the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the F_1 reverse index(F_1C).

$$\begin{aligned}
BP &= -139.599(\pm 50.6099) + 5.8628(\pm 0.4724)FC_1,\\
N &= 22, \quad S_e = 34.3542, \quad F = 154.0119, \quad SF = 7.4901 \times 10^{-14},\\
S &= 33.5407(\pm 6.3572) + 0.7297(\pm 0.0593)FC_1,\\
N &= 22, \quad S_e = 4.3153, \quad F = 151.2147, \quad SF = 8.8162 \times 10^{-11},\\
\omega &= 0.0845(\pm 0.0285) + 0.0036(\pm 0.0002)FC_1,\\
N &= 11, \quad S_e = 0.0164, \quad F = 165.714, \quad SF = 4.2243 \times 10^{-7},\\
\log P &= -1.1516(\pm 0.5054) + 0.0690(\pm 0.0047)FC_1,\\
N &= 22, \quad S_e = 0.3431, \quad F = 214.1772, \quad SF = 3.7880 \times 10^{-12},\\
RI &= -167.702(\pm 45.0011) + 5.7725(\pm 0.4200)FC_1,\\
N &= 22, \quad S_e = 30.5469, \quad F = 188.842, \quad SF = 1.1965 \times 10^{-11},\\
\Delta H_f &= -44.494(\pm 21.4989) + 3.1401(\pm 0.2006)FC_1,\\
N &= 22, \quad S_e = 14.5935, \quad F = 244.8355, \quad SF = 1.1015 \times 10^{-12}.
\end{aligned}$$

3.8 The Linear Regression Models for the Reverse Harmonic Index(CH)

Here, we studied the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the reverse Geometric-arithmetic index(CH).

$$BP = 99.1192(\pm 31.1384) + 23.1013(\pm 1.8283)CH,$$

$$N = 22, \quad S_e = 33.8113, \quad F = 159.6438, \quad SF = 5.4370 \times 10^{-11},$$
$$S = 65.7657(\pm 5.2555) + 2.7237(\pm 0.3085)CH,$$
$$N = 22, \quad S_e = 5.7067, \quad F = 77.9033, \quad SF = 2.4717 \times 10^{-8},$$
$$\omega = 0.2354(\pm 0.0255) + 0.0148(\pm 0.0017)CH,$$
$$N = 11, \quad S_e = 0.0237, \quad F = 74.6246, \quad SF = 1.1924 \times 10^{-5},$$
$$\log P = 1.7560(\pm 0.3752) + 0.2662(\pm 0.0220)CH,$$
$$N = 22, \quad S_e = 0.4074, \quad F = 146.0308, \quad SF = 1.2012 \times 10^{-10},$$
$$RI = 76.5204(\pm 33.4974) + 22.1915(\pm 1.9668)CH,$$
$$N = 22, \quad S_e = 36.3728, \quad F = 127.2982, \quad SF = 4.0082 \times 10^{-10},$$
$$\Delta H_f = 100.6307(\pm 23.0193) + 11.3309(\pm 1.3516)CH,$$
$$N = 22, \quad S_e = 24.9953, \quad F = 70.2779, \quad SF = 5.6156 \times 10^{-8}.$$

3.9 The Linear Regression Models for the Reverse Randić Index(CR)

Now, we studied the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the reverse Randić index(CR).

$$BP = 90.5596(\pm 27.2692) + 23.4017(\pm 1.5886)CR,$$
$$N = 22, \quad S_e = 29.4377, \quad F = 216.9886, \quad SF = 3.3602 \times 10^{-12},$$
$$S = 66.1633(\pm 5.5825) + 2.6777(\pm 0.3252)CR,$$
$$N = 22, \quad S_e = 6.0265, \quad F = 67.7880, \quad SF = 7.4546 \times 10^{-8},$$
$$\omega = 0.2336(\pm 0.0253) + 0.0146(\pm 0.0016)CR,$$
$$N = 11, \quad S_e = 0.0234, \quad F = 76.7948, \quad SF = 1.0612 \times 10^{-5},$$
$$\log P = 1.6354(\pm 0.3134) + 0.2713(\pm 0.0182)CR,$$
$$N = 22, \quad S_e = 0.3383, \quad F = 220.8095, \quad SF = 2.8616 \times 10^{-12},$$
$$RI = 64.6816(\pm 27.5087) + 22.7196(\pm 1.6026)CR,$$
$$N = 22, \quad S_e = 29.6963, \quad F = 200.9766, \quad SF = 6.7840 \times 10^{-12},$$
$$\Delta H_f = 97.5498(\pm 22.3071) + 11.42315(\pm 1.2995)CR,$$
$$N = 22, \quad S_e = 24.0811, \quad F = 77.2621, \quad SF = 2.6416 \times 10^{-8}.$$

3.10 The Linear Regression Models for the Reverse Sombor Index(CSO)

In this section, we studied the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the reverse Sombor index(CSO).

$$BP = -48.9076(\pm 22.5196) + 10.2338(\pm 0.4274)CSO,$$
$$N = 22, \quad S_e = 18.6051, \quad F = 573.2999, \quad SF = 3.3909 \times 10^{-16},$$
$$S = 46.5139(\pm 4.4377) + 1.2412(\pm 0.0842)CSO,$$
$$N = 22, \quad S_e = 3.6663, \quad F = 217.1912, \quad SF = 3.3315 \times 10^{-12},$$
$$\omega = 0.1189(\pm 0.0139) + 0.0071(\pm 0.0002)CSO,$$
$$N = 11, \quad S_e = 0.0090, \quad F = 571.6767, \quad SF = 1.8704 \times 10^{-9},$$
$$logP = 0.0929(\pm 0.3394) + 0.1171(\pm 0.0064)CSO,$$

$$N = 22, \quad S_e = 0.2804, \quad F = 330.4937, \quad SF = 6.6232 \times 10^{-14},$$
$$RI = -74.1859(\pm 20.2286) + 9.9948(\pm 0.3839)CSO,$$
$$N = 22, \quad S_e = 16.7123, \quad F = 677.7159, \quad SF = 6.6872 \times 10^{-17},$$
$$\Delta H_f = 15.5078(\pm 17.0293) + 5.2609(\pm 0.3232)CSO,$$
$$N = 22, \quad S_e = 14.0691, \quad F = 264.9467, \quad SF = 5.2842 \times 10^{-13}.$$

3.11 The Linear Regression Models for the Reverse Geometric-Arithmetic Index(CG)

In this section, we studied the linear regression models of the boiling point(BP), entropy (S), acentric factor(ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) for the reverse Geometric-arithmetic index(CG).

$$BP = 56.6302(\pm 37.7686) + 18.9226(\pm 1.6442)CG,$$
$$N = 22, \quad S_e = 36.7033, \quad F = 132.4495, \quad SF = 2.8355 \times 10^{-10},$$
$$S = 61.7886(\pm 6.5490) + 2.1846(\pm 0.2851)CG,$$
$$N = 22, \quad S_e = 6.3643, \quad F = 58.7153, \quad SF = 2.2534 \times 10^{-7},$$
$$\omega = 0.1829(\pm 0.0219) + 0.0131(\pm 0.0001)CG,$$
$$N = 11, \quad S_e = 0.0170, \quad F = 152.882, \quad SF = 5.9647 \times 10^{-9},$$
$$\log P = 1.1904(\pm 0.4065) + 0.2214(\pm 0.0177)CG,$$
$$N = 22, \quad S_e = 0.3951, \quad F = 156.5837, \quad SF = 6.4625 \times 10^{-11},$$
$$RI = 29.2803(\pm 36.3602) + 18.4685(\pm 1.5828)CG,$$
$$N = 22, \quad S_e = 35.3346, \quad F = 136.0811, \quad SF = 2.2374 \times 10^{-10},$$
$$\Delta H_f = 82.3901(\pm 27.7455) + 9.1656(\pm 1.2078)CG,$$
$$N = 22, \quad S_e = 26.9629, \quad F = 57.8525, \quad SF = 2.6107 \times 10^{-7}.$$

We have noticed that the models obtained by using the first reverse Zagreb index ($CM1$), second reverse Zagreb index ($CM2$), first hyper reverse Zagreb index, and reverse Sombor index (CSO) are the best models to predicting the boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) of polycyclic aromatic hydrocarbons. The scatter plot of boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index with Randić index (R) are shown in Fig. 1, respectively. The scatter plot of boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f), and Kovats retention index with other reverse topological indices mentioned in this paper can be drawn similarly.

4 Physicochemical Properties of Some Benzenoid Hydrocarbons

Here in this section, we calculated boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) of some benzenoid hydrocarbons by using our desired models are shown in Table 4.

5 Conclusion

In this paper, we considered some well-known reverse vertex degree-based topological indices and have studied their predictive ability of some physicochemical properties of polycyclic aromatic hydrocarbons comparatively. Using these reverse indices, we have established the models for predicting boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f)

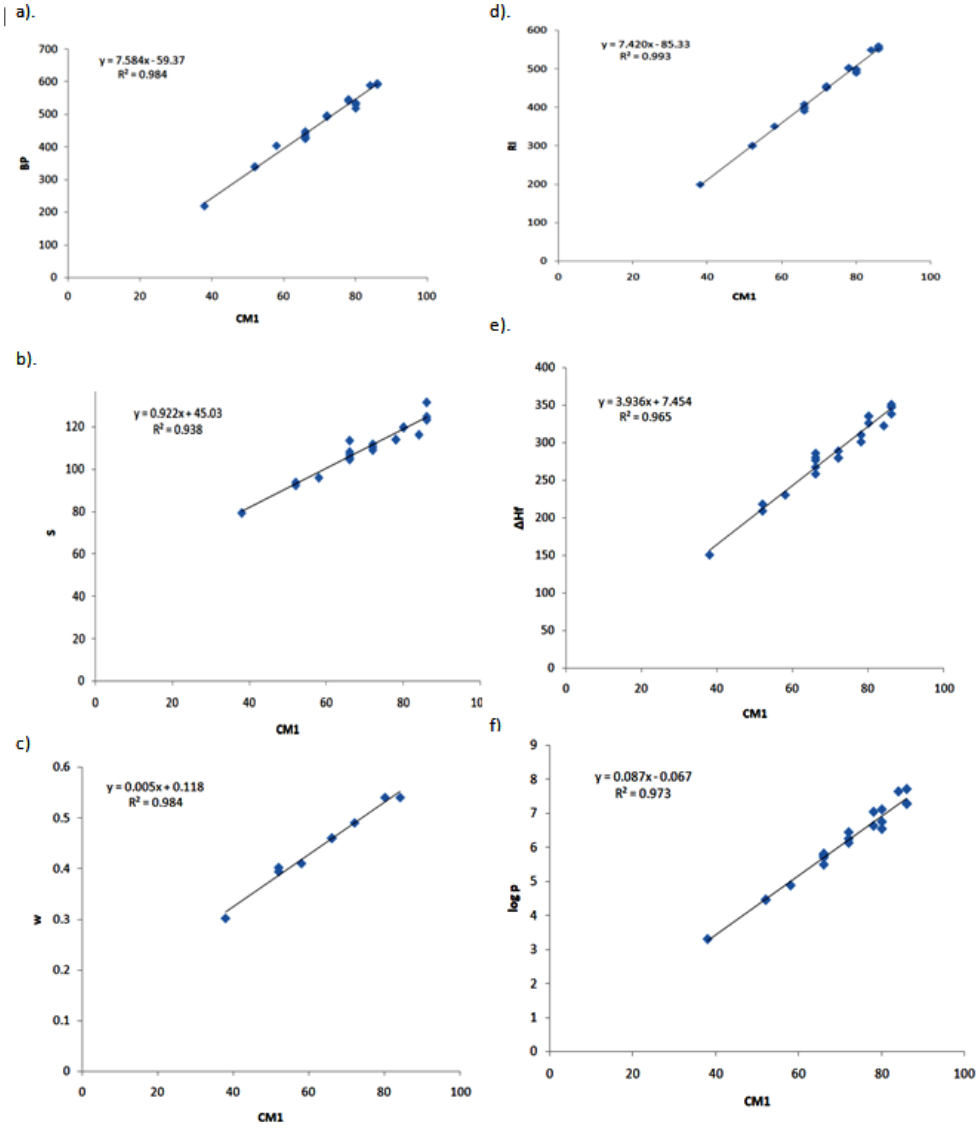

Figure 1: Scatter diagram of boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI).

Benzenoid hydrocarbons	BP	S	ω	$log\ P$	RI	ΔH_f
Pentaphene	547.35	118.79	0.518	6.893	508.27	322.3354
Benzo[b]chrysene	524.598	116.024	0.503	6.632	486.01	310.5274
Benzo[c]chrysene	547.35	118.79	0.518	6.893	508.27	322.3354
Pentacene	547.35	118.79	0.518	6.893	508.27	322.3354
Dibenzo[c,g]phenanthrene	547.35	118.79	0.518	6.893	508.27	322.3354
Benzo[a]naphthacene	532.182	116.946	0.508	6.719	493.43	314.4634
Dibenzo[a,j]naphthacene	653.526	131.698	0.588	8.111	612.15	377.4394
Dibenzo[a,l]naphthacene	653.526	131.698	0.588	8.111	612.15	377.4394
Dibenzo[a,c]naphthacene	668.694	133.542	0.598	8.285	626.99	385.3114
Dibenzo[a,l]pyrene	592.854	124.322	0.548	7.415	552.79	345.9514
Dibenzo[de,qr]naphthacene	592.854	124.322	0.548	7.415	552.79	345.9514
Dibenzo[g,p]chrysene	638.358	129.854	0.578	7.937	597.31	369.5674
Benzo[c]picene	653.526	131.698	0.588	8.111	612.15	377.4394
Benzo[ghi]perylene	517.014	115.102	0.498	6.545	478.59	306.5914
Dibenzo[b,k]chrysene	638.358	129.854	0.578	7.937	597.31	369.5674
Dibenzo[c,l]chrysene	653.526	131.698	0.588	8.111	612.15	377.4394
Benzo[b]perylene	592.854	124.322	0.548	7.415	552.79	345.9514
Dibenzo[de,mn]naphthacene	592.854	124.322	0.548	7.415	552.79	345.9514
Benzo[a]pentacene	653.526	131.698	0.588	8.111	612.15	377.4394

Table 4: Physiochemical properties (predicted) of some benzenoid hydrocarbons.

and Kovats retention index (RI) of polycyclic aromatic hydrocarbons. We have noticed that the models obtained by using the first reverse Zagreb index ($CM1$), second reverse Zagreb index ($CM2$), first hyper reverse Zagreb index, and reverse Sombor index (CSO) are the best models for predicting these properties of polycyclic aromatic hydrocarbons. That is, the predictive ability of boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f) and Kovats retention index (RI) of polycyclic aromatic hydrocarbons is approximately the same for the first reverse Zagreb index ($CM1$). The second reverse Zagreb index ($CM2$), first hyper reverse Zagreb index and reverse Sombor index (CSO) is also good to predict these properties of polycyclic aromatic hydrocarbons. We predicted boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($log\ P$), enthalpy of formation (ΔH_f), and Kovats retention index (RI) of some polycyclic aromatic hydrocarbons by using our derived models.

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