Correlation of Some Molecular Descriptors with Polycyclic Aromatic Hydrocarbons and Topological Indices of Fullerenes

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Abstract

The aspiration of the present article is to assess the performance of some molecular descriptors like re–defined version of Zagreb indices and F–index with some interesting class of hydrocarbons in terms of their physico–chemical properties: melting point, boiling point and partition coefficient. Further, results for re–defined version of Zagreb indices and F–index are computed for particular class of fullerenes.

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Keywords: Re–defined version of Zagreb indices, F–index, polycyclic aromatic hydrocarbons.

1 Introduction

For many decades chemists have come across the challenges to obtain the relationship between the properties of molecules and their structures. The quantification of chemical structures can be done in many ways, the most admired one these days is Graph Theory, notably more economical and affordable being topological indices. Topological indices are molecular descriptors which characterize the topology of a graph through numerical parameters. These are well used nowadays in chemical structure analysis using quantitative structure–activity relationship (QSAR) models and quantitative structure–property relationship (QSPR) models for modeling physico–chemical properties of biological activities.

Alkenes are attractive class of hydrocarbons which find a wide variety of applications in molecular modeling procedures. The interesting class of cyclic alkenes which are unsaturated hydrocarbons are polycyclic aromatic hydrocarbons (PAH). These are organic compounds made of only carbon and hydrogen atoms and are composed of aromatic rings. The physico–chemical properties of PAH which are necessary for environmental studies like melting point (MP), boiling point (BP), partion coefficient n–octanol/water (LogP), critical temperature, density and others are well modeled by a single molecular descriptor.

Let $G = (V, E)$ be a simple and finite graph with $|V(G)| = n$ as the vertex set and $|E(G)| = m$ as the edge set. The degree of vertex v in a graph G is denoted

as $d_G(v)$ and is defined as the number of edges of a graph G incident with v [1]. For undefined terminologies refer [6].

2 Description of Indices

The process of correlating molecular structures is critical, hence significant models are required to meet the demand. Graph Theory plays a vital role in this case by providing a tool through topological indices which have rapid computation capability. These days topological indices are accepted as a powerful tool for correlation purpose. Abundant number of topological indices are identified these days. Amongst these, the first degree based topological index is first Zagreb index devised in 1972 [5]. Further, second Zagreb index [4], F–index [2] were stated and studied. Later these Zagreb indices were re–defined by Ranjini et al.[9] This section provides definitions for re–defined versions of Zagreb indices and F–index.

Let $G = (V, E)$ be a molecular graph and d_u is the degree of the vertex u, similarly d_v is the degree of vertex v.

Now the re–defined version of Zagreb indices are defined as follows [9],

The first re–defined Zagreb index of a graph G i.e., $ReZG_1(G)$ is defined by

$$ReZG_1(G) = \sum_{e=uv \in E(G)} \frac{d_u + d_v}{d_u d_v} \tag{2.1}$$

The third re–defined Zagreb index of a graph G i.e., $ReZG_3(G)$ is defined by

$$ReZG_3(G) = \sum_{e=uv \in E(G)} (d_u d_v)\,(d_u + d_v) \tag{2.2}$$

The F–index of a graph G i.e., $F(G)$ is defined by [2],

$$F(G) = \sum_{(v) \in V(G)} (d_G(v))^3 = \sum_{uv \in E(G)} ((d_G(u))^2 + (d_G(v))^2) \tag{2.3}$$

3 On the chemical applicability of re–defined version of Zagreb indices and F–index

Quantitative structure–property relationships (QSPR) and quantitative structure–activity relationships (QSAR) analysis are widely studied using topological indices having high correlation factor. This section accounts for the linear regression analysis of re–defined version of Zagreb indices and F–index with MP, BP and LogP of PAH. A data set of PAH available on http://www.moleculardescriptors.eu/dataset.htm. is investigated for MP, BP and LogP with three topological indices first re–defined Zagreb index $ReZG_1(G)$, third re–defined Zagreb index $ReZG_3(G)$ and F–index $F(G)$. The dataset of PAH (columns 1–5 of Table 1) are refered from web link mentioned above, the last three columns of Table 1 are calculated by using equations (1), (2) and (3).

Tab. 1: Data for polycyclic aromatic hydrocarbons (PAH) indicating MP, BP and LogP and the corresponding values of $ReZG_1(G)$, $ReZG_3(G)$ and $F(G)$.

No.	**Molecule**	**MP**	**BP**	**LogP**	**ReZG$_1$(G)**	**ReZG$_3$(G)**	**F(G)**
1	naphtalene	81	218	3.35	10	270	118
2	1-methylnaphthalene	-22	245	3.87	11	320	138
3	2-methylnaphthalene	35	241	4	11	310	138
4	1-ethylnaphthalene	-14	259	4.39	12	344	146
5	2-ethylnaphthalene	-7	258	4.38	12	334	146
6	2-6-dimethylnaphthalene	110	262	4.31	12	350	158
7	2-7-dimethylnaphthalene	97	262	-	12	350	158
8	1-7-dimethylnaphthalene	-14	263	4.44	12	360	158
9	1-5-dimethylnaphthalene	80	269	4.31	12	370	158
10	1-2-dimethylnaphthalene	-4	271	4.31	12	370	158
11	1-3-7-trimethylnaphthalene	14	280	-	13	400	178
12	2-3-5-trimethylnaphthalene	25	285	-	13	410	178
13	2-3-6-trimethylnaphthalene	101	286	4.73	13	400	178
14	phenalene	85	-	-	13	438	180
15	1-phenylnaphthalene	45	334	-	16	486	204
16	2-phenylnaphthalene	104	360	-	16	476	204
17	anthracene	216	340	4.5	14	444	188
18	1-methylanthracene	86	363	-	15	494	208
19	2-methylanthracene	209	-	-	15	484	208
20	2-7-dimethylanthracene	241	370	-	16	524	228
21	2-6-dimethylanthracene	250	370	-	16	524	228
22	2-3-dimethylanthracene	252	-	-	16	534	228
23	9-10-dimethylanthracene	183	-	5.69	16	564	228
24	phenanthrene	101	338	4.52	14	454	188
25	1-methylphenanthrene	123	359	5.08	15	504	208
26	2-methylphenanthrene	56	355	5.24	15	494	208
27	3-methylphenanthrene	65	352	5.15	15	494	208
28	4-methylphenanthrene	50	-	-	15	504	208
29	9-methylphenanthrene	91	355	-	15	504	208

No.	Molecule	MP	BP	LogP	$ReZG_1(G)$	$ReZG_3(G)$	F(G)
30	3-6-dimethylphenanthrene	141	363	-	16	534	228
31	4-5-methylenephenanthrene	116	359	-	15	590	234
32	tetracene	257	-	5.76	18	618	258
33	benzo[a]anthracene	162	-	5.91	18	628	258
34	chrysene	256	441	5.86	18	638	258
35	benzo[c]phenanthrene	68	-	-	18	638	258
36	triphenylene	199	439	5.49	18	648	258
37	pyrene	156	393	5	16	606	242
38	1-methylpyrene	70	410	-	17	656	262
39	2-methylpyrene	144	410	-	17	646	262
40	4-methylpyrene	148	410	-	17	656	262
41	2-7-dimethylpyrene	-	396	-	18	686	282
42	pentacene	271	-	-	22	792	328
43	dibenzo[ai]anthracene	264	-	6.81	22	802	328
44	dibenzo[ah]anthracene	270	-	5.8	22	812	328
45	dibenzo[aj]anthracene	198	-	-	22	812	328
46	benzo[b]chrysene	294	-	-	22	812	328
47	dibenzo[ac]anthracene	205	-	-	22	822	328
48	pycene	-	519	-	22	822	328
49	benzo[a]pyrene	177	496	5.97	20	790	312
50	benzo[e]pyrene	179	493	-	20	800	312
51	perylene	278	-	6.25	20	800	312
52	coronene	360	-	6.5	24	1104	420
53	anthranthrene	261	-	-	22	942	366
54	benzo[ghi]perylene	283	-	6.9	22	952	366
55	dibenzo[ae]pyrene	234	-	-	24	984	382
56	1-methylchrysene	161	-	-	19	688	278
57	6-methylchrysene	257	-	-	19	688	278
58	3-methylcholanthrene	180	-	6.75	21	840	332
59	indeno[1-2-3-cd]pyrene	163	-	-	22	952	366
60	pentaphene	263	-	-	22	802	328
61	hexaphene	308	-	-	26	976	398

Note: The index is considered to be better when $|r|$ is closer to 1.

From the Table 2 we draw following conclusions

1. Among the considered PAH properties, the best correlated property is BP, the second well correlated property is LogP, while MP shows least correlation for the considered topological indices.

2. $ReZG_1(G)$ highly correlates with BP ($|r|$ = 0.986174) as good as $F(G)$ and better than $ReZG_3(G)$. Next, $ReZG_1(G)$ highly correlates with LogP ($|r|$ = 0.95434) compared to $F(G)$ and $ReZG_3(G)$. In the case of MP, $F(G)$ ($|r|$ =

No.	Molecule	MP	BP	LogP	$\mathbf{ReZG_1(G)}$	$\mathbf{ReZG_3(G)}$	F(G)
62	indano	-51	178	-	9	254	110
63	indene	-2	183	2.92	9	254	110
64	azulene	100	270	3.22	10	270	118
65	acenaphthene	96	279	3.92	12	422	172
66	acenaphthylene	93	270	-	12	422	172
67	fluorene	117	294	4.18	13	438	180
68	1-methylfluorene	87	318	4.97	14	488	200
69	2-methylfluorene	104	318	-	14	478	200
70	3-methylfluorene	88	316	-	14	478	200
71	4-methylfluorene	71	-	-	14	488	200
72	9-methylfluorene	47	-	-	14	498	200
73	1-2-benzofluorene	190	407	5.4	17	502	250
74	fluoranthene	111	383	5.2	16	616	242
75	2-3-benzofluorene	209	402	5.75	17	612	250
76	3-4-benzofluorene	125	406	-	17	622	250
77	benzo[ghi]fluoranthene	149	432	5.78	18	768	296
78	benzo[k]fluoranthene	217	481	-	20	790	312
79	benzo[b]fluoranthene	168	481	-	20	800	312
80	benzo[j]fluoranthene	166	480	-	20	800	312
81	ovalene	473	-	-	27	1602	598
82	quaterryllene	483	-	-	40	1860	700

Tab. 2: Correlation of PAH properties with selected topological indices.

Property	Total No. of molecules	$\mathbf{ReZG_1(G)}$	$\mathbf{ReZG_3(G)}$	F(G)
MP	80	0.844605	0.834389	0.85062
BP	53	0.986174	0.967631	0.978041
LogP	37	0.95434	0.917761	0.93557

0.85062) shows better correlation than $ReZG_1(G)$ and $ReZG_3(G)$.

3. The results of correlation for MP, BP and LogP for Wiener index W obtained are 0.748, 0.955 and 0.905 respectively [11]. Comparing these values with the Table 2 we conclude that the correlation of PAH properties with $ReZG_1(G)$, $ReZG_3(G)$ and $F(G)$ are in high correlation with MP, BP and LogP then for Wiener index $W(G)$.

The linear regression models for MP, BP and LogP using the Table 1 are obtained by using the least squares fitting procedure as implemented in R software [10]. The fitted models are,

4 Re–defined version of Zagreb indices and F–index for fullerenes

Fullerenes are allotropes of carbon. The molecules of fullerenes are made up of carbon atoms in the form of a closed mesh or partially closed mesh. The empirical formula of fullerene is denoted by C_n, where n indicates the number of carbon

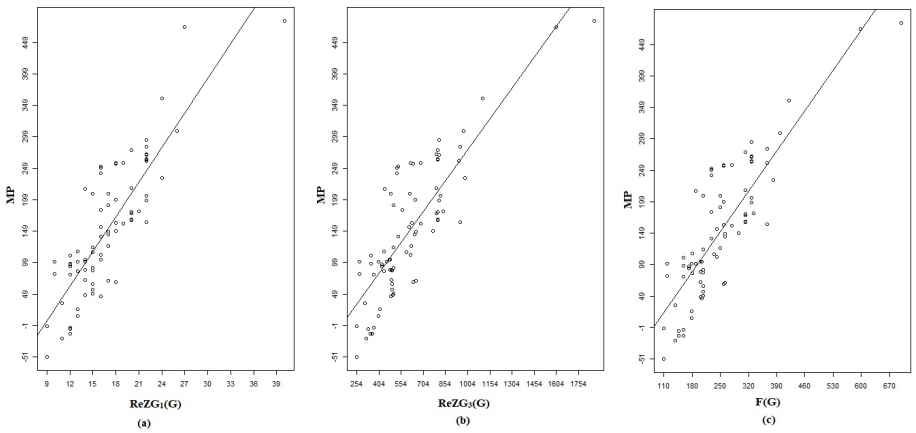

Fig. 1: Scatter diagram of (a) MP on $ReZG_1(G)$, (b) MP on $ReZG_3(G)$ and MP on $F(G)$ superimposed by the fitted regression line.

atoms. The closed fullerenes are refered as buckyballs and cylindrical fullerenes refered to as buckytubes(carbon nanotubes). Applications of fullerenes are innumerable in various fields like chemistry, genetics, biology etc. [7, 8]

Closed fullerenes: The closed fullerenes are series of n carbon atoms that form a closed cage and are also called as buckyballs. Kroto et al. [8] discovered fullerenes in the year 1985 for which they were awarded the Nobel prize in the year 1996. Closed fullerenes have 12 pentagonal and $(\frac{n}{2} - 10)$ hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20 [3, 7, 8]. These graphs are planar and 3–regular i.e., all vertices are of degree 3.

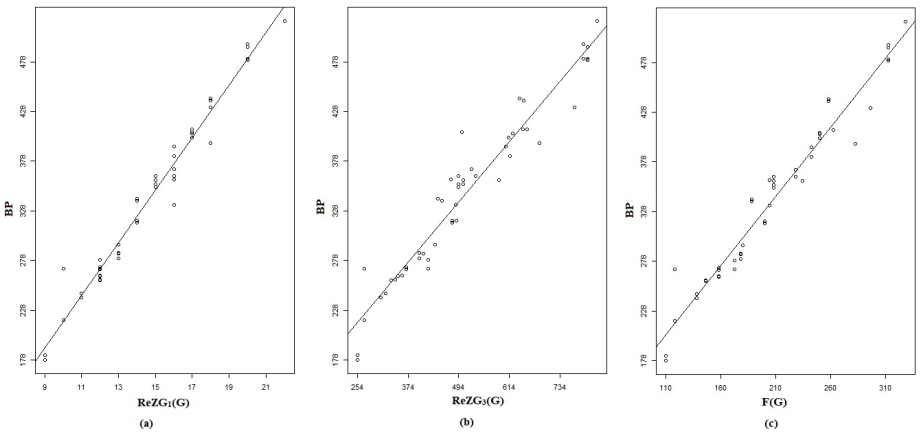

Fig. 2: Scatter diagram of (a) BP on $ReZG_1(G)$, (b) BP on $ReZG_3(G)$ and BP on $F(G)$ superimposed by the fitted regression line.

Theorem 1. *If C_n is a closed fullerene graph with n vertices, then the first re–defined Zagreb index of C_n is $ReZG_1(C_n) = n$.*

Proof.

Let C_n be the closed fullerene graph with n vertices. The number of edges in C_n are $\frac{3n}{2}$.

The first re–defined Zagreb index of a graph G is

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

Since fullerene graph is a 3–regular graph, then

$$ReZG_1(C_n) = n.$$

□

Theorem 2. *If C_n is a closed fullerene graph with n vertices, then the third re–defined Zagreb index of C_n is $ReZG_3(C_n) = 81n$.*

Proof.

Let C_n be the closed fullerene graph with n vertices. The number of edges in C_n are $\frac{3n}{2}$.

The third re–defined Zagreb index of a graph G is

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

Since fullerene graph is a 3–regular graph, then

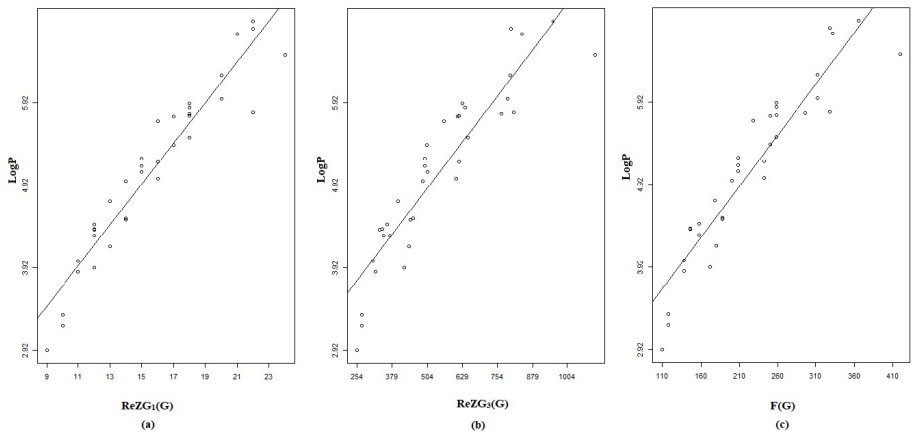

Fig. 3: Scatter diagram of (a) $LogP$ on $ReZG_1(G)$, (b) $LogP$ on $ReZG_3(G)$ and $LogP$ on $F(G)$ superimposed by the fitted regression line.

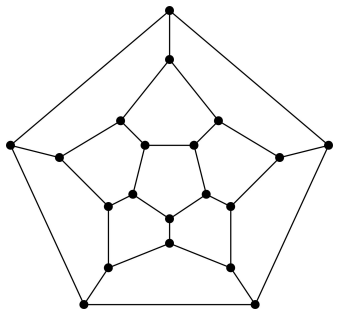

Fig. 4: 2–dimensional graph of fullerene C_{20}.

$$ReZG_3(C_n) = 81n.$$

□

Theorem 3. *If C_n is a closed fullerene graph with n vertices, then the F–index of C_n is $F(C_n) = 27n$.*

Proof.

Let C_n be the fullerene graph with n vertices.
The F–index of a graph G is

$$F(G) = \sum_{(v)\in V(G)} (d_G(v))^3$$

Since fullerene graph is a 3–regular graph, then

$$F(C_n) = 27n.$$

□

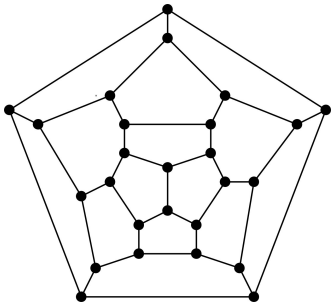

Fig. 5: 2–dimensional graph of fullerene C_{26}.

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