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Connectivity indices and QSPR analysis of benzenoid hydrocarbons

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Abstract: In mathematical chemistry, a large number of topological indices are used to predict the physicochemical properties of compounds, especially in the study of quantitative structure-proerty relationship (QSPR). However, many topological indices have almost the same predictive ability. In this paper, we focus on how to use fewer topological indices to predict the physicochemical properties of compounds through the QSPR analysis of connectivity indices of benzene hydrocarbons.

Keywords: Connectivity indices; QSPR; Benzene hydrocarbons.

MSC: 05C09, 05C92.

1. Introduction

In mathematical chemistry, topological indices (or molecular structure descriptors) have been extensively studied in various areas of mathematics [1,2], physics [3], informatics [4], biology [5], especially in chemistry [6–9], such as chemical documentation, isomer discrimination, molecular complexity, chirality, similarity/dissimilarity, drug design, database selection, lead optimization, quantitative structure-activity/proerty relationship (QSAR/QSPR), and etc. A degree-based topological indices is a common type of topological index which is calculated using the degrees of a chemical graph, such as Zagreb indices [10], Narumi-Katayama index [11], Albertson index [12], reduced second Zagreb index [13], the second Hyper-Zagreb index [14], the Hyper-Zagreb index [15], the forgotten topological index [16], Sombor index [17], the face index [18]. Some of the degree-based topological indices are called the connectivity indices or branching indices originating from Randić's seminal paper [19], which includes Randić index [19], harmonic index [20], sum-connectivity indices [21], atom-bond-connectivity index [22] and atom-bond sum-connectivity index [23]. The connectivity indices are the best known and widely applied in mathematical chemistry.

Let G be a simple undirected connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $u \in V(G)$ is the number of edges that are incident to u, denoted by $d_u(G)$, d_u for short. The maximum degree of G are denoted by $\Delta(G)$, or simply Δ. A chemical graph (or molecular graph) is a graph with $2 \le \Delta \le 4$. The first Zagreb index (M_1), Randić index (R) and atom-bond-connectivity index (ABC) are classical degree-based topological indices, and defined as

$$\begin{aligned} M_1(G) &= \sum_{uv\in E(G)} (d_u + d_v), \\ R(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}, \\ ABC(G) &= \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}, \end{aligned}$$

which are frequently used to predict the physicochemical properties and biological activity of chemical compounds in QSAR/QSPR.

The Sombor index (SO), harmonic index (H), sum-connectivity index (SCI) and atom-bond sum-connectivity index (ABS) are introduced and defined as

$$\begin{aligned} SO(G) &= \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}, \\ H(G) &= \sum_{uv\in E(G)} \frac{2}{d_u + d_v}, \\ SCI(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}, \\ ABS(G) &= \sum_{uv\in E(G)} \sqrt{1 - \frac{2}{d_u + d_v}}. \end{aligned}$$

In particular, research shows that the Sombor index, sum-connectivity index and atom-bond sum-connectivity index are useful in predicting physicochemical properties for octane isomers (see [21,24,25]). However, professor Gutman [26] believes that Sombor index is not of great applicability in QSPR and QSAR studies. Indeed, Sombor index and the first Zagreb index are almost the same correlation with physicochemical properties for octane isomers (see [25]) and lower benzenoid hydrocarbons (see Table 2.3 in Second 2).

From a mathematical perspective, it is not difficult to find such a fact that

$$\frac{1}{\sqrt{2}}(a+b) \le \sqrt{a^2+b^2} \le \frac{5}{6}(a+b)$$

for any integer number $1 \le a \le 4$ and $1 \le b \le 4$. Thus, for the chemical graph, we have

$$\frac{1}{\sqrt{2}} M_1 \le SO \le \frac{5}{6} M_1.$$

Similarly, we consider connectivity indices. Note that the degree of benzenoid hydrocarbons is only 2 and 3. We obtain the following relationship of connectivity indices for benzenoid hydrocarbons:

$$\frac{40}{41} R < H \le R,$$

$$R \le SCI \le \frac{\sqrt{30}}{5} R,$$

$$ABC \le ABS \le \frac{\sqrt{30}}{5} ABC.$$

On the other hand, we find that the difference between these corresponding indices is very small for lower benzenoid hydrocarbons. Let $e_{i,j}$ be the number of edges in G joining vertices of degree i and j. For benzenoid hydrocarbons, we have

$$\begin{aligned} M_1 &= 4e_{2,2} + 5e_{2,3} + 6e_{3,3}, \\ \sqrt{2}SO &= 4e_{2,2} + \sqrt{26}e_{2,3} + 6e_{3,3}, \\ R &= \frac{1}{2}e_{2,2} + \frac{1}{\sqrt{6}}e_{2,3} + \frac{1}{3}e_{3,3}, \\ H &= \frac{1}{2}e_{2,2} + \frac{2}{5}e_{2,3} + \frac{1}{3}e_{3,3}, \\ SCI &= \frac{1}{2}e_{2,2} + \frac{1}{\sqrt{5}}e_{2,3} + \frac{1}{\sqrt{6}}e_{3,3}, \\ ABC &= \frac{1}{\sqrt{2}}e_{2,2} + \frac{1}{\sqrt{2}}e_{2,3} + \frac{2}{3}e_{3,3}, \\ ABS &= \frac{1}{\sqrt{2}}e_{2,2} + \frac{\sqrt{15}}{5}e_{2,3} + \frac{\sqrt{6}}{3}e_{3,3}. \end{aligned}$$

If a benzenoid graph contains n vertices, h hexagons and r inlets, then $e_{2,2} = n - 2h - r + 2$, $e_{2,3} = 2r$ and $e_{3,3} = 3h - r - 3$ (see [27]). Thus we obtain

$$\begin{aligned} M_1 &= 4n + 10h - 10, \\ \sqrt{2}SO &= 4n + 10h - 10 + 0.198039r, \\ R &= 0.5n - 0.016837r, \\ H &= 0.5n - 0.033333r, \\ SCI &= 0.5n + 0.224745(h-1) - 0.013821r, \\ ABC &= 0.5n + 0.585786(h-1) + 0.040440r, \\ ABS &= 0.5n + 1.035276(h-1) + 0.025590r. \end{aligned}$$

The above discussion reveals to us why these corresponding indices have almost the same correlation and predictive ability for lower benzenoid hydrocarbons (see Table 2.3 and Table 2.4 in Section 2). This means that using connectivity indices to study the QSPR of benzene hydrocarbons, only calculating R and ABC is sufficient. Therefore, we should first consider the degree composition of the chemical graph in order to select the degree-based topological indices with significant differences for predicting physicochemical properties of compounds, which has guiding significance for the study of quantitative structure-proerty relationship of chemical compounds. Meanwhile, we should make reasonable use of existing topological indices (especially classical topological indices) to reduce the generation of similar topological indices from chemical point of view.

2. Numerical results

In this section, we study the correlation between some degree-based topological indices and physicochemical properties of twenty-two lower benzenoid hydrocarbons. The data on the physicochemical properties of twenty-two lower benzenoid hydrocarbons, including boiling point (Bp), entropy (S), octanol-water partition coefficient (logP), Kovats retention index (RI), enthalpy of formation (ΔH_f), π-electronic energy (E_π), and Gibb's energy (GE), is derived from reference [28,29]. The data in Tables 2.3 and 2.4 confirm our viewpoint.

Table 2.1 Experimental values of physiochemical properties for benzenoid hydrocarbons

Molecule	Bp	S	logP	RI	ΔH_f	E_π	GE
Naphthalene	218	79.38	3.3	200	150.6	13.6832	252.38
Phenanthrene	338	93.79	4.46	300	209.1	19.4483	383.08
Anthracene	340	92.43	4.45	301.69	218.3	19.3137	383.08
Chrysene	431	106.83	5.81	400	267.7	25.1922	513.78
Tetraphene	425	108.22	5.76	398.5	276.9	25.1012	513.78
Triphenylene	429	104.66	5.49	400	258.5	25.2745	513.78
Naphthacene	440	105.47	5.76	408.3	286.1	13.6832	-
Benzo[a]pyrene	496	111.85	6.13	453.44	279.9	28.222	621.88
Benzo[e]pyrene	493	110.46	6.44	450.73	289.1	28.3361	621.88
Perylene	497	109.10	6.25	456.22	279.9	28.2453	621.88
Anthanthrene	547	114.10	7.04	503.89	310.5	31.253	-
Benzo[ghi]perylene	542	114.10	6.63	501.32	301.3	31.4251	729.98
Dibenz[a,h]anthracene	536	119.87	6.75	495.45	335.5	30.8805	644.48
Dibenz[a,j]anthracene	531	119.87	6.54	489.8	335.5	30.8795	644.48
Picene	519	119.87	7.11	500	326.3	30.9432	644.48
Coronene	590	116.36	7.64	549.67	322.7	34.5718	838.08
Benzo[c]phenanthrene	448	113.61	5.7	391.12	280.5	25.1875	-
Pyrene	404	96.06	4.88	351.22	230.5	22.5055	491.18
Dibenzo[a,e]pyrene	592	124.89	7.28	551.53	338.5	-	-
Dibenzo[a,h]pyrene	596	123.50	7.28	559.9	347.7	33.928	-
Dibenzo[a,i]pyrene	594	123.50	7.28	556.47	347.7	-	-
Dibenzo[a,l]pyrene	595	131.69	7.71	553	351.2	-	-

Table 2.2 The values of different degree-based topological indices for benzenoid hydrocarbons

Molecule	M_1	SO	R	H	SCI	ABC	ABS
Naphthalene	50	35.6354	4.9663	4.9333	5.1971	7.7377	8.1575
Phenanthrene	76	54.1602	6.9495	6.9	7.4080	11.1924	12.0468
Anthracene	76	54.3003	6.9327	6.8667	7.3942	11.2328	12.0724
Chrysene	102	72.6850	8.9327	8.8667	9.6190	14.6470	15.9361
Tetraphene	102	72.8251	8.9158	8.8333	9.6051	14.6875	15.9617
Triphenylene	102	72.5450	8.9495	8.9	9.6328	14.6066	15.9105
Naphthacene	102	72.9651	8.8990	8.8	9.5913	14.7279	15.9873
Benzo[a]pyrene	120	85.5530	9.9158	9.8333	10.8299	16.6875	18.4112
Benzo[e]pyrene	120	85.4130	9.9327	9.8667	10.8437	16.6470	18.3856
Perylene	120	85.4130	9.9327	9.8667	10.8437	16.6470	18.3856
Anthanthrene	138	98.4209	10.8990	10.8	12.0408	18.7279	20.8863
Benzo[ghi]perylene	138	98.2809	10.9158	10.8333	12.0546	18.6875	20.8607
Dibenz[a,h]anthracene	128	91.3499	10.8990	10.8	11.8161	18.1421	19.8510
Dibenz[a,j]anthracene	128	91.3499	10.8990	10.8	11.8161	18.1421	19.8510
Picene	128	91.2098	10.9158	10.8333	11.8299	18.1017	19.8254
Coronene	156	111.1489	11.8990	11.8	13.2655	20.7279	23.3358
Benzo[c]phenanthrene	102	72.6850	8.9327	8.8667	9.6190	14.6470	15.8942
Pyrene	94	67.0282	8.9327	7.8667	7.9327	13.2328	14.5219
Dibenzo[a,e]pyrene	146	103.9377	11.9158	11.8333	13.0546	20.1017	22.2749
Dibenzo[a,h]pyrene	146	104.0778	11.8990	11.8	13.0408	20.1421	22.3005
Dibenzo[a,i]pyrene	146	104.0778	11.8990	11.8	13.0408	20.1421	22.3005
Dibenzo[a,l]pyrene	146	103.9378	11.9158	11.8333	13.0546	20.1017	22.2749

Table 2.3 The correlation coefficient of different degree-based topological indices with some physicochemical properties of benzenoid hydrocarbons

Physico-chemical property	M_1	SO	R	H	SCI	ABC	ABS
Bp	0.9924	0.9925	0.9958	0.9957	0.9965	0.9964	0.9951
S	0.9236	0.9238	0.9591	0.9593	0.9507	0.9443	0.9349
logP	0.9828	0.9829	0.9890	0.9890	0.9889	0.9881	0.9862
RI	0.9922	0.9923	0.9988	0.9987	0.9986	0.9979	0.9959
ΔH_f	0.9410	0.9418	0.9731	0.9724	0.9656	0.9614	0.9524
E_π	0.9069	0.9057	0.9039	0.9055	0.9066	0.9046	0.9062
GE	0.9963	0.9962	0.9737	0.9738	0.9822	0.9865	0.9918

Table 2.4 The correlation coefficient of different degree-based topological indices

	M_1	SO	R	H	SCI	ABC	ABS
M_1	1	1	0.9916	0.9916	0.9957	0.9975	0.9993
SO	1	1	0.9917	0.9917	0.9958	0.9976	0.9993
R	0.9916	0.9917	1	1	0.9993	0.9981	0.9957
H	0.9916	0.9917	1	1	0.9993	0.9980	0.9956
SCI	0.9957	0.9958	0.9993	0.9993	1	0.9997	0.9984
ABC	0.9975	0.9976	0.9981	0.9980	0.9997	1	0.9995
ABS	0.9993	0.9993	0.9957	0.9956	0.9984	0.9995	1

3. Conclusion

In this paper, we discussed how to achieve almost identical physicochemical property predictions with fewer connectivity indices in QSPR analysis of benzenoid hydrocarbons. The following question is of interest and further research:

Question 1. *How to achieve almost identical physicochemical property predictions with fewer topological indices in QSPR analysis of the similar compounds.*

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