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Prediction Potential of Degcity Indices for Physico-Chemical Properties of Polycyclic Aromatic Hydrocarbons: A QSPR Study

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Abstract: Polycyclic aromatic hydrocarbons(PAHs), formed by natural and anthropogenic processes, can be found everywhere in the environment. They are a special class of organic compounds attracted by scientists because of their pollutant power. The physicochemical properties of PAHs play an important role in accumulating or dispersing them in the environment. In this article, we have studied the QSPR (Quantitative Structure-Property Relationship) of some physicochemical properties of polycyclic aromatic hydrocarbons (PAHs) using degcity indices. Also, we compare degcity indices with the other topological indices and further examine the degeneracy of the degcity indices.

Keywords: QSPR analysis; polycyclic aromatic hydrocarbons; topological indices; degcity indices; physicochemical properties.

1. Introduction

Polycyclic aromatic hydrocarbons(PAHs) are a large class of organic compounds containing two or more benzene rings bonded in linear, cluster, or angular structures. They have been receiving attention from researchers due to their impact on health and the environment, see [1 - 7]. As a result of anthropogenic activities and natural processes, hundreds of PAHs are released into the environment daily. The physicochemical properties play a prominent role in predicting the fate of PAHs in the environment [8, 9]. A topological index is a real number associated with the molecular graph of a chemical structure. Topological indices are widely used in QSPR studies since only the molecular structure of the chemical compound is required, and no additional experimental data is needed to compute them [10]. The role of topological indices in QSPR analysis to predict physicochemical properties of chemical compounds is exceptional these days, refer [11 - 18] for more details on QSPR studies and applications. We introduce degree-eccentricity-related topological indices, called degcity indices, and are defined as

$$DC_1(G) = \sum_{e=uv\in E(G)} [e_u + e_v][d_u + d_v],$$

$$DC_2(G) = \sum_{e=uv\in E(G)} \frac{e_u + e_v}{d_u + d_v},$$

$$DC_3(G) = \sum_{e=uv\in E(G)} \frac{d_u + d_v}{e_u + e_v},$$

$$DC_4(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{e_u + e_v}{d_u + d_v}},$$

$$DC_5(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{d_u + d_v}{e_u + e_v}},$$

$$DC_6(G) = \sum_{e=uv\in E(G)} \frac{e_u + e_v}{d_u d_v},$$

$$DC_7(G) = \sum_{e=uv\in E(G)} \frac{d_u + d_v}{e_u e_v},$$

where d_u and d_v represent the degree of the vertices u, v in the vertex set $V(G)$ respectively, $e = uv$ is an edge in the edge set $E(G)$ and e_u, e_v denote the eccentricity of the vertices u, v respectively, of a simple connected graph G. For undefined graph notations and terminologies, one can refer [19]. The purpose of this paper is to study the prediction ability of the degcity indices for PAHs.

2. Materials and Methods

QSPR models have been developed to predict some physicochemical properties of PAHs. Further, we have compared the degcity indices with the following well-known indices. The first and second Zagreb indices were introduced by I. Gutman and N. Trinajstić [20] and are defined as:

$$M_1 = M_1(G) = \sum_{u\in V(G)} d_u^2 ,$$

$$M_2 = M_2(G) = \sum_{uv\in E(G)} d_u d_v .$$

The Randic index was introduced by Milan Randic [21] and is defined as:

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

with summation going over all pairs of adjacent vertices of the molecular graph G.

The Forgotten index (F-index) was introduced by B. Furtula and Gutman [22] and is defined as:

$$F = F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} (d_u^2 + d_v^2).$$

The first and second Zagreb eccentricity indices [23, 24] are defined as:

$$FZE = \xi_1(G) = \sum_{u \in V(G)} e_u^2,$$

$$SZE = \xi_2(G) = \sum_{uv \in E(G)} e_u e_v.$$

The eccentric connectivity index was introduced by V. Sharma et al. [25] and is defined as:

$$ECI = \xi^c(G) = \sum_{u \in V(G)} d_u e_u = \sum_{uv \in E(G)} (e_u + e_v).$$

The experimental values of physico-chemical properties [Molecular weight(mw) in g/mol, Boiling point(bp) in $^\circ C$, Complexity(C), Enthalpy of Vaporization at Normal bp (ΔH_{vb}) in cal/mol, Critical temperature (ct), Organic carbon-water partition coefficient($log K_{oc}$).

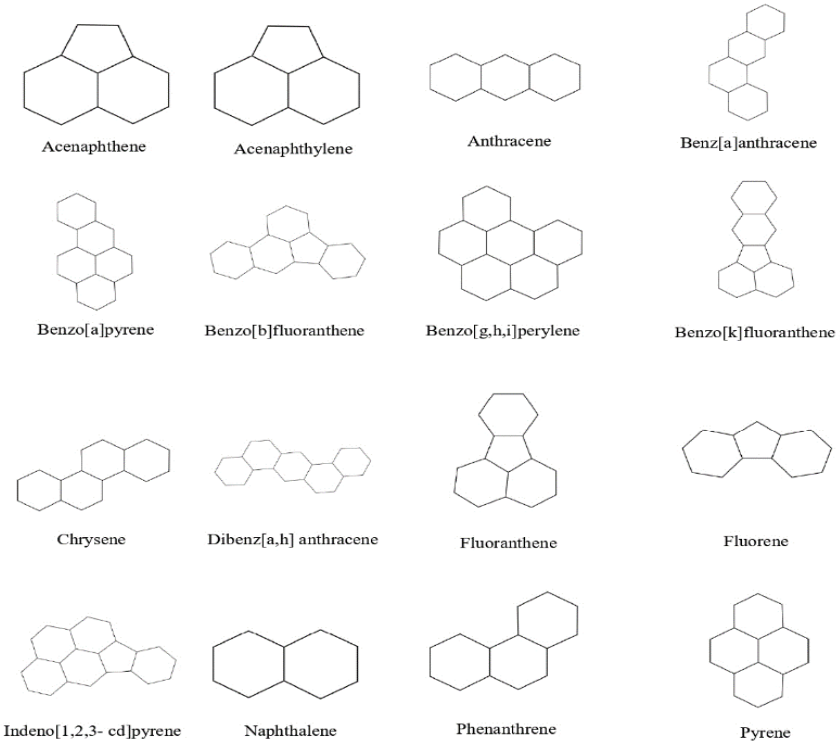

Figure 1. Molecular graphs of PAHs.

Octanol air partition coefficient ($log K_{oa}$), Octanol water partition coefficient($log K_{ow}$)] for 16 PAHs are shown in Table 1 and are taken from the risk assessment information system (RAIS) and Pubchem. The corresponding degcity indices and other topological indices of the PAHs are listed in Table 2 and Table 3, respectively. The molecular graphs of 16 PAHs are shown in Figure 1.

Table 1. The experimental values of physicochemical properties of PAHs.

PAHs	mw	bp	C	ΔH_{vb}	ct	log Koc	logKoa	logKow
Acenaphthene	154.21	279	155	12155	803.15	3.7013	6.044	3.92
Acenaphthylene	152.19	280	184	11714.63	792	3.7013	6.272	3.93

PAHs	mw	bp	C	ΔH_{vb}	ct	log Koc	logKoa	logKow
Anthracene	178.23	342	154	13121	873	4.2138	7.093	4.45
Benz[a]anthracene	228.3	437.6	294	16000	979	5.2476	9.069	5.76
Benzo[a]pyrene	252.3	496	372	14412.52	969.27	5.7689	10.859	6.13
Benzo[b] fluoranthene	252.3	481	372	14412.52	969.27	5.7777	10.351	5.78
Benzo[g,h,i]perylene	276.3	550	411	17747.61	1092.5	6.2902	11.499	6.63
Benzo[k] fluoranthene	252.3	480	338	16412.05	1019.7	5.7689	10.732	6.11
Chrysene	228.3	448	264	16467.5	979	5.2564	9.48	5.73
Dibenz[a,h] anthracene	278.3	524	361	17341.3	990.41	6.2814	11.779	6.5
Fluoranthene	202.25	384	243	13757.17	905	4.7439	8.601	5.16
Fluorene	166.22	294	165	12666	826	3.9619	6.585	4.18
Indeno[1,2,3- cd]pyrene	276.3	536	453	17747.61	1078.2	6.2902	11.547	6.7
Naphthalene	128.17	218	80.6	10325.05	748.3	3.1887	5.045	3.3
Phenanthrene	178.23	338.4	174	12915.15	869	4.2226	7.222	4.46
Pyrene	202.25	394	217	14370	936	4.7351	8.193	4.88

Table 2. Degcity indices for PAHs.

PAHs	DC_1	DC_2	DC_3	DC_4	DC_5	DC_6	DC_7
Acenaphthene	544	24.4333	8.6929	18.3163	10.9192	21.7222	51.2000
Acenaphthylene	544	24.4333	8.6929	18.3163	10.9192	21.7222	51.2000
Anthracene	840	39.3333	7.0426	24.8343	10.5153	35.5556	114.8333
Benz[a]anthracene	1356	60.7833	7.8920	35.3496	12.7422	53.9722	214.0667
Benzo[a]pyrene	1564	66.2500	9.4748	39.4372	14.9245	57.4167	228.2667
Benzo[b] fluoranthene	1487	63.4833	9.8762	38.6104	15.2402	55.3056	207.8333
Benzo[g,h,i]perylene	1638	66.5333	11.8118	41.9878	17.6936	56.5556	206.4500
Benzo[k] fluoranthene	1538	65.3000	9.5833	39.1684	15.0160	56.6667	221.1667
Chrysene	1338	60.0667	8.0209	35.1211	12.8392	53.4444	209.1667
Dibenz[a,h] anthracene	2058	89.4000	8.2198	47.6923	14.4750	78.3333	381.2667
Fluoranthene	904	39.7667	10.0025	27.1607	13.6206	35.1111	101.6667
Fluorene	676	31.4000	7.8434	21.4578	10.7274	28.3333	78.4000
Indeno[1,2,3- cd]pyrene	1750	71.0167	11.0787	43.3576	17.1392	60.3611	234.4333
Naphthalene	400	20.6000	6.4349	14.8951	8.3122	19.3333	43.6000
Phenanthrene	792	37.3333	7.4616	24.1912	10.8096	33.8889	102.5833
Pyrene	972	42.1333	9.2656	28.0169	13.1410	36.8889	114.5000

Table 3. Well-known topological indices for PAHs.

PAHs	M_1	M_2	R	F	FZE	SZE	ECI
Acenaphthene	68	83	5.94948	172	214	235	114
Acenaphthylene	68	83	5.94948	172	214	235	114
Anthracene	76	90	6.93265	188	472	516	180
Benz[a]anthracene	102	124	8.91581	258	882	983	284
Benzo[a]pyrene	120	151	9.91581	312	943	1080	318
Benzo[b] fluoranthene	120	154	9.8409	312	853	973	303
Benzo[g,h,i]perylene	138	178	10.9158	366	856	995	326
Benzo[k] fluoranthene	120	151	9.91581	312	909	1041	313
Chrysene	102	125	8.93265	258	858	959	280
Dibenz[a,h] anthracene	128	158	10.899	328	1562	1780	424
Fluoranthene	94	118	7.94948	242	421	468	187
Fluorene	72	87	6.44948	180	324	352	144
Indeno[1,2,3 - d]pyrene	138	183	10.7491	366	966	1127	346
Naphthalene	50	57	4.96632	118	182	187	90
Phenanthrene	76	91	6.94948	188	424	459	170
Pyrene	94	117	7.93265	242	474	534	200

2.1. QSPR model for PAHs.

The following linear regression model has been studied:

$$P = c + (TI)m, \quad (2.1)$$

where P is the physicochemical property, TI is the topological index, m is the slope, and c is the intercept. Using (2.1), we have the following linear regression models for each degcity index:

1. DC_1 index [$DC_1(G)$]:

$$mw = 101.6534227 + [DC_1(G)]0.096717311$$

$$bp = 173.50885 + [DC_1(G)]0.201394403$$

$$C = 30.79328691 + [DC_1(G)]0.203516516$$

$$\Delta H_{vb} = 9664.5475 + [DC_1(G)]4.180878593$$

$$ct = 714.3557376 + [DC_1(G)]0.184781164$$

$$logKoc = 2.6302948 + [DC_1(G)]0.002014303$$

$$logKoa = 3.806778439 + [DC_1(G)]0.004318382$$

$$logKow = 2.805220662 + [DC_1(G)]0.002105128$$

2. DC_2 index [$DC_2(G)$]:

$$mw = 94.41891705 + [DC_2(G)]2.362615083$$

$$bp = 158.8771847 + [DC_2(G)]4.911041688$$

$$C = 20.38848645 + [DC_2(G)]4.875416591$$

$$\Delta H_{vb} = 9330.003433 + [DC_2(G)]102.5657122$$

$$ct = 702.5852657 + [DC_2(G)]4.472933873$$

$$logKoc = 2.482366783 + [DC_2(G)]0.049150779$$

$$logKoa = 3.489993292 + [DC_2(G)]0.105365349$$

$$logKow = 2.647684752 + [DC_2(G)]0.051425599$$

3. DC_3 index [$DC_3(G)$]:

$$mw = 10.02196081 + [DC_3(G)]22.95571278$$

$$bp = -32.2820842 + [DC_3(G)]49.49655872$$

$$C = -257.801376 + [DC_3(G)]59.14271956$$

$$\Delta H_{vb} = 6071.155525 + [DC_3(G)]950.7240594$$

$$ct = 485.8511498 + [DC_3(G)]49.90476755$$

$$logKoc = 0.658668559 + [DC_3(G)]0.485248548$$

$$logKoa = -0.43621649 + [DC_3(G)]1.042127167$$

$$logKow = 0.752123636 + [DC_3(G)]0.506287772$$

4. DC_4 index [$DC_4(G)$]:

$$mw = 63.56589259 + [DC_4(G)]4.798220111$$

$$bp = 92.97120197 + [DC_4(G)]10.03079195$$

$$C = -50.4482991 + [DC_4(G)]10.13183777$$

$$\Delta H_{vb} = 8015.397141 + [DC_4(G)]207.5036648$$

$$ct = 637.659751 + [DC_4(G)]9.293380287$$

$$logKoc = 1.835099399 + [DC_4(G)]0.099994013$$

$$logKoa = 2.110839684 + [DC_4(G)]0.214088777$$

$$logKow = 1.96936006 + [DC_4(G)]0.104657338$$

5. DC_5 index [$DC_5(G)$]:

$$mw = -19.1044461 + [DC_5(G)]17.75700371$$

$$bp = -87.2110385 + [DC_5(G)]37.68462989$$

$$C = -268.23475 + [DC_5(G)]40.80363802$$

$$\Delta H_{vb} = 4606.017118 + [DC_5(G)]755.2296707$$

$$ct = 450.7872649 + [DC_5(G)]36.44022659$$

$$logKoc = 0.083027683 + [DC_5(G)]0.372290542$$

$$logKoa = -1.63627337 + [DC_5(G)]0.79676613$$

$$logKow = 0.13967292 + [DC_5(G)]0.389339312$$

6. DC_6 index [$DC_6(G)$]:

$$mw = 91.61239003 + [DC_6(G)]2.753791033$$

$$bp = 153.2682306 + [DC_6(G)]5.719053031$$

$$C = 17.03798606 + [DC_6(G)]5.627206498$$

$$\Delta H_{vb} = 9198.146387 + [DC_6(G)]119.7749559$$

$$ct = 698.3234006 + [DC_6(G)]5.18963657$$

$$logKoc = 2.425351492 + [DC_6(G)]0.057257508$$

$$logKoa = 3.367918951 + [DC_6(G)]0.122740467$$

$$logKow = 2.586651523 + [DC_6(G)]0.059938844$$

7. DC_7 index [$DC_7(G)$]:

$$mw = 134.9450679 + [DC_7(G)]0.487000188$$

$$bp = 244.7368868 + [DC_7(G)]1.002177773$$

$$C = 108.3849472 + [DC_7(G)]0.97766471$$

$$\Delta H_{vb} = 11584.06598 + [DC_7(G)]18.05024201$$

$$ct = 782.7152212 + [DC_7(G)]0.90071719$$

$$logKoc = 3.468797962 + [DC_7(G)]0.009235658$$

$$logKoa = 5.59199069 + [DC_7(G)]0.019877562$$

$$logKow = 3.709951704 + [DC_7(G)]0.00947452$$

The statistical parameters of the linear regression model for the degcity indices DC_1, DC_2, DC_3, DC_4, DC_5, DC_6 and DC_7 are listed in Tables 4, 5, 6, 7, 8, 9, and 10, respectively, where r = correlation coefficient, SE = standard error, F = F-test, and SF = significance F.

Table 4. Statistical parameters for $DC_1(G)$.

Property	c	m	R	SE	F	SF
mw	101.6534	0.0967	0.9826	9.5018	391.0215	1.25E-11
bp	173.5088	0.2014	0.9700	26.2207	222.6424	5.46E-10
C	30.7933	0.2035	0.9293	41.9893	88.6594	1.96E-07
ΔH_{vb}	9664.5475	4.1809	0.9198	926.2766	76.8877	4.63E-07
ct	714.3557	0.1848	0.9135	42.7166	70.6196	7.69E-07
logKoc	2.6303	0.0020	0.9804	0.2100	347.1533	2.80E-11
logKoa	3.8068	0.0043	0.9791	0.4653	325.0501	4.37E-11
logKow	2.8052	0.0021	0.9717	0.2658	236.7976	3.63E-10

Table 5. Statistical parameters for $DC_2(G)$.

Property	c	m	R	SE	F	SF
mw	94.4189	2.3626	0.9668	13.0603	200.3776	1.09E-09
bp	158.8772	4.9110	0.9527	32.7531	137.6625	1.25E-08
C	20.3885	4.8754	0.8967	50.3235	57.4717	2.55E-06
ΔH_{vb}	9330.0034	102.5657	0.9089	984.4156	66.4691	1.10E-06
ct	702.5853	4.4729	0.8907	47.7343	53.7646	3.72E-06
logKoc	2.4824	0.0492	0.9636	0.2851	181.9732	2.05E-09
logKoa	3.4900	0.1054	0.9623	0.6229	175.1819	2.63E-09
logKow	2.6477	0.0514	0.9561	0.3295	149.1057	7.48E-09

Table 6. Statistical parameters for $DC_3(G)$.

Property	c	m	R	SE	F	SF
mw	10.0220	22.9557	0.6717	37.8600	11.5110	0.0044
bp	-32.2821	49.4966	0.6866	78.3718	12.4889	0.0033
C	-257.8014	59.1427	0.7779	71.4536	21.4509	0.0004
ΔH_{vb}	6071.1555	950.7241	0.6024	1883.7579	7.9754	0.0135
ct	485.8511	49.9048	0.7107	73.8856	14.2842	0.0020
logKoc	0.6587	0.4852	0.6803	0.7818	12.0613	0.0037
logKoa	-0.4362	1.0421	0.6806	1.6777	12.0808	0.0037
logKow	0.7521	0.5063	0.6731	0.8319	11.5982	0.0043

Table 7. Statistical parameters for $DC_4(G)$.

Property	c	m	R	SE	F	SF
mw	63.5659	4.7982	0.9922	6.3505	892.7260	4.41E-14
bp	92.9712	10.0308	0.9834	19.5620	411.1645	8.92E-12
C	-50.4483	10.1318	0.9417	38.2402	109.7758	5.23E-08
ΔH_{vb}	8015.3971	207.5037	0.9292	872.1263	88.5245	1.98E-07
ct	637.6598	9.2934	0.9352	37.1759	97.7226	1.08E-07
logKoc	1.8351	0.1000	0.9907	0.1450	743.2747	1.56E-13
logKoa	2.1108	0.2141	0.9881	0.3522	577.6431	8.79E-13
logKow	1.9694	0.1047	0.9833	0.2045	409.5919	9.16E-12

Table 8. Statistical parameters for $DC_5(G)$.

Property	c	m	R	SE	F	SF
mw	-19.1044	17.7570	0.9347	18.1609	96.8702	1.14E-07
bp	-87.2110	37.6846	0.9404	36.6456	107.1545	6.08E-08
C	-268.2347	40.8036	0.9654	29.6360	192.0805	1.44E-09
ΔH_{vb}	4606.0171	755.2297	0.8609	1200.7896	40.0820	1.856E-05
ct	450.7873	36.4402	0.9335	37.6591	94.8738	1.29E-07
logKoc	0.0830	0.3723	0.9389	0.3671	104.2322	7.22E-08
logKoa	-1.6363	0.7968	0.9361	0.8055	99.1311	9.86E-08
logKow	0.1397	0.3893	0.9312	0.4100	91.3517	1.63E-07

Table 9. Statistical parameters for $DC_6(G)$.

Property	c	m	R	SE	F	SF
mw	91.6124	2.7538	0.9564	14.9278	150.0962	7.16E-09
bp	153.2682	5.7191	0.9416	36.2905	109.5371	5.30E-08
C	17.0380	5.6272	0.8784	54.3371	47.3033	7.59E-06
ΔH_{vb}	9198.1464	119.7750	0.9008	1024.8994	60.2376	1.94E-06
ct	698.3234	5.1896	0.8771	50.4396	46.6905	8.15E-06
logKoc	2.4254	0.0573	0.9527	0.3241	137.6720	1.25E-08
logKoa	3.3679	0.1227	0.9514	0.7053	133.5833	1.51E-08
logKow	2.5867	0.0599	0.9458	0.3653	118.7744	3.19E-08

Table 10. Statistical parameters for $DC_7(G)$.

Property	c	m	R	SE	F	SF
mw	134.9451	0.4870	0.9089	21.3081	66.5374	1.09E-06
bp	244.7369	1.0022	0.8868	49.8307	51.5222	4.72E-06
C	108.3849	0.9777	0.8202	65.0529	28.7704	9.993E-05
ΔH_{vb}	11584.0660	18.0502	0.7295	1614.1995	15.9276	0.0013
ct	782.7152	0.9007	0.8181	60.3941	28.3326	0.0001
logKoc	3.4688	0.0092	0.8259	0.6015	30.0311	8.107E-05
logKoa	5.5920	0.0199	0.8280	1.2840	30.5283	7.478E-05
logKow	3.7100	0.0095	0.8034	0.6697	25.4940	0.0002

3. Results and Discussion

To predict the quality of degcity indices of the physicochemical properties for PAHs, we adopt the following scale given by M. Randic [26]:

Table 11. Quality prediction scale for topological indices based on Correlation coefficient (r).

Correlation coefficient (r)	Quality
0.990 (and higher)	Outstanding
0.975 (and higher)	Excellent
0.950 (and higher)	Very good
0.925 (and higher)	Good
0.900 (and higher)	Fair
0.800 (and higher)	Mediocre
Below 0.800	Uninteresting

Correlation coefficient (r)	Quality
Below 0.100	Non-existent

Table 12. Correlation (r) of degcity indices with physicochemical properties of PAHs.

Index	Mw	bp	C	ΔH_{vb}	Ct	log Koc	logKoa	logKow
DC_1	0.9826	0.9700	0.9293	0.9198	0.9135	0.9804	0.9791	0.9717
DC_2	0.9668	0.9527	0.8967	0.9089	0.8907	0.9636	0.9623	0.9561
DC_3	0.6717	0.6866	0.7779	0.6024	0.7107	0.6803	0.6806	0.6731
DC_4	0.9922	0.9834	0.9417	0.9292	0.9352	0.9907	0.9881	0.9833
DC_5	0.9347	0.9404	0.9654	0.8609	0.9335	0.9389	0.9361	0.9312
DC_6	0.9564	0.9416	0.8784	0.9008	0.8771	0.9527	0.9514	0.9458
DC_7	0.9089	0.8868	0.8202	0.7295	0.8181	0.8259	0.8280	0.8034

From Table 12, the correlation of degcity indices with the physicochemical properties of PAHs is as follows:

First degcity index $DC_1(G)$: It shows an excellent correlation with mw, logKoc, logKoa, very good with bp, logKow, good with C, and fair with ΔH_{vb}, ct.

Second degcity index $DC_2(G)$: It shows a very good correlation with mw, bp, logKoc, logKoa, logKow, fair with ΔH_{vb} and mediocre with C, ct.

Third degcity index $DC_3(G)$: It does not show a good correlation with the physical properties of PAHs.

Fourth degcity index $DC_4(G)$: It shows an outstanding correlation with mw, logKoc, excellent with bp, logKoa, logKow, good with C, ΔH_{vb}, ct.

Fifth degcity index $DC_5(G)$: It has a very good correlation with C, good with mw, bp, ct, logKoc, logKoa, logKow and mediocre with ΔH_{vb}.

Sixth degcity index $DC_6(G)$: It has a very good correlation with mw, logKoc, logKoa, good with bp, logkow, fair with ΔH_{vb} and mediocre with C, ct.

Seventh degcity index $DC_7(G)$: It has a fair correlation with mw and mediocre with bp, c, ct, logKoc, logKoa, logKow.

3.1. Correlation of degcity indices with well-known topological indices.

In this part, the degcity indices are compared with well-known topological indices viz. First and second Zagreb indices (M_1, M_2), Randic index (R), Forgotten index(F), First and Second Zagreb eccentricity indices (FZE, SZE), and Eccentric connectivity index (ECI).

Table 13. Correlation of degcity indices with other topological indices.

Index	M_1	M_2	R	F	FZE	SZE	ECI
DC_1	0.9584	0.9402	0.9810	0.9467	0.9698	0.9752	0.9988
DC_2	0.9318	0.9849	0.9650	0.9165	0.9849	0.9877	0.9991
DC_3	0.7537	0.3451	0.6758	0.7794	0.3451	0.3691	0.5081
DC_4	0.9717	0.9539	0.9912	0.9613	0.9539	0.9599	0.9950
DC_5	0.9699	0.7191	0.9365	0.9786	0.7191	0.7360	0.8395
DC_6	0.9163	0.9892	0.9545	0.8993	0.9892	0.9907	0.9962
DC_7	0.8594	1.0000	0.9064	0.8394	1.0000	0.9994	0.9779

From Table 13, the quality [Outstanding = O, Excellent = E, Very Good = VG, Good = G, Fair = F, Mediocre = M] of the degcity indices with the other topological indices is depicted as (Table 14).

Table 14. Quality of degcity indices with other topological indices.

Index	O	E	VG	G	F	M
DC_1	ECI	R, SZE	M_1, FZE	M_2, F	-	-
DC_2	ECI	M_2,FZE, SZE	R	M_1	F	-
DC_4	R, ECI	-	M_1, M_2, F, FZE, SZE	-	-	-
DC_6	-	F	M1	R	-	ECI
DC_7	SZE, ECI	M_2, FZE	R	-	M_1	F

3.2. Correlation among degcity indices.

From Table 15, it follows that the first degcity index DC_1 has an outstanding correlation with DC_2, DC_4 and DC_6, very good with DC_7 and a mediocre with DC_5. The second degcity index DC_2 has an outstanding correlation with DC_4, DC_6, excellent with DC_7, and mediocre with DC_5. The third degcity index DC_3 has a mediocre correlation with DC_5. The fourth degcity index DC_4 has an excellent correlation with DC_6, very good with DC_7 and mediocre with DC_5. The sixth degcity index DC_6 has an excellent correlation with DC_7.

Table 15. Correlation among degcity indices.

Index	DC_1	DC_2	DC_3	DC_4	DC_5	DC_6	DC_7
DC_1	1						
DC_2	0.9959	1					
DC_3	0.5450	0.4730	1				
DC_4	0.9975	0.9909	0.5807	1			
DC_5	0.8619	0.8173	0.8902	0.8858	1		
DC_6	0.9909	0.9990	0.4369	0.9848	0.7934	1	
DC_7	0.9686	0.9842	0.3409	0.9525	0.7158	0.9887	1

3.3. Degeneracy of degcity indices.

The quality of a topological index depends on its discrimination ability among all graphs. The degeneracy(discrimination power) of topological indices should therefore be evaluated and ranked [27]. For more details on this, one can refer [28, 29]. Sensitivity, which is the measure of degeneracy, was introduced by E. V. Konstantinova [28] and is defined as:

$$S = \frac{a - b}{a},$$

where a is the total number of nonisomorphic graphs considered (PAHs in our case) and b is the number of them that cannot be distinguished by the topological index. For PAHs, all degcity indices show good sensitivity compared to other topological indices which are shown in Table 16.

Table 16. Sensitivity of degcity indices and other topological indices.

Index	Sensitivity
DC_1	0.9375
DC_2	0.9375
DC_3	0.9375
DC_4	0.9375
DC_5	0.9375
DC_6	0.9375
DC_7	0.9375
FZE	0.9375
SZE	0.9375
ECI	0.9375
M_2	0.875

Index	Sensitivity
R	0.875
M_1	0.5625
F	0.5625

4. Conclusions

Finally, we conclude that all the degcity indices except DC_3 and DC_7 exhibit good prediction ability with respect to the physicochemical properties of PAHs and with the well-known topological indices that we considered. Also, they possess good sensitivity compared to other topological indices.

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Conflicts of Interest

The authors declare no conflict of interest.

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