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QSPR Analysis of Certain Degree Based Topological Indices

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Abstract: In QSAR/QSPR study, topological indices are utilized to guess the bioactivity of chemical compounds. In this paper, we study the QSPR analysis of ten degree-based topological indices. Our study reveals some important results which help us to characterize the useful topological indices based on their predicting power.

Keywords: Degree; topological indices; QSPR analysis.

1 Introduction

The molecular descriptor is the final result of logic and mathematical procedure which transform chemical information encoded within a symbolic representation of a molecule into a useful member or the result of some standardized experiments. Attention is paid to the term ”useful” with its double meanings. It means that the number can give more insights into the interpretation of the molecular properties and / or is able to take part in a model for the prediction of some interesting property of the molecules.

A fundamental concept of chemistry is that the structural characteristics of a molecule are responsible for its properties. Topological indices are a convenient means of translating chemical constitution into numerical values which can be used for correlation with physical properties in quantitative structure-property/activity relationship (QSPR/QSAR) studies. The use of graph invariant (topological indices) in QSPR and QSAR studies has become of major interest in recent years. Topological indices have found application in various areas of chemistry, physics, mathematics, informatics, biology, etc [1,22,26], but their most important use to date is in the non-empirical Quantitative Structure- Property Relationships (QSPR) and Quantitative Structure -Activity Relationships (QSAR) [3,21,23,25].

The first genuine degree- based topological index was put -forward in 1975 by Milan randic in his seminar paper ”on characterization of molecular branching [20]” his index was defined as

$$R(G) = \sum_{u\sim v} \frac{1}{\sqrt{d_G(u)d_G(v)}} \tag{1}$$

With summation going over all pairs of adjacent vertices of the molecular graph G. Randić himself named ”branching index ”, but soon it was Re- named to ”connectivity index”. Now a days, most authors refer to it as to the ”Randić index”. The reciprocal Randić index is defined as

$$RR(G) = \sum_{u\sim v} \sqrt{d_G(u)d_G(v)}. \tag{2}$$

Analyzing the structure dependency of total π-electron energy [10], an approximate formula was obtained in which terms of the forms occurred.

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 \tag{3}$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)\, d_G(v) \tag{4}$$

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It was immediately recognized that these terms increase with the increasing extent of branching of the carbon atom skeleton,that is provide quantitative measures of molecular branching ten years later, in a review article, Balaban[1] included M_1 and M_2 among topological indices and named them "Zagreb group indices".

The Forgotten Topological Index [6] is defined as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3. \tag{5}$$

Ernesto Estrada conceived a new topological index, that is an amended version of equation (2.1). He named it "atom -bond connectivity index" [4] which is conveniently abbreviated by *ABC*. It is defined as

$$ABC(G) = \sum_{u \sim v} \sqrt{\frac{d_u(G) + d_v(G) - 2}{d_u(G) d_v(G)}} \tag{6}$$

Motivated by the success of the ABC index , Furtula et. al[7] put forward its modified version. that they some what inadequately named "augmented Zagreb index ". It is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u) d_G(v)}{d_G(u) + d_G(v) - 2} \right)^3. \tag{7}$$

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

$$GA(G) = \sum_{u \sim v} \frac{2\sqrt{d_u(G) d_v(G)}}{d_u(G) + d_v(G)} \tag{8}$$

where of course, $\sqrt{d_u(G) d_v(G)}$ and $\frac{d_u(G)+d_v(G)}{2}$ 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[27] and was named "Geometric - Arithmetic index". In the 1980s, Siemion Fajtlowicz [5] 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.

$$H(G) = \sum_{u \sim v} \frac{2}{d_u(G) + d_v(G)} \tag{9}$$

With a single exception $H(G)$ did not attract anybody's attention, especially not of chemists. The so called "sum connectivity index" is a recent invention by Bo Zhou and Nenad Trinajstic [28]

$$SCI(G) = \sum_{u \sim v} (d_u(G) + d_G(v))^{\frac{-1}{2}} \tag{10}$$

A number of properties of the sum connectivity index has been determined. Which again are bounds and characterization of graphs of various types, extremal with respect to SCI. By comparing the product and sum- connectivity indices, it was found that these have remarkable similar correlation properties. For recent work on degree-based topological indices, we refer the interested reader to the articles [11, 12, 16, 17, 19, 20, 18].

2 The Use of Selected Degree Based Topological Indices in QSPR Studies

We have used here 10 degree based topological indices, namely, first Zagreb index $M_1(G)$, second Zagreb index $M_2(G)$, Forgotten index $F(G)$, Randić index $R(G)$, atom-bond connectivity index (ABC(G)), augumented Zagreb index (AZI(G)), geometric-arithmetic index (GA(G)), harmonic index ($H(G)$), sum-connectivity index ($SCI(G)$) and reciprocal Randić index ($RR(G)$) for modeling eight representative physical properties [boiling points(bp), molar volumes (mv) at 20°C, molar refractions (mr) at 20°C, heats of vaporization (hv) at 25°C, surface tensions (st) 20°C and melting points (mp)] of the 67 alkanes from n-butanes to nonanes. Values for these property were taken from Needham et. al [5]. The above said degree-based topological indices and the experimental values for the physical properties of 67 alkanes are listed in Table 1 and 2 respectively.

Table 1.

S.No.	Alkane	bp($^{\circ}C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^{\circ}C$)	cp(atm)	st(dyne/cm)	mp($^{\circ}C$)
1	Butane	-0.500				152.01	37.47		-138.35
2	2-methyl propane	-11.730				134.98	36		-159.60
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00	-129.72
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00	-159.90
5	2,2 dimethylpropane	9.503	112.074	25.7243	21.78	160.60	31.57		-16.55
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42	-95.35
7	2-methylpentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38	-153.67
8	3-methyalpentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12	-118.00
9	2,2-methylbutane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30	-99.87
10	2,3-dimethylbutane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37	-128.54
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26	-90.61
12	2-methylhexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29	-118.28
13	3-methylhexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79	-119.40
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44	-118.60
15	2,2-dimethylpentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02	-123.81
16	2,3-dimethylpentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96	-119.10
17	2,4-dimethylpentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15	-119.24
18	3,3-dimethylpentane	86.064	144.530	34.3323	33.02	263.00	30	19.59	-134.46
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76	-56.79
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60	-109.04
21	3-methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17	-120.50
22	4-methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00	-120.95
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51	
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60	-121.18
25	2,3-dimethylhexane	115.607	160.39	38.98	38.79	293.00	26.6	20.99	
26	2,4-dimethylhexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05	-137.50
27	2,5-dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73	-91.20
28	3,3-dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63	-126.10
29	3,4-dimethylhexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64	
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52	-114.96
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99	-90.87
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67	-112.27
33	2,2,4-trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77	-107.38
34	2,3,3-trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56	-100.70
35	2,3,4-trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14	-109.21
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92	-53.52
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88	-80.40
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34	-107.64
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34	-113.20
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81	-114.90
41	4-ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81	
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80	-113.00
43	2,3-dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34	-116.00
44	2,4-dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30	
45	2,5-dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30	
46	2,6- dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83	-102.90
47	3,3- dimethylheptane	137.300	176.897	43.6870	42.66	314.00	24.19	22.01	
48	3,4- dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80	
49	3,5- dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77	
50	4,4- dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01	
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80	
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77	
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22	
54	2,2,4- trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51	-120.00
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80	

continued...

S.No.	Alkane	bp($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87	
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-99.0
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37	-66.54
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12

Table 2.

S.No.	Alkane	$M_1(G)$	$F(G)$	$M_2(G)$	$R(G)$	$ABC(G)$	$AZI(G)$	$GA(G)$	$H(G)$	$SCI(G)$	$RR(G)$
1	Butane	10	18	8	1.9142	2.1213	24	2.8856	1.833	1.6547	4.8284
2	2-methyl propane	12	30	4	1.7320	2.4494	10.125	2.5980	1.5	1.5	5.1961
3	Pentane	14	26	12	2.4142	2.8284	32	3.8856	2.333	2.1547	6.8284
4	2-methyl butane	16	38	14	2.2700	3.0472	22.75	3.6546	2.0666	2.0245	7.3278
5	2,2 dimethylpropane	20	68	16	2	3.4641	9.48	3.2	1.6	1.7888	8
6	Hexane	18	34	16	2.9142	3.5355	40	5.8856	2.8333	2.6567	8.8284
7	2-methylpentane	20	46	18	2.77	3.7543	30.75	4.6546	2.5666	2.5245	9.3278
8	3-methyalpentane	20	46	19	2.808	3.6449	35.375	4.7112	2.6333	2.5491	9.1416
9	2,2-methylbutane	24	76	22	2.5606	4.0122	23.1109	4.2856	2.5666	2.3272	10.2426
10	2,3-dimethylbutane	22	58	21	2.6427	3.9326	24.89	4.4641	2.3333	2.4082	9.9282
11	Heptanes	22	42	20	3.4142	4.2426	48	5.8856	3.3337	3.1547	10.8284
12	2-methylhexane	24	54	22	3.27	4.4614	38.75	5.8082	3.0666	3.0245	11.3278
13	3-methylhexane	24	54	23	3.3080	4.3320	43.375	5.7112	3.1333	3.0491	11.4594
14	3-ethylpentane	24	54	24	3.3460	4.2426	48	5.7880	3.2	3.0736	11.5911
15	2,2-dimethylpentane	28	84	26	2.8321	4.7193	31.1111	5.2856	3.0666	2.8272	11.8637
16	2,3-dimethylpentane	26	66	26	3.1807	4.5303	37.515	5.5206	2.9	2.9328	12.0598
17	2,4-dimethylpentane	26	66	24	3.1258	4.6801	29.5	5.4236	2.8	2.8944	11.8271
18	3,3-dimethylpentane	28	84	28	3.1213	4.5604	36.7407	5.3712	2.8	2.8656	12.4852
19	Octane	26	50	24	3.9142	4.9497	56	6.8856	3.8333	3.6547	12.8284
20	2-methylheptane	28	62	26	3.77	4.4614	46.75	6.6546	3.5666	3.4855	13.3278
21	3-methylheptane	28	62	27	3.8080	5.0591	51.325	6.7112	3.3	3.5491	13.4594
22	4-methylheptane	28	62	27	3.8080	5.0591	51.325	6.7112	3.6333	3.5491	13.459
23	3-ethylhexane	28	62	28	3.8460	4.9497	56	6.7678	3.7	3.5736	13.5911
24	2,2-dimethylhexane	32	92	30	3.5606	5.4265	41.481	6.2856	3.2	3.3272	14.2426
25	2,3-dimethylhexane	30	74	30	3.6807	5.2374	45.5136	6.7510	2.9	3.4328	14.0598
26	2,4-dimethylhexane	30	74	29	3.6639	5.2779	42.125	6.4802	3.3666	3.4189	13.9588
27	2,5-dimethylhexane	30	74	28	3.6258	5.3870	37.5	6.4236	3.3	3.3944	13.8271
28	3,3-dimethylhexane	32	92	32	3.6213	5.2675	44.7407	6.3712	3.3	3.3656	14.4852
29	3,4-dimethylhexane	30	74	31	3.7187	5.1280	50.1406	6.5772	3.4666	3.4573	14.1915
30	3-ethyl-2-methylpentane	30	74	22	3.7187	5.1280	50.1406	6.5772	3.4666	3.4573	14.015
31	3-ethyl-3-methylpentane	32	92	34	3.6819	5.1086	50.3703	6.4568	3.4	3.4567	14.7279
32	2,2,3-trimethylpentane	34	104	35	3.4813	5.4742	40.3101	6.1783	3.052	3.2441	15.0598
33	2,2,4-trimethylpentane	34	104	32	3.4165	5.6452	34.4861	6.0546	2.9333	3.1971	14.7420
34	2,3,3-trimethylpentane	34	104	36	3.5040	5.4247	50.398	6.2074	3.0857	3.2579	15.1708
35	2,3,4-trimethylpentane	32	86	33	3.5534	5.4158	39.6562	6.3301	3.1666	3.3164	14.6602
36	Nonane	30	58	28	4.4142	5.6568	64	7.8856	4.3333	4.1547	14.8284
37	2-methyloctane	32	70	30	4.27	5.8756	54.75	7.6546	4.0666	4.0245	15.3278
38	3-methyloctane	32	70	31	4.3080	5.7662	59.375	7.7112	4.1333	4.0491	15.4594
39	4-methyloctane	32	70	31	4.3080	5.7662	59.375	7.7112	4.1333	4.0491	15.4594
40	3-ethylheptane	32	70	32	4.3460	5.6568	64	7.7678	4.2	4.0736	15.5911
41	4-ethylheptane	32	70	32	4.3460	5.6568	63	7.7678	4.2	4.0736	15.5911
42	2,2-dimethylheptane	36	100	34	4.0606	6.1336	47.1111	7.2856	3.7	3.8272	16.2426
43	2,3-dimethylheptane	34	82	34	4.1807	5.9445	53.5156	7.5206	3.9	3.9328	16.0598
44	2,4-dimethylheptane	34	82	33	4.1639	5.9850	50.125	7.4802	3.8666	3.9189	15.9588
45	2,5-dimethylheptane	34	82	33	4.1639	5.9850	50.125	7.4802	3.8666	3.9189	15.9588

S.No.	Alkane	$M_1(G)$	$F(G)$	$M_2(G)$	$R(G)$	$ABC(G)$	$AZI(G)$	$GA(G)$	$H(G)$	$SCI(G)$	$RR(G)$
46	2,6- dimethylheptane	34	82	32	4.1258	5.9850	69.125	7.4236	3.8	3.8944	15.8271
47	3,3- dimethylheptane	36	100	36	4.1213	6.0944	52.7407	7.4082	3.8	3.8656	16.4852
48	3,4- dimethylheptane	34	82	35	4.2187	5.8351	58.1406	7.5772	3.9666	3.9573	16.1915
49	3,5- dimethylheptane	34	82	34	4.2019	5.8756	54.75	7.5368	3.9333	3.9435	16.0904
50	4,4- dimethylheptane	36	100	36	4.1213	5.9746	52.7407	7.3712	3.8	3.8656	16.4852
51	3-ethyl-2-methylhexane	34	82	35	4.2187	5.8351	58.1406	7.5772	3.9666	3.9573	16.1915
52	4-ethyl-2-methylhexane	34	82	34	4.2019	5.8756	54.75	7.5368	3.9333	3.9435	16.0904
53	3-ethyl-3-methylhexane	36	100	36	4.2567	5.8157	62.7656	7.4568	3.9	3.9040	16.7279
54	2,2,4- trimethylhexane	38	112	37	3.9545	6.2429	48.4861	7.1112	3.5	3.7216	16.8736
55	2,2,5- trimethylhexane	38	112	36	3.9165	6.3523	37.8611	7.0546	3.4333	3.6971	16.7420
56	2,3,3- trimethylhexane	38	112	40	4.0040	6.1318	43.5063	7.2074	3.5857	3.7579	17.1708
57	2,3,4- trimethylhexane	36	112	44	4.0914	6.0135	52.2812	7.3867	3.7333	3.8410	16.7919
58	2,3,5- trimethylhexane	36	94	36	4.0365	6.1633	44.2656	7.2897	3.6333	3.8800	16.5592
59	3,3,4- trimethylhexane	38	112	41	4.0420	6.0224	53.9397	7.2639	3.6523	3.7925	17.3024
60	3,3-diethylpentane	44	112	40	4.2446	5.6568	64	7.5424	4	3.9423	16.9705
61	2,2-dimethyl-3-ethylpentane	54	116	40	4.0193	5.9234	55.949	7.2349	3.6190	3.7687	17.1915
62	2,3-dimethyl-3-ethylpentane	46	144	42	4.0646	5.9729	54.9443	7.2930	3.6857	3.7963	17.4134
63	2,4-dimethyl-3-ethylpentane	44	136	38	4.0914	6.0135	52.2812	7.3867	3.7333	3.8410	16.7919
64	2,2,3,3-tetramethylpentane	42	142	46	3.8106	6.3567	46.8148	6.8856	3.25	3.5752	18.2426
65	2,2,3,4- tetramethylpentane	40	124	42	3.8540	6.3597	42.4507	6.9878	3.3190	3.6278	17.6602
66	2,2,4,4- tetramethylpentane	42	142	40	3.7071	6.6103	30.2222	6.6856	3.06666	3.4997	17.6568
67	2,3,3,4- tetramethylpentane	40	124	44	4.2540	6.2890	45.8887	7.0435	3.3714	3.6503	17.8564

3 Regression Models

We have tested the following linear regression model

$$P = A + B(TI) \tag{11}$$

where P = physical property, TI = topological index .

Using (11), we have obtained the following different linear models for each degree based topological index, which are listed below.

1.**First Zagreb index** $M_1(G)$**:**

$$bp = 16.9427 + [M_1(G)]3.0529 \tag{12}$$
$$mv = 65.8469 + [M_1(G)]3.1056 \tag{13}$$
$$mr = 20.3361 + [M_1(G)]0.614 \tag{14}$$
$$hv = 13.1094 + [M_1(G)]0.8266 \tag{15}$$
$$ct = 135.3490 + [M_1(G)]4.8692 \tag{16}$$
$$cp = 34.9036 - [M_1(G)]0.2657 \tag{17}$$
$$st = 14.5896 + [M_1(G)]0.2038 \tag{18}$$
$$mp = -135.2755 + [M_1(G)]0.8934 \tag{19}$$

2.**Second Zagreb index** $M_2(G)$**:**

$$bp = 0.0831 + [M_2(G)]3.6857 \tag{20}$$
$$mv = 83.0532 + [M_2(G)]2.5335 \tag{21}$$
$$mr = -141.6210 + [M_2(G)]5.9622 \tag{22}$$
$$hv = 18.0481 + [M_2(G)]0.6647 \tag{23}$$
$$ct = 121.3978 + [M_2(G)]5.4413 \tag{24}$$
$$cp = 28.5274 - [M_2(G)]0.0767 \tag{25}$$
$$st = 0.3013 + [M_2(G)]0.3013 \tag{26}$$
$$mp = -109.3121 + [M_2(G)]0.0660 \tag{27}$$

3.**Forgotten index** $F(G)$**:**

$$bp = 40.6893 + [F(G)]0.8644 \quad (28)$$
$$mv = 129.1337 + [F(G)]0.3998 \quad (29)$$
$$mr = 29.8717 + [F(G)]0.1150 \quad (30)$$
$$hv = 30.9511 + [F(G)]0.0945 \quad (31)$$
$$ct = 199.0880 + [F(G)]1.0812 \quad (32)$$
$$cp = 30.9385 - [F(G)]0.0529 \quad (33)$$
$$st = 17.5492 + [F(G)]0.0410 \quad (34)$$
$$mp = -135.1700 + [F(G)]0.3862 \quad (35)$$

4.**Randić index** $R(G)$**:**

$$bp = -98.6135 + [R(G)]57.5074 \quad (36)$$
$$mv = 50.5734 + [R(G)]30.2112 \quad (37)$$
$$mr = 5.9622 + [R(G)]9.0465 \quad (38)$$
$$hv = 3.1679 + [R(G)]9.6368 \quad (39)$$
$$ct = 36.0566 + [R(G)]68.8462 \quad (40)$$
$$cp = 42.8740 - [R(G)]4.4586 \quad (41)$$
$$st = 8.2806 + [R(G)]3.4046 \quad (42)$$
$$mp = -150.8451 + [R(G)]13.1312 \quad (43)$$

5.**Atom-Bond Connectivity Index** $ABC(G)$**:**

$$bp = -64.7160 + [ABC(G)]33.6873 \quad (44)$$
$$mv = 76.1097 + [ABC(G)]16.2563 \quad (45)$$
$$mr = 13.1497 + [ABC(G)]4.9545 \quad (46)$$
$$hv = 14.7594 + [ABC(G)]4.5345 \quad (47)$$
$$ct = 85.4513 + [ABC(G)]38.6361 \quad (48)$$
$$cp = 38.6749 - [ABC(G)]2.3100 \quad (49)$$
$$st = 12.3796 + [ABC(G)]1.6096 \quad (50)$$
$$mp = -157.1321 + [ABC(G)]10.3371 \quad (51)$$

6.**Augumented Zagreb Index** $AZI(G)$**:**

$$bp = -6.9694 + [AZI(G)]2.5772 \quad (52)$$
$$mv = 86.3797 + [AZI(G)]1.6020 \quad (53)$$
$$mr = 18.4166 + [AZI(G)]0.4449 \quad (54)$$
$$hv = 15.3597 + [AZI(G)]0.4981 \quad (55)$$
$$ct = 119.2045 + [AZI(G)]3.6270 \quad (56)$$
$$cp = 28.6614 - [AZI(G)]0.0534 \quad (57)$$
$$st = 10.3607 + [AZI(G)]0.2215 \quad (58)$$
$$mp = -106.8160 + [AZI(G)]0.0164 \quad (59)$$

7.**Geometric-Airthmetic Index** $GA(G)$**:**

$$bp = -71.0005 + [GA(G)]28.2980 \quad (60)$$
$$mv = 63.8346 + [GA(G)]15.0577 \quad (61)$$
$$mr = 9.9345 + [GA(G)]4.5087 \quad (62)$$
$$hv = 28.9943 + [GA(G)]1.5901 \quad (63)$$
$$ct = 68.6852 + [GA(G)]33.9443 \quad (64)$$
$$cp = 40.7758 - [GA(G)]2.2006 \quad (65)$$
$$st = 10.1002 + [GA(G)]1.6478 \quad (66)$$
$$mp = -147.7301 + [GA(G)]6.9956 \quad (67)$$

8.**Harmonic Index** $H(G)$**:**

$$bp = -79.2906 + [H(G)]56.7151 \quad (68)$$
$$mv = 65.6773 + [H(G)]28.3820 \quad (69)$$
$$mr = 10.7879 + [H(G)]8.4097 \quad (70)$$
$$hv = 6.5238 + [H(G)]9.4834 \quad (71)$$
$$ct = 61.9426 + [H(G)]67.0777 \quad (72)$$
$$cp = 41.5159 - [H(G)]4.4392 \quad (73)$$
$$st = 9.6866 + [H(G)]3.2849 \quad (74)$$
$$mp = -132.8786 + [H(G)]8.7228 \quad (75)$$

9.**Sum-Connectivity Index** $SCI(G)$**:**

$$bp = -87.5509 + [SCI(G)]58.4106 \quad (76)$$
$$mv = 54.8446 + [SCI(G)]31.1247 \quad (77)$$
$$mr = 7.3150 + [SCI(G)]9.2986 \quad (78)$$
$$hv = 4.9328 + [SCI(G)]9.8115 \quad (79)$$
$$ct = 49.0257 + [SCI(G)]70.0084 \quad (80)$$
$$cp = 42.1462 - [SCI(G)]4.5669 \quad (81)$$
$$st = 9.0043 + [SCI(G)]3.4385 \quad (82)$$
$$mp = -152.6617 + [SCI(G)]14.6904 \quad (83)$$

10.**Reciprocal Randić Index** $RR(G)$**:**

$$bp = -33.6900 + [RR(G)]10.3117 \quad (84)$$
$$mv = 53.8976 + [RR(G)]7.0504 \quad (85)$$
$$mr = 9.2765 + [RR(G)]2.0924 \quad (86)$$
$$hv = 10.1679 + [RR(G)]1.9853 \quad (87)$$
$$ct = 72.2490 + [RR(G)]15.1722 \quad (88)$$
$$cp = 29.0700 - [RR(G)]0.2027 \quad (89)$$
$$st = 8.1983 + [RR(G)]0.8754 \quad (90)$$
$$mp = -104.9739 + [RR(G)]0.1913 \quad (91)$$

Table 3. Statical parameters for the linear QSPR model for $M_1(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	16.9427	3.0529	0.8168	21.4370	135.797
Molar volume	65	65.8469	3.1056	0.800	10.7804	111.939
Molar refraction	65	20.3361	0.6139	0.837	2.92267	147.601
Heats of vaporization	65	13.1094	0.8266	0.714	3.8422	65.631
Critical temperature	67	135.3490	4.8692	0.856	23.8350	178.878
Critical Pressure	67	34.9036	-0.2657	0.686	2.2970	57. 891
Surface tension	64	14.5896	0.2038	0.329	1.8716	7.531
Melting point	51	-135.2755	0.8934	0.286	39.2743	4.350

Table 4. Statical parameters for the linear QSPR model for $M_2(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	0.0831	3.6857	0.859	19.3021	182.290
Molar volume	65	83.0532	2.5335	0.806	11.6501	117.038
Molar refraction	65	-141.6210	5.9622	0.854	24.0913	170.172
Heats of vaporization	65	18.0481	0.6647	0.737	3.4930	74.858
Critical temperature	67	121.3978	5.4413	0.898	20.9913	271.031
Critical Pressure	67	28.5274	-0.0767	0.688	0.4882	58.450
Surface tension	64	0.3012	0.3012	0.777	1.4420	94.571
Melting point	51	-109.3121	0.06607	0.267	0.5939	3.830

Table 5. Statical parameters for the linear QSPR model for $F(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	40.6893	0.8644	0.673	27.86510	53.802
Molar volume	65	129.1337	0.3998	0.595	14.4374	34.539
Molar refraction	65	29.8717	0.1150	0.613	4.2221	37.917
Heats of vaporization	65	30.9511	0.0945	0.498	4.7615	20.757
Critical temperature	67	199.0880	1.0812	0.704	32.7746	63.982
Critical Pressure	67	30.9385	-0.0529	0.486	2.7595	20.148
Surface tension	64	17.5492	0.0410	0.595	1.5932	33.957
Melting point	51	-135.1700	0.3862	0.283	39.3090	4.256

Table 6. Statical parameters for the linear QSPR model for $R(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	-98.6135	57.5074	0.986	6.3398	2227.243
Molar volume	65	50.5734	30.2112	0.954	5.1516	633.831
Molar refraction	65	5.9622	9.0465	0.960	1.4943	742.626
Heats of vaporization	65	3.1679	9.6368	0.995	0.5237	6858.829
Critical temperature	67	36.0566	68.8462	0.962	12.084	813.917
Critical Pressure	67	42.8740	-4.4586	0.911	1.3024	317.224
Surface tension	64	8.2806	3.4046	0.909	0.8278	293.379
Melting point	51	-150.8451	13.1312	0.219	40.0107	2.404

Table 7. Statical parameters for the linear QSPR model for $ABC(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	-64.7160	33.6873	0.909	15.7398	307.340
Molar volume	65	76.1097	16.2563	0.802	10.7319	113.523
Molar refraction	65	13.1497	4.9545	0.822	3.0456	130.942
Heats of vaporization	65	14.7594	4.5345	0.732	3.7407	72.707
Critical temperature	67	85.4531	38.6361	0.850	24.3046	169.545
Critical Pressure	67	38.6749	-2.310	0.743	2.1135	80.147
Surface tension	64	12.3796	1.6096	0.7	1.4153	59.598
Melting point	51	-157.1321	10.3371	0.28	39.3439	4.161

Table 8. Statical parameters for the linear QSPR model for $AZI(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	-6.9694	2.5772	0.874	18.3086	209.855
Molar volume	65	86.3797	1.6020	0.736	12.1528	74.673
Molar refraction	65	18.4166	0.4449	0.754	3.5124	82.803
Heats of vaporization	65	15.3597	0.4981	0.884	2.5599	225.327
Critical temperature	67	119.2045	3.6270	0.85	24.2238	169.745
Critical Pressure	67	28.6614	-0.0534	0.718	2.1981	69.191
Surface tension	64	10.3607	0.2215	0.834	1.0922	142.177
Melting point	51	-106.8160	-0.0164	0.248	26.6226	3.288

Table 9. Statical parameters for the linear QSPR model for $GA(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	-71.0005	28.2980	0.985	6.4949	2119.065
Molar volume	65	63.8346	15.0577	0.966	4.6216	888.866
Molar refraction	65	9.9345	4.5087	0.973	1.2389	1108.954
Heats of vaporization	65	28.1143	1.5901	0.987	0.87	2445.486
Critical temperature	67	68.6852	33.9443	0.964	12.3561	842.477
Critical Pressure	67	40.7758	-2.2006	0.913	1.2876	326.062
Surface tension	64	10.1002	1.6478	0.9	0.8688	260.665
Melting point	51	-147.73	6.9956	0.235	31.8327	2.684

Table 10. Statical parameters for the linear QSPR model for $H(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	-79.2906	56.7151	0.941	12.7832	499.372
Molar volume	65	65.6773	28.3820	0.879	8.5769	213.372
Molar refraction	65	10.7879	8.4097	0.875	2.5844	206.325
Heats of vaporization	65	6.5238	9.4834	0.961	1.5249	753.562
Critical temperature	67	61.9426	67.0777	0.908	19.3752	304.072
Critical Pressure	67	41.5159	-4.4392	0.878	1.5112	218.902
Surface tension	64	9.6866	3.2849	0.847	1.0534	157.487
Melting point	51	-132.8786	8.7228	0.487	10.1211	15.193

Table 11. Statical parameters for the linear QSPR model for $SCI(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	-87.5509	58.4106	0.988	5.9054	2576.911
Molar volume	65	54.8446	31.1247	0.965	4.7229	848.465
Molar refraction	65	7.3150	9.2986	0.969	1.3194	970.321
Heats of vaporization	65	4.9328	9.8115	0.995	0.5385	6484.601
Critical temperature	67	49.0257	70.0084	0.963	12.3871	837.949
Critical Pressure	67	42.1462	-4.5669	0.920	1.2342	360.616
Surface tension	64	9.001	3.4385	0.901	0.8581	268.756
Melting point	51	-152.6617	14.6904	0.240	39.7853	2.988

Table 12. Statical parameters for the linear QSPR model for $RR(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	67	-33.6900	10.3117	0.938	13.0131	479.064
Molar volume	65	53.8976	7.0504	0.934	6.4264	429.341
Molar refraction	65	9.2765	2.0924	0.962	1.4521	790.070
Heats of vaporization	65	10.1679	1.9852	0.871	2.6928	197.584
Critical temperature	67	72.2490	15.1722	0.951	14.2558	612.794
Critical Pressure	67	29.0700	-0.2027	0.827	1.7728	140.787
Surface tension	64	8.1983	0.8754	0.848	1.0505	158.701
Melting point	51	-104.9739	-0.1913	0.277	26.4055	4.168

4 Discussion and Concluding Remarks

By inspection of the data given in tables 3 to 12, it is possible to draw a number of conclusions for the given degree based topological indices.

First, the famous and much studied Zagreb indices (first Zagreb index and second Zagreb index) were found to be completely inadequate for any structure-property correlation, except the correlation of second Zagreb index with the critical temperature of the alkanes with correlation coefficient value $r = 0.898$. This important details seems to have been ignored in recent comprehensive surveys [1,2,3,5], in Zagreb indices.

In addition, the results for forgotten index revealed that the recent advocated idea of using forgotten index does not pass the test.

The Randić index is one of the most often applied molecular-graph-based structure descriptor. In table 6, one can easily verify that Randić index shows good correlation with all physical properties of alkanes, except their melting points with correlation coefficient value $r = 0.219$. Further, we can see that the range of correlation coefficient values lies between 0.881 to 0.995. Surprisingly, Randić index shows very high correlation with heats of vaporization of the alkanes with correlation coefficient value $r = 0.995 \approx 1$.

The QSPR study of atom-bond connectivity(ABC) index reveals that the ABC-index is an useful tool to predict the boiling points of alkanes with correlation coefficient value $r = 0.909$.

In [7] Furtula et. al., have shown that the prediction power of augumented Zagreb index (AZI) is better than the ABC-index in the study of heats of formation for heptanes and octanes. In table 8, one could see that the above argument is true for alkanes for predicting the heats of formations with correlation coefficient value $r = 0.884$.

The QSPR study of the geometric-arithmetic index revealed that the predicting power of geometric-arithmetic index for the physical properties of alkanes is equally good as Randić index. The correlation coefficient values lies between 0.889 to 0.987 except for melting points of alkanes, with correlation coefficient value $r = 0.235$. Surprisingly, we could see that the correlation of GA-index with heats of vaporization of alkanes is very high with correlation coefficient $r = 0.987 \approx 1$. Thus GA-index found to be useful tool in predicting the physical properties of alkanes.

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 10, reveals that harmonic index is also an useful tool in predicting the heats of vaporization and critical temperatures of alkanes with correlation coefficient values $r = 0.961$ and $r = 0.908$ respectively. Further, harmonic index shows good correlation with physical properties of alkanes with correlation coefficient values lies between 0.807 to 0.961 except melting points of the alkanes, where the correlation coefficient value of harmonic index with melting points of alkanes is 0.487.

The so called sum-connectivity index shows remarkably similar correlation properties [5]. The QSPR study in table 11 reveals that the predicting power of sum-connectivity index is very high compared to other degree based topological indices. The value of correlation coefficient of sum-connectivity index with physical properties of alkanes lies between 0.887 to 0.995 except melting points of alkanes, where the correlation coefficient value of sum-connectivity index with melting points of alkanes is very low viz, r = 0.240. Further, the r value of sum-connectivity index is very high for the heats of valorizations of alkanes with $r = 0.995 \sim 1$. Thus the QSPR study reveals that the sum-connectivity index is an useful tool in predicting the physical properties of alkanes.

In addition, the QSPR study of reciprocal Randić index shows that the predicting power of reciprocal Randić index is better than Zagreb indices, forgotten index and augumented Zagreb index. Table 12 reveals that the predicting power of reciprocal Randić index with boiling points, molar volumes, molar refractions and critical temperatures of alkanes is reasonably good with correlation coefficient values $r = 0.938, 0.934, 0.962$ and 0.951 respectively.

From practical point of view, topological indices for which the absolute value of correlation coefficient is less than 0.8 can be characterized as useless. Thus, the QSPR study of these 10 degree-based topological indices with physical properties of 67 alkanes helps us to characterize useful topological indices with absolute value of correlation coefficient lies between 0.8 to 0.995.

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