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QSPR Analysis of Chemical Graph Theory

Rachanna Kanabur^{a,*}, S.K.Giregol^a, Akshata Nagaral, Priyanka Badave, Rekha Sannakkai, Renuka Sasalatti^a

^aDepartment of Mathematics BLDEA's, Commerce, B.H.S. Arts and T.G.P. Science College, Jamkhandi Karnataka, India.

Abstract

In this paper, we find the values of four important degree-based topological indices of molecular graph of alkane isomers. Further, we show that these parameters are highly correlated with physical properties of alkane isomers. . ©2019 All rights reserved.

Keywords: Alkane isomers,, Degree-based topological indices.

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1. Introduction

Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u . The edge connecting the vertices u and v is denoted by uv [4].

Chemical graph theory is the branch of mathematical chemistry. It is concerned with handling chemical graphs that represent chemical system. Hence chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. It has found to be a useful tool in QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) [8, 5, 14]. Numerous studies have been made relating to the above mentioned fields by using what are called topological indices. In 1975, Randic [10] proposed a topological index that has become one of the most widely used in both QSAR and QSPR studies.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [4, 2, 11]. This theory had an important effect on the development of the chemical sciences.

*Corresponding author

Email addresses: rachukanabur@gmail.com (Rachanna Kanabur), oladalalaa@yahoo.com (S.K.Giregol), olimat_anas@yahoo.com (Akshata Nagaral, Priyanka Badave, Rekha Sannakkai, Renuka Sasalatti)

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2. Computing Some New Degree-Based Topological Indices

We consider the following most studied degree based topological indices for QSPR study [12, 14, 15, 16].

Definition 2.1. Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u , then Arithmetic-Geometric Index (AG_1 index) of G is defined as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) \cdot d_G(v)}}$$

Where, (AG_1 index) is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v , where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex u (or v).

Definition 2.2. The SK index of a graph $G = (V, E)$ is defined as $SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G .

Definition 2.3. The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) \cdot d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G .

Definition 2.4. The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G .

Motivation

By looking at the earlier results QSPR Analysis of Certain Degree-Based Topological Indices and QSPR Analysis of Degree-Based Topological Indices with physical properties of Benzenoid Hydrocarbons [7, 5, 6, 13].

3. Data Sources and Analytical Method

Energy of Alkane isomers are taken from [19, 7, 12, 5]. Seven physicochemical properties of Alkane isomers have been selected on the availability of a suitable body of data: *boiling point* (BP), *critical temperature* (CT), *critical pressure* (CP), *Molar volume* (CV), *Molar refraction* (MR), *Heat of Vaporization* (HV), *Surface tension* (ST). The values are compiled in Table 2.

4. Results and Discussion

In Table 3, the correlation coefficient of topological indices with physicochemical properties of alkane isomers are found to be good.

4.1. Regression Models

We have tested the following linear regression model

$$P = a + b(TI) \quad (4.1)$$

where, P =Physical property, TI =Topological Index. Using (4.1), we have obtained the following different linear models for each degree-based topological index, which are listed below.

Table 1: The topological indices (AG1 Index, SK Index, SK1 Index and SK2 Index) values of Alkane Isomers.

S.NO.	Compound Name	AG1	SK	SK1	SK2
		Index	Index	Index	Index
1	Butane	3.1213	5	4	8.5
2	2-methyl propane	3.46410	6	4.5	12
3	Pentane	4.123	7	6	12.5
4	2-methyl butane	4.3906	8	7	16.5
5	2,2 dimethyl propane	5	10	8	25
6	Hexane	5.1213	9	8	16.5
7	2-methyl pentane	5.2359	10	9	20.5
8	3- methyl pentane	5.3172	10	9.5	21
9	2,2-dimethyl butane	5.8713	12	11	30
10	2,3- dimethyl butane	5.6188	11	10.5	25
11	Heptanes	6.1213	11	10	20.5
12	2-methyl hexane	6.3906	12	11	24.5
13	3- methyl hexane	6.5767	12	11.5	25
14	3-ethylpentane	6.2438	12	12	25.5
15	2,2-dimethyl pentane	6.8713	14	13	34
16	2,3- dimethyl pentane	6.54530	13	13	29.5
17	2,4- dimethyl pentane	6.6600	13	12	28.5
18	3,3- dimethyl pentane	6.7426	14	14	35
19	Octane	7.1213	13	12	24.5
20	2-methylheptane	7.3906	14	13	28.5
21	3- methylheptane	7.3172	14	13.5	29
22	4- methylheptane	7.3172	14	13.5	29
23	3-ethylhexane	7.2438	14	14	29.5
24	2,2-dimethylhexane	7.8713	16	15	38
25	2,3- dimethylhexane	7.5453	15	15	33.5
26	2,4- dimethylhexane	7.5866	15	14.5	33
27	2,5- dimethylhexane	7.6600	15	14	32.5
28	3,3- dimethylhexane	7.7426	16	16	39
29	3,4- dimethylhexane	7.4719	15	15.5	34
30	3-ethyl-2-methylpentane	7.4719	15	15.5	34
31	3-ethyl-3-methylpentane	7.6139	16	17	40
32	2,2,3-trimethylpentane	7.9963	17	17.5	43.5
33	2,2,4- trimethylpentane	8.1406	17	16	42
34	2,3,3- trimethylpentane	7.9410	17	18	44
35	2,3,4- trimethylpentane	8.4401	16	16.5	38
36	Nonane	8.1213	15	14	28.5
37	2-methyloctane	8.3906	16	15	32.5
38	3-methyloctane	8.3172	16	15.5	33
39	4-methyloctane	8.3172	16	15.5	33
40	3-ethylheptane	8.2438	16	16	33.5
41	4- ethylheptane	8.2438	16	16	33.5
42	2,2-dimethylheptane	8.8713	18	17	42
43	2,3- dimethylheptane	8.5453	17	17	37.5
44	2,4- dimethylheptane	10.8960	17	16.5	37
45	2,5- dimethylheptane	8.5866	17	16.5	37
46	2,6- dimethylheptane	8.6600	17	16	36.5
47	3,3- dimethylheptane	8.7426	18	18	43
48	3,4- dimethylheptane	7.4719	17	17.5	38
49	3,5- dimethylheptane	8.5132	17	17	37.5
50	4,4- dimethylheptane	8.7426	18	18	43
51	3-ethyl-2-methylhexane	8.4719	17	17.5	38
52	4-ethyl-2-methylhexane	8.5132	17	17	37.5
53	3-ethyl-3-methylhexane	7.0229	18	19	44
54	2,2,4-trimethylhexane	9.0672	19	18.5	46.5
55	2,2,5- trimethylhexane	9.1406	19	18	46
56	2,3,3- trimethylhexane	8.9410	19	20	48
57	2,3,4- trimethylhexane	8.7000	18	19	42.6
58	2,3,5- trimethylhexane	8.8147	18	18	41.5
59	3,3,4- trimethylhexane	8.8676	19	20.5	48.5
60	3,3-diethylpentane	8.4852	18	20	40.5
61	2,2-dimethyl-3-ethylpentane	8.9229	19	20	44.75
62	2,3-dimethyl-3-ethylpentane	8.8124	19	21	49
63	2,4-dimethyl-3-ethylpentane	8.7000	18	19	42.5
64	2,2,3,3-tetramethylpentane	9.3713	21	23	58.5
65	2,2,3,4- tetramethylpentane	9.2244	20	21	52
66	2,2,4,4- tetramethylpentane	9.6213	21	20	55.5
67	2,3,3,4- tetramethylpentane	9.1395	20	22	53

1. AG_1 Index ($AG_1(G)$)

$$Bp = 3.992 + 0.033AG_1(G) \quad (4.2)$$

$$CT = -0.976 + 0.03AG_1(G) \quad (4.3)$$

$$CP = 18.622 - 0.414AG_1(G) \quad (4.4)$$

$$MV = -3.525 + 0.069AG_1(G) \quad (4.5)$$

$$ST = -2.608 + 0.495AG_1(G) \quad (4.6)$$

Table 2: The physical and chemical properties (BP, MV, MR, HV, CT, CP, ST) of Alkane Isomers.

S.NO.	Compound Name	Bp(0C)	mv(cm3)	mr(cm3)	hv(kJ)	ct(0C)	cp(atm)	St(dyne/cm)
1	Butane	-0.500		20.68	22.44	152.01	37.47	12.46
2	2-methyl propane	-11.730		20.85	21.6	134.98	36	14.1
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00
5	2,2 dimethyl propane	9.503	112.074	25.7243	21.78	160.60	31.57	12.05
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42
7	2-methyl pentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38
8	3- methyl pentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12
9	2,2-dimethyl butane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30
10	2,3- dimethyl butane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26
12	2-methyl hexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29
13	3- methyl hexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44
15	2,2-dimethyl pentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02
16	2,3- dimethyl pentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96
17	2,4- dimethyl pentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15
18	3,3- dimethyl pentane	86.064	144.530	34.3323	33.02	263.00	30	19.59
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60
21	3- methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17
22	4- methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00
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
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
27	2,5- dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73
28	3,3- dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63
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
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67
33	2,2,4- trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77
34	2,3,3- trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56
35	2,3,4- trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81
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
43	2,3- dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34
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
47	3,3- dimethylheptane	137.00	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
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38
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
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31

Table 3: Correlation of topological indices with physicochemical properties of Alkane isomers.

	Bp (⁰)	ct (⁰ C)	cp (atm)	mv (cm ³)	st ($\frac{\text{dyne}}{\text{cm}}$)	hv (kJ)	mr (cm ³)
AG ₁	0.8463	0.8946	-0.8514	0.9186	0.8308	0.8614	0.9467
SK	0.8211	0.8945	-0.7661	0.8736	0.8097	0.8176	0.927
SK ₁	0.8112	0.8959	-0.6730	0.8047	0.8290	0.7910	0.8864
SK ₂	0.6841	0.7784	-0.5897	0.8047	0.6870	0.6522	0.7987

$$HV = -0.7 + 0.216AG_1 (G) \quad (4.7)$$

$$MR = -1.586 + 0.236AG_1 (G) \quad (4.8)$$

2. SK Index

$$Bp = 7.116 + 0.074SK (G) \quad (4.9)$$

$$CT = -4.689 + 0.069SK (G) \quad (4.10)$$

$$CP = 38.327 - 0.867SK (G) \quad (4.11)$$

$$MV = -9.553 + 0.155SK (G) \quad (4.12)$$

$$ST = -7.885 + 1.122SK (G) \quad (4.13)$$

$$HV = -3.07 + 0.478SK (G) \quad (4.14)$$

$$MR = -5.664 + 0.538SK (G) \quad (4.15)$$

3. SK₁ Index

$$Bp = 5.565 + 0.087SK_1 (G) \quad (4.16)$$

$$CT = -8.611 + 0.083SK_1 (G) \quad (4.17)$$

$$CP = 39.199 - 0.905SK_1 (G) \quad (4.18)$$

$$MV = -12.542 + 0.172SK_1 (G) \quad (4.19)$$

$$ST = -13.031 + 1.365SK_1 (G) \quad (4.20)$$

$$HV = -5.945 + 0.549SK_1 (G) \quad (4.21)$$

$$MR = -8.648 + 0.611SK_1 (G) \quad (4.22)$$

4. SK₂ Index

$$Bp = 15.014 + 0.182SK_2 (G) \quad (4.23)$$

$$CT = -16.102 + 0.178SK_2 (G) \quad (4.24)$$

$$CP = 87.24 - 1.965SK_2 (G) \quad (4.25)$$

$$MV = -12.542 + 0.172SK_2 (G) \quad (4.26)$$

$$ST = -22.813 + 2.802SK_2 (G) \quad (4.27)$$

$$HV = -8.052 + 1.122SK_2 (G) \quad (4.28)$$

$$MR = -18.07 + 1.364SK_2 (G) \quad (4.29)$$

By inspection of the data in Table 4 to Table 7, it is possible to draw a number of conclusions for the given topological indices like invariants.

The QSPR study of $AG_1 (G)$ index reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 4, one can easily verify that $AG_1 (G)$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $AG_1 (G)$ index with physical properties of alkane isomers lies between -0.8514 to 0.9467.

Further, the correlation coefficient value of $AG_1 (G)$ index is very high for the MR of alkane isomers with $r = 0.9467$. Thus the QSPR study reveals that the $AG_1 (G)$ index is an useful tool in predicting the

Table 4: Statistical parameters for the linear QSPR model for AG₁ (G).

Physical Properties	N	a	b	r
Boiling point	67	3.992	0.033	0.8463
Critical temperature	67	-0.976	0.03	0.8946
Critical pressure	67	18.622	-0.414	-0.8514
Molar volume	65	-3.525	0.069	0.9186
ST	67	-2.608	0.495	0.8308
HV	67	-0.7	0.216	0.8614
MR	67	-1.586	0.236	0.9467

Table 5: Statistical parameters for the linear QSPR model for SK (G).

Physical Properties	N	a	b	r
Boiling point	67	7.116	0.074	0.8211
Critical temperature	67	-4.689	0.069	0.8945
Critical pressure	67	38.327	-0.867	-0.7661
Molar volume	65	-9.553	0.155	0.8736
ST	67	-7.885	1.122	0.8097
HV	67	-3.07	0.478	0.8176
MR	67	-5.664	0.538	0.927

Table 6: Statistical parameters for the linear QSPR model for SK₁ (G).

Physical Properties	N	a	b	r
Boiling point	67	5.565	0.087	0.8112
Critical temperature	67	-8.611	0.083	0.8959
Critical pressure	67	39.199	-0.905	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-13.031	1.365	0.829
HV	67	-5.945	0.549	0.791
MR	67	-8.648	0.611	0.8864

Table 7: Statistical parameters for the linear QSPR model for SK₂ (G).

Physical Properties	N	a	b	r
Boiling point	67	15.014	0.182	0.6841
Critical temperature	67	-16.102	0.178	0.7784
Critical pressure	67	87.24	-1.965	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-22.813	2.802	0.687
HV	67	-8.052	1.122	0.6522
MR	67	-18.07	1.364	0.7987

physical properties of alkane isomers. The QSPR study of SK (G) index reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 5, one can easily verify that SK (G) index index shows good correlation with all physical properties of alkane isomers. We can see that the corre-

lation coefficient value of SK (G) index with physical properties of alkane isomers lies between -0.7661 to 0.927. Further, the correlation coefficient value of SK (G) index is very high for the MR of alkane isomers with $r = 0.927$. Thus the QSPR study reveals that the SK (G) index is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of SK_1 (G) index reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 6, one can easily verify that SK_1 (G) index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of SK_1 (G) index with physical properties of alkane isomers lies between -0.673 to 0.8959. Further, the correlation coefficient value of SK_1 index is very high for the CT of alkane isomers with $r = 0.8959$. Thus the QSPR study reveals that the SK_1 (G) index is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of SK_2 (G) index reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 7, one can easily verify that SK_2 (G) index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of SK_2 (G) index with physical properties of alkane isomers lies between -0.673 to 0.7987. Further, the correlation coefficient value of SK_2 (G) index is very high for the MR of alkane isomers with $r = 0.7987$. Thus the QSPR study reveals that the SK_2 (G) index is an useful tool in predicting the physical properties of alkane isomers.

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