

Analysis of Distance 2 Topological Models of Alkanes

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Abstract: Topological Indices serve as mathematical models for the QSPR/QSAR study, which provides the optimum theoretical analysis for expensive practical drug discovery experiments. In this paper, some of the degree-based topological indices concerning the vertices at distance 2 are obtained for alkane groups. And then, some physiochemical properties of Alkanes are analyzed using linear and double regression models.

Keywords: Topological Indices; QSPR/QSAR; correlation and regression models.

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1. Introduction

Let $\mathbb{G}(V, E)$ be a simple, connected, undirected graph of order n and size m . The degree of a vertex v is the number of vertices adjacent to v in \mathbb{G} and is denoted by $d_{\mathbb{G}}(v)$. The distance between two vertices u, v in \mathbb{G} is the length of the shortest path connecting u and v and is denoted by $d(u, v)$.

In the study of quantitative structure-activity and structure-property relationships (QSAR/ QSPR), topological indices (TIs) have great importance. TIs are used to form different regression models, which are powerful tools in the prediction of the physiochemical properties of chemical compounds. TIs widespread application in QSAR/QSPR studies has created a research interest, and several authors have published many papers in this field. For some of the related work, we refer to [1-23].

Zagreb indices [24] were defined in the earlier stage of the study, which was introduced by Gutman and Trinajstic and are defined as $M_1(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})}[d_{\mathbb{G}}(u) + d_{\mathbb{G}}(v)]$ and $M_2(\mathbb{G}) = \sum_{uv \in E(\mathbb{G})}[d_{\mathbb{G}}(u) \times d_{\mathbb{G}}(v)]$. These indices are defined over the edges of \mathbb{G} . B. Sooryanarayana *et al.* [25] generalized the first and the second Zagreb indices of a graph \mathbb{G} , namely the first Zagreb index and the second Zagreb index at a distance l , $1 \leq l \leq diam(\mathbb{G})$ respectively as

$${}_lM_1(\mathbb{G}) = \sum_{d(u,v)=l}[d_{\mathbb{G}}(u) + d_{\mathbb{G}}(v)] \text{ and } {}_lM_2(\mathbb{G}) = \sum_{d(u,v)=l}[d_{\mathbb{G}}(u) \times d_{\mathbb{G}}(v)].$$

From the above idea, in this paper, we have introduced some new topological indices based on the vertices at a distance of two ($l = 2$) instead of adjacent vertices. These indices are computed and are used to obtain regression models with the selected physiochemical properties of a wide range of alkanes. Alkanes are the simplest family of hydrocarbons. They

contain only single-bonded carbon and hydrogen atoms. Each carbon atom forms four bonds, and each hydrogen atom forms one bond.

2. Materials and Methods

Some degree-based TIs at a distance-2 and their definitions are listed in Table 1

Table 1. Definition of some degree-based Topological Indices at distance-2 of a graph G .

Sl.No.	Topological Indices	Definition
1	First Zagreb Index at distance 2	${}_2M_1(G) = \sum_{d(u,v)=2} [d_G(u) + d_G(v)]$
2	Second Zagreb Index at distance 2	${}_2M_2(G) = \sum_{d(u,v)=2} [d_G(u) \times d_G(v)]$
3	Third Zagreb Index at distance 2	${}_3M_1(G) = \sum_{d(u,v)=2} [d_G(u) - d_G(v)]$
4	ABC Index at distance 2	${}_2ABC_2(G) = \sum_{d(u,v)=2} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) \times d_G(v)}}$
5	Randic index at distance 2	${}_2R(G) = \sum_{d(u,v)=2} \frac{1}{\sqrt{d_G(u) \times d_G(v)}}$
6	Sum-connectivity index at distance 2	${}_2SCI(G) = \sum_{d(u,v)=2} \frac{1}{\sqrt{d_G(u) + d_G(v)}}$
7	Reciprocal Randic index at distance 2	${}_2RR(G) = \sum_{d(u,v)=2} \sqrt{d_G(u) \times d_G(v)}$
8	First Gourava index at distance 2	${}_2GO_1(G) = \sum_{d(u,v)=2} [d_G(u) + d_G(v) + d_G(u) \times d_G(v)]$
9	Second Gourava index at distance 2	${}_2GO_2(G) = \sum_{d(u,v)=2} [(d_G(u) \times d_G(v)) (d_G(u) + d_G(v))]$
10	First hyper Gourava index at distance 2	${}_2HGO_1(G) = \sum_{d(u,v)=2} [d_G(u) + d_G(v) + d_G(u) \times d_G(v)]^2$
11	Second hyper Gourava index at distance 2	${}_2HGO_2(G) = \sum_{d(u,v)=2} [(d_G(u) \times d_G(v)) (d_G(u) + d_G(v))]^2$
12	Inverse sum Index at distance 2	${}_2I(G) = \sum_{d(u,v)=2} \frac{d_G(u) \times d_G(v)}{d_G(u) + d_G(v)}$
13	Geometric Arithmetic Index at distance 2	${}_2GA(G) = \frac{2\sqrt{d_G(u) \times d_G(v)}}{d_G(u) + d_G(v)}$
14	Sum connectivity Gourava index at distance 2	${}_2SGO(G) = \sum_{d(u,v)=2} [(d_G(u) \times d_G(v)) + (d_G(u) + d_G(v))]^{-\frac{1}{2}}$

Some physical properties: CT - Critical Temperature; CP - Critical Pressure; BP - Boiling Point; ST- Surface Tension; MR- Molar Refraction; MV-Molar Volumes of 67 alkanes are considered to develop regression models. The values are shown in Table 2.

Table 2. 67-Alkanes and their properties.

no.	Alkanes	bp (°C)	mv (cm ³)	mr (cm ³)	hv(kJ)	ct(°C)	cp (atm)	St
								(dyne/cm)
1	2,2,3,3-Tetramethyl pentane	140.274	169.495	43.2147	41	334.5	27.04	23.38
2	2,2,3,4-Tetramethyl pentane	133.016	173.557	43.4359	41	319.6	25.66	21.8
3	2,2,3-Trimethyl pentane	109.84	159.52	38.92	36.91	294	28.2	20.67
4	2,2,4,4-Tetramethyl pentane	122.284	178.256	43.8747	38.1	301.6	24.58	20.37

no.	Alkanes	bp (°C)	mv (cm3)	mr (cm3)	hv(kJ)	ct(°C)	cp (atm)	St
								(dyne/cm)
5	2,2,4-Trimethyl hexane	126.54	179.22	43.7638	40.57	301	23.39	20.51
6	2,2,4-Trimethyl pentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77
7	2,2,5-Trimethyl hexane	124.084	181.346	43.9356	40.17	296.6	22.41	20.04
8	2,2-Di Methyl butane	49.741	132.744	29.9347	27.69	216.2	30.67	16.3
9	2,2-Dimethyl heptane	132.69	180.5	43.91	42.28	302	22.8	20.8
10	2,2-Dimethyl hexane	107.84	164.28	39.25	37.29	279	25.6	19.6
11	2,2-Dimethyl pentane	79.197	148.695	34.6166	32.43	247.7	28.4	18.02
12	2,2-Dimethyl propane	9.503	112.074	25.7243	21.78	160.6	31.57	-
13	2,2-Dimethyl-3-ethyl pentane	133.83	174.537	43.4571	42.02	322.6	25.96	22.38
14	2,3,3,4-Tetramethyl pentane	141.551	169.928	43.2016	41.75	334.5	26.85	23.31
15	2,3,3-Trimethyl hexane	137.68	173.78	43.4347	42.23	326.1	25.56	22.41
16	2,3,3-Trimethyl pentane	114.76	157.29	38.76	37.22	303	29	21.56
17	2,3,4-Trimethyl hexane	139	173.498	43.4917	42.93	324.2	25.46	22.8
18	2,3,4-Trimethyl pentane	113.46	158.85	38.86	37.61	295	27.6	21.14
19	2,3,5-Trimethyl hexane	131.34	177.656	43.6474	41.42	309.4	23.49	21.27
20	2,3-Dimethyl butane	57.988	130.24	29.8104	29.12	227.1	30.99	17.37
21	2,3-Dimethyl heptane	140.5	176.65	43.63	43.79	315	23.79	22.34
22	2,3-Dimethyl hexane	115.607	160.39	38.98	38.79	293	26.6	20.99
23	2,3-Dimethyl pentane	89.784	144.153	34.3237	34.24	264.6	29.2	19.96
24	2,3-Dimethyl-3-ethyl pentane	142	170.093	42.9542	42.55	338.6	26.94	23.87
25	2,4-Dimethyl heptane	133.5	179.12	43.73	42.87	306	22.7	23.3
26	2,4-Dimethyl hexane	109.42	163.09	39.13	37.76	282	25.8	20.05
27	2,4-dimethyl pentane	80.5	148.949	34.6192	32.88	247.1	27.4	18.15
28	2,4-Dimethyl-3-ethyl pentane	136.73	173.804	43.4037	42.93	324.2	25.46	22.8
29	2,5-Dimethyl heptane	136	179.37	43.84	43.87	307.8	22.7	21.3
30	2,5-Dimethyl hexane	109.1	164.69	39.25	37.86	279	25	19.73
31	2,6-Dimethyl heptane	135.21	180.91	43.92	42.82	306	23.7	20.83
32	2-Methyl butane	27.852	116.426	25.2923	24.59	187.7	32.9	15
33	2-Methyl heptane	117.647	163.663	39.2316	39.68	288	24.8	20.6
34	2-Methyl hexane	90.052	147.656	34.5908	34.8	257.9	27.2	19.29
35	2-Methyl octane	143.26	179.77	43.87	44.65	315	23.6	21.88
36	2-Methyl pentane	60.271	131.933	29.945	29.86	224.9	29.95	17.38
37	2-Methyl propane	-11.73	-	-	-	134.98	36	-
38	3,3,4-Trimethyl hexane	140.46	172.055	43.3407	42.28	330.6	26.45	23.27
39	3,3-Diethyl pentane	146.168	170.185	43.1134	43.36	342.8	26.94	23.75
40	3,3-Dimethyl heptane	137.3	176.897	43.687	42.66	314	24.19	22.01
41	3,3-Dimethyl hexane	111.96	160.87	39	37.93	290.84	27.2	20.63
42	3,3-Dimethyl pentane	86.064	144.53	34.3323	33.02	263	30	19.59
43	3,4-Dimethyl heptane	140.6	175.349	43.5473	43.84	322.7	24.77	22.8
44	3,4-Dimethyl hexane	117.72	158.81	38.84	39.02	298	27.4	21.64
45	3,5-Dimethyl heptane	136	177.386	43.6379	42.98	312.3	23.59	21.77
46	3-Ethyl heptane	143	176.41	43.64	44.81	318	23.98	22.81
47	3-Ethyl hexane	118.53	160.07	38.94	39.4	292	25.74	21.51

no.	Alkanes	bp (°C)	mv (cm3)	mr (cm3)	hv(kJ)	ct(°C)	cp (atm)	St
								(dyne/cm)
48	3-Ethyl pentane	93.475	143.517	34.2827	35.22	267.6	28.6	20.44
49	3-Ethyl-2-methyl hexane	138	175.445	43.655	43.84	322.7	24.77	22.8
50	3-Ethyl-2-methyl pentane	115.65	158.79	38.83	38.52	295	27.4	21.52
51	3-Ethyl-3-methyl hexane	140.6	173.077	43.268	44.04	327.2	25.66	23.22
52	3-Ethyl-3-methyl pentane	118.25	157.02	38.71	37.99	305	28	21.99
53	3-Methyl heptane	118.925	161.832	39.1001	39.83	292	25.6	21.17
54	4-Methyl heptane	117.709	162.105	39.1174	39.67	290	25.6	21
55	3-Methyl hexane	91.85	145.821	34.4597	35.08	262.4	28.1	19.79
56	3-Methyl octane	144.18	177.5	43.72	44.75	318	23.7	22.34
57	3-Methyl pentane	63.282	129.717	29.8016	30.27	231.2	30.83	18.12
58	4,4-Dimethyl heptane	135.2	176.897	43.6022	42.66	317.8	24.18	22.01
59	4-Ethyl heptane	141.2	175.68	43.69	44.81	318.3	23.98	22.81
60	4-Ethyl-2-methyl hexane	133.8	177.386	43.6472	42.98	330.3	25.56	21.77
61	4-Methyl octane	142.48	178.15	43.76	44.75	318.3	23.06	22.34
62	Butane	-0.05	-	-	-	152.01	37.47	-
63	Heptane	98.427	146.54	34.5504	36.55	267.55	27.01	20.26
64	Hexane	68.74	130.688	29.9066	31.55	234.7	29.92	18.42
65	Nonane	150.76	178.71	43.84	46.44	322	22.74	22.92
66	Octane	125.665	162.592	39.1922	41.48	296.2	24.64	21.76
67	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16

The computation of all the TIs mentioned in Table 1 is computed for all the 67 alkanes and is listed in Table 3.

The most used techniques for investigating the relationship between two or more quantitative variables are linear and multiple regression models. Correlation quantifies the strength of the linear relationship between a pair of variables, whereas regression expresses the relationship as an equation. In this paper, we establish a relation between the properties of alkanes and the TIs of the molecular graphs.

In Table 4. Linear regression Model $y = mx + c$ for different properties of alkanes and TIs are listed. Here y represents properties of Alkanes, and x represents TIs at a distance-2 of Alkanes. Also, the correlation coefficient between the properties and the TIs is computed and listed.

Double regression Model $y = a + bx_1 + cx_2$ for properties of alkanes and for all possible combinations of TIs are computed. Here y represents the properties of Alkanes and x_1 and x_2 represents two different TIs at a distance-2 of Alkanes. The correlation coefficient between the properties and the TIs is computed. And also, their error analysis is calculated.

Table 3. Computed TI's at distance-2 for alkanes.

no.	Alkanes	$_2M_1$	$_2M_2$	$_2M_3$	$_2ABC$	$_2R_2$	$_2SCI$	$_2RR$	$_2GO_1$	$_2GO_2$	$_2HGO_1$	$_2HGO_2$	$_2I$	$_2GA$	$_2SGO$
1	2,2,3,3-tetramethylpentane	36	24	8	12.7	10.1	7.94	17.3	60	72	300	560	8.33	12.5	6.24
2	2,2,3,4-Tetramethylpentane	44	38	16	20.7	8.25	6.65	19.8	82	184	772	8336	9.21	10.9	5.14
3	2,2,3-Trimethylpentane	31	25	11	14.0	6.37	5.10	14.1	56	108	444	2928	6.50	8.35	3.95

no.	Alkanes	${}_2M_1$	${}_2M_2$	${}_2M_3$	${}_2ABC$	${}_2R_2$	${}_2SCI$	${}_2RR$	${}_2GO_1$	${}_2GO_2$	${}_2HGO_1$	${}_2HGO_2$	${}_2I$	${}_2GA$	${}_2SGO$
4	2,2,4,4-Tetramethyl pentane	38	34	6	8.48 5	10.4 93	8.06 0	18.4 85	72	176	780	1662 4	9.00 0	12.6 57	6.35 2
5	2,2,4-Trimethyl hexane	36	32	8	13.5 17	7.90 2	6.38 6	17.2 67	68	148	626	7648	8.29 8	10.5 70	4.92 9
6	2,2,4-Trimethyl pentane	30	26	6	9.65 3	7.82 4	6.09 3	14.5 35	56	122	522	7252	7.04 8	9.70 4	4.77 5
7	2,2,5-Trimethyl hexane	34	28	8	12.0 21	8.29 7	6.57 1	16.3 49	62	116	478	3400	7.86 7	10.6 37	5.11 4
8	2,2-Di Methyl butane	20	13	6	7.70 7	5.62 1	4.30 1	9.24 3	33	44	183	520	4.50 0	6.62 8	3.40 7
9	2,2-Dimethyl heptane	32	27	6	11.3 14	7.18 2	5.83 9	15.4 85	59	110	451	2972	7.50 0	9.71 4	4.49 5
10	2,2-Dimethyl hexane	28	23	6	9.89 9	6.68 2	5.33 9	13.4 85	51	94	387	2716	6.50 0	8.71 4	4.14 2
11	2,2-Dimethyl pentane	24	19	6	8.48 5	6.18 2	4.83 9	11.4 85	43	78	323	2460	5.50 0	7.71 4	3.78 8
12	2,2-Dimethyl propane	12	6	0	0.00 0	6.00 0	4.24 3	6.00 0	18	12	54	24	3.00 0	6.00 0	3.46 4
13	2,2-Dimethyl-3-ethyl pentane	42	38	14	19.3 19	7.09 4	5.93 8	19.3 17	80	178	728	5596	8.91 7	10.2 16	4.51 0
14	2,3,3,4-Tetramethyl pentane	48	40	20	25.6 54	7.64 3	6.31 8	20.9 28	88	188	772	5104	10.0 00	10.6 64	4.83 5
15	2,3,3-Trimethyl hexane	42	36	16	21.0 20	7.03 8	5.89 6	18.9 85	78	164	670	4408	9.03 3	10.0 83	4.48 8
16	2,3,3-Trimethyl pentane	38	30	16	20.2 41	6.47 7	5.35 8	16.7 42	68	130	530	2468	8.03 3	8.99 7	4.10 7
17	2,3,4-Trimethyl hexane	40	36	14	20.2 32	5.91 3	5.14 0	18.2 56	76	164	674	4720	8.36 7	9.11 9	3.85 2
18	2,3,4-Trimethyl pentane	26	17	8	10.9 35	6.82 0	5.37 8	12.2 17	43	52	217	368	5.75 0	8.52 3	4.21 6
19	2,3,5-Trimethyl hexane	36	32	10	15.7 12	6.59 5	5.50 2	16.8 88	68	142	586	4364	7.95 0	9.40 6	4.19 0
20	2,3-Dimethyl butane	20	14	8	9.79 8	4.30 9	3.41 4	8.92 8	34	52	214	584	4.00 0	5.46 4	2.66 7
21	2,3-Dimethyl heptane	34	30	10	15.8 34	5.46 3	4.75 6	15.9 24	64	126	512	2564	7.48 3	8.44 3	3.56 2
22	2,3-Dimethyl hexane	32	32	8	14.1 77	4.81 3	4.17 8	15.0 25	64	158	656	6340	7.08 3	7.48 4	3.12 2
23	2,3-Dimethyl pentane	26	21	10	13.3 33	4.42 5	3.73 2	11.7 92	47	86	351	1516	5.36 7	6.38 7	2.83 8
24	2,3-Dimethyl-3-ethyl pentane	44	37	18	23.3 77	6.80 8	5.75 2	19.4 59	81	168	683	3624	9.48 3	9.91 1	4.36 3
25	2,4-Dimethyl heptane	32	30	6	12.6 07	5.77 7	4.94 9	15.5 21	62	132	544	4256	7.53 3	8.69 4	3.72 7
26	2,4-Dimethyl hexane	28	25	6	11.5 21	5.23 9	4.42 5	13.3 89	53	108	447	3464	6.41 7	7.63 7	3.35 6
27	2,4-dimethyl pentane	22	19	4	7.65 7	5.16 2	4.13 2	10.6 57	41	82	343	3068	5.16 7	6.77 1	3.20 2
28	2,4-Dimethyl-3-ethyl pentane	40	38	12	18.4 90	6.03 7	5.21 7	18.5 59	78	178	730	5444	8.65 0	9.29 0	3.90 6
29	2,5-Dimethyl heptane	29	23	7	11.6 42	6.31 4	5.17 1	13.8 38	52	86	352	1452	6.61 7	8.61 7	3.97 7
30	2,5-Dimethyl hexane	26	22	6	9.89 9	5.64 5	4.61 8	12.5 56	48	88	360	1952	6.06 7	7.73 1	3.54 7

no.	Alkanes	$2M_1$	$2M_2$	$2M_3$	$2ABC$	$2R_2$	$2SCI$	$2RR$	$2GO_1$	$2GO_2$	$2HGO_1$	$2HGO_2$	$2I$	$2GA$	$2SGO$
31	2,6-Dimethyl heptane	30	26	6	11.3 14	6.14 5	5.11 8	14.5 56	56	104	424	2208	7.06 7	8.73 1	3.90 0
32	2-Methyl butane	12	8	4	5.27 8	2.99 2	2.36 2	5.56 0	20	26	108	220	2.58 3	3.75 2	1.85 0
33	2-Methyl heptane	24	21	4	9.19 2	4.53 0	3.88 6	11.6 92	45	82	333	1524	5.70 0	6.80 8	2.92 8
34	2-Methyl hexane	20	17	4	7.77 8	4.03 0	3.38 6	9.69 2	37	66	269	1268	4.70 0	5.80 8	2.57 4
e35	2-Methyl octane	28	25	4	10.6 07	5.03 0	4.38 6	13.6 92	53	98	397	1780	6.70 0	7.80 8	3.28 1
36	2-Methyl pentane	16	13	4	6.36 4	3.53 0	2.88 6	7.69 2	29	50	205	1012	3.70 0	4.80 8	2.22 1
37	2-Methyl propane	6	3	0	0.00 0	3.00 0	2.12 1	3.00 0	9	6	27	12	1.50 0	3.00 0	1.73 2
38	3,3,4-Trimethyl hexane	44	38	18	23.4 69	6.61 5	5.68 9	19.7 17	82	174	710	4548	9.28 3	9.94 9	4.28 8
39	3,3-Diethyl pentane	44	40	12	22.3 42	5.00 0	4.78 9	20.0 00	84	176	708	3136	10.0 00	9.20 0	3.45 5
40	3,3-Dimethyl heptane	36	31	10	16.1 92	6.38 9	5.44 9	16.8 99	67	132	539	3400	8.16 7	9.45 7	4.12 1
41	3,3-Dimethyl hexane	32	27	10	14.7 78	5.88 9	4.94 9	14.8 99	59	116	475	3144	7.16 7	8.45 7	3.76 8
42	3,3-Dimethyl pentane	28	21	10	13.9 99	5.32 8	4.41 1	12.6 57	49	82	335	1204	6.16 7	7.37 1	3.38 6
43	3,4-Dimethyl heptane	36	33	12	17.9 55	5.07 8	4.57 4	16.7 87	69	144	585	3240	7.85 0	8.36 6	3.38 0
44	3,4-Dimethyl hexane	32	28	12	16.8 69	4.54 0	4.04 9	14.6 56	60	120	488	2448	6.73 3	7.30 9	3.00 9
45	3,5-Dimethyl heptane	34	31	8	15.3 84	5.31 6	4.71 8	16.1 21	65	134	551	3860	7.66 7	8.50 3	3.51 0
46	3-Ethyl heptane	32	30	6	14.0 91	4.27 0	4.02 5	15.3 28	62	124	500	2248	7.36 7	7.65 5	2.91 9
47	3-Ethyl hexane	28	26	6	12.6 77	3.77 0	3.52 5	13.3 28	54	108	436	1992	6.36 7	6.65 5	2.56 5
48	3-Ethyl pentane	24	21	6	11.5 91	3.23 2	3.00 0	11.1 96	45	84	339	1200	5.25 0	5.59 8	2.19 5
49	3-Ethyl-2-methyl hexane	36	34	10	16.5 41	5.16 4	4.62 6	16.9 59	70	150	608	3428	8.01 7	8.48 0	3.41 7
50	3-Ethyl-2-methyl pentane	32	29	10	15.4 55	4.62 6	4.10 2	14.8 27	61	126	511	2636	6.90 0	7.42 4	3.04 6
51	3-Ethyl-3-methyl hexane	40	36	12	19.6 56	5.68 2	5.11 2	18.4 85	76	160	650	4016	9.00 0	9.31 4	3.78 3
52	3-Ethyl-3-methyl pentane	36	30	12	18.8 78	5.12 1	4.57 4	16.2 43	66	126	510	2076	8.00 0	8.22 8	3.40 2
53	3-Methyl heptane	26	23	6	11.6 42	4.10 7	3.67 9	12.4 24	49	92	373	1664	5.95 0	6.67 4	2.72 8
54	4-Methyl heptane	26	24	6	11.3 14	4.14 5	3.70 4	12.5 56	50	100	406	2200	6.06 7	6.73 1	2.74 5
55	3-Methyl hexane	22	19	6	10.2 28	3.60 7	3.17 9	10.4 24	41	76	309	1408	4.95 0	5.67 4	2.37 5
56	3-Methyl octane	30	27	6	13.0 56	4.60 7	4.17 9	14.4 24	57	108	437	1920	6.95 0	7.67 4	3.08 2
57	3-Methyl pentane	18	14	6	9.14 2	3.06 9	2.65 5	8.29 3	32	52	212	616	3.83 3	4.61 8	2.00 4
58	4,4-Dimethyl heptane	36	33	10	15.5 56	6.45 0	5.48 8	17.1 42	69	150	615	5084	8.16 7	9.54 2	4.14 9
59	4-Ethyl heptane	32	31	6	13.7 63	4.30 8	4.04 9	15.4 59	63	132	533	2784	7.48 3	7.71 1	2.93 6
60	4-Ethyl-2-methyl hexane	34	32	6	13.9 70	5.40 2	4.77 0	16.2 93	66	140	574	4048	7.83 3	8.61 8	3.54 7

no.	Alkanes	${}_2M_1$	${}_2M_2$	${}_2M_3$	${}_2ABC$	${}_2R_2$	${}_2SCI$	${}_2RR$	${}_2GO_1$	${}_2GO_2$	${}_2HGO_1$	${}_2HGO_2$	${}_2I$	${}_2GA$	${}_2SGO$	
61	4-Methyl octane	30	28	6	12.7	4.64	4.20	14.5	58	116	470	2456	7.06	7.73	3.09	
62	Butane	6	4	2	2.82	1.41	1.15	2.82	8	10	12	50	72	1.33	1.88	0.89
63	Heptane	18	16	2	7.07	2.91	2.65	8.82	5	34	60	242	840	4.33	4.88	1.95
64	Hexane	14	12	2	5.65	2.41	2.15	6.82	8	26	44	178	584	3.33	3.88	1.60
65	Nonane	26	24	2	9.89	3.91	3.65	12.8	28	50	92	370	1352	6.33	6.88	2.66
66	Octane	22	20	2	8.48	3.41	3.15	10.8	28	42	76	306	1096	5.33	5.88	2.30
67	Pentane	10	8	2	4.24	1.91	1.65	4.82	8	18	28	114	328	2.33	2.88	1.24

Table 4. Linear regression models for different properties of alkanes and TI's.

Model	y=	BP	MV	MR	HV	CT	CP	ST
${}_2M_1$	r	0.848	0.778	0.833	0.740	0.896	-0.645	0.802
	m	3.365	1.616	0.515	0.468	4.350	-0.214	0.189
	c	11.651	113.481	23.877	24.643	158.457	32.939	15.200
${}_2M_2$	r	0.875	0.819	0.862	0.803	0.909	-0.698	0.830
	m	3.615	1.757	0.551	0.526	4.593	-0.242	0.205
	c	19.00	116.451	25.051	25.075	169.971	32.761	15.560
${}_2ABC$	r	0.748	0.585	0.656	0.638	0.815	-0.451	0.756
	m	5.183	2.055	0.687	0.684	6.906	-0.262	0.308
	c	44.079	135.061	30.325	29.729	197.722	29.999	16.825
${}_2R$	r	0.486	0.528	0.546	0.301	0.518	-0.474	0.336
	m	10.385	5.619	1.728	0.976	13.550	-0.848	0.391
	c	54.797	131.410	29.923	33.408	213.538	31.197	18.808
${}_2SCI$	r	0.625	0.649	0.673	0.450	0.657	-0.579	0.471
	m	17.455	9.239	2.849	1.954	22.446	-1.353	0.735
	c	31.594	119.510	26.230	29.732	184.750	32.767	17.548
${}_2RR$	r	0.879	0.832	0.879	0.783	0.917	-0.705	0.820
	m	7.779	3.889	1.223	1.116	9.929	-0.522	0.435
	c	3.193	107.149	22.087	22.969	149.257	33.851	14.733
${}_2GO_1$	r	0.867	0.804	0.854	0.777	0.908	-0.675	0.822
	m	1.765	0.855	0.270	0.252	2.262	-0.115	0.100
	c	13.979	114.149	24.211	24.609	162.525	32.943	15.281
${}_2GO_2$	r	0.806	0.759	0.800	0.727	0.844	-0.639	0.746
	m	0.654	0.312	0.098	0.091	0.837	-0.043	0.035
	c	40.226	127.580	28.538	28.654	196.266	31.308	17.010
${}_2HGO_1$	r	0.795	0.755	0.794	0.710	0.832	-0.635	0.725
	m	0.156	0.075	0.024	0.022	0.200	-0.010	0.008
	c	41.694	128.067	28.710	28.967	198.088	31.250	17.161
${}_2HGO_2$	r	0.431	0.504	0.505	0.333	0.451	-0.431	0.271
	m	0.006	0.004	0.001	0.001	0.008	-0.001	0.000
	c	92.198	151.545	36.211	36.607	262.830	28.179	20.302
${}_2I$	r	0.884	0.840	0.885	0.790	0.919	-0.715	0.825
	m	16.410	8.238	2.583	2.363	20.887	-1.112	0.916

Model	y=	BP	MV	MR	HV	CT	CP	ST
$_2GA$	c	2.274	106.456	21.912	22.774	148.468	33.984	14.694
	r	0.751	0.771	0.799	0.612	0.789	-0.680	0.620
	m	13.073	6.936	2.140	1.681	16.612	-0.980	0.615
	e	8.841	107.021	22.364	25.390	157.038	34.272	16.038
$_2SGO$	r	0.566	0.597	0.618	0.385	0.599	-0.534	0.412
	m	20.103	10.683	3.292	2.100	26.004	-1.586	0.807
	e	41.510	124.737	27.848	31.392	196.971	32.093	18.115

3. Results and Discussion

3.1. Single regression.

In Table 5, linear correlation between the properties and the distance-2 TI's with $r \geq 0.8$ are listed. The physicochemical properties such as BP, HV, CP, ST are highly correlated with $_2M_2$ with the correlation values 0.8753, 0.8031, 0.6985, 0.8297, respectively, and the properties BP, MV, MR, and CT show a high correlation with $_2I$ with a correlation value of 0.8837, 0.8403, 0.8853 and 0.9193. It can also be observed that CT has a good correlation with all the considered TIs having a correlation coefficient greater than 0.8.

Table 5. Linear correlation between the properties and the TIs at a distance-2 with $r \geq 0.8$.

Properties/ TI's	$_2M_1$	$_2M_2$	$_2ABC$	$_2RR$	$_2G0_1$	$_2G0_2$	$_2HGO_1$	$_2I$
BP	0.8481	0.8753		0.8789	0.8668	0.8066		0.8837
MV		0.8187		0.8321	0.8042			0.8403
MR	0.8328	0.8622		0.8788	0.8537			0.8853
HV		0.8031						
CT	0.8959	0.9090	0.8148	0.9169	0.9079	0.8439	0.8323	0.9193
CP		0.6985						
ST	0.8016	0.8297		0.8196	0.8220			0.8247

3.2 Double regression.

From the computation, we have observed that many double regression models of properties with two different combinations of distance 2 TIs have a good correlation which varies from 0.9 to 0.97. Properties having a good correlation greater than 0.9 with different double regression models are listed in Table 6. Among the different double regression models, we have observed the one which has the best fit with a high correlation coefficient, and the least sum of the squares of the error is given in Table 7.

Table 6. Double correlation between the properties and the TIs at a distance of 2 with $r > 0.9$.

Properties	TI Pairs			
B.P	• $_2M_1, _2M_3$ • $_2M_1, _2RR$ • $_2M_1, _2SDD$	$_2RR$ with all the TIs considered except with $_2M_2, _2ABC, _2SCI$	$_2R, _2SCI$	
MV	• $_2M_1, _2M_3$ • $_2M_1, _2RR$ • $_2M_1, _2I$	$_2R, _2M_2$		
MR	• $_2M_1, _2M_3$ • $_2M_1, _2RR$ • $_2M_1, _2I$ • $_2M_1, _2SDD$	• $_2M_2, _2M_3$ • $_2M_2, _2HM$ • $_2M_2, _2F$ • $_2M_2, _2GO_2$	• $_2M_2, _2RR$ • $_2M_2, _2GO_1$ • $_2M_2, _2I$	• $_2R, _2SCI$ • $_2R, _2GA$

Properties	TI Pairs			
HV	• ${}_{2}R2$, ${}_{2}SCI$ • ${}_{2}R2$, ${}_{2}GA$			
CT	• ${}_{2}R2$, ${}_{2}SCI$ • ${}_{2}R2$, ${}_{2}GA$			
CP	${}_{2}M1$, ${}_{2}RR$			
ST	M2, GO2	• ${}_{2}R$, ${}_{2}SCI$ • ${}_{2}R$, ${}_{2}I$ • ${}_{2}R$, ${}_{2}SGO$		

Table 7. Properties of Alkanes and the topological indices with maximum correlation coefficient in the double regression model.

Properties	Two highly correlated models with the property	r	Double Regression Model	The sum of the square of errors
BP	${}_{2}R$, ${}_{2}SCI$	0.956328	$B.P = 7.39113 - 86.865 {}_{2}R + 129.19646 {}_{2}SCI$	7871.307
MV	${}_{2}M1$, ${}_{2}RR$	0.945853	$MV = 93.9910 - 8.5993 {}_{2}M1 + 23.1342 {}_{2}RR$	2140.800
MR	${}_{2}M1$, ${}_{2}RR$	0.955646	$MR = 18.8173 - 2.13716 {}_{2}M1 + 6.0054 {}_{2}RR$	156.134
HV	${}_{2}R2$, ${}_{2}GA$	0.923498	$HV = 21.04966 - 5.85292 {}_{2}R + 6.25564 {}_{2}GA$	278.049
CT	${}_{2}R2$, ${}_{2}SGO$	0.974126	$CT = 135.8107 - 199.2530 {}_{2}R + 355.336657 {}_{2}GA$	7035.971
CP	${}_{2}M1$, ${}_{2}RR$	0.907328	$CP = 36.2337 + 1.91921 {}_{2}M1 - 4.7814 {}_{2}RR$	114.034
ST	${}_{2}R2$, ${}_{2}SGO$	0.942627	$ST = 13.5657 - 11.19118 {}_{2}R + 19.5593 {}_{2}SGO$	27.109

It can be observed from Table 7 that there is a high correlation between the double regression model of ${}_{2}M1$, ${}_{2}RR$ with the Physical properties MV, MR, and CP of alkanes which have the correlation coefficient of 0.945853, 0.955646, and 0.907328, respectively. Also, a very good correlation coefficient of 0.956328 between BP and ${}_{2}R$, ${}_{2}SCI$. Using the computed values of properties of 67 Alkanes obtained from double regression and of practical values of BP, plotted the curves as Figure 1.

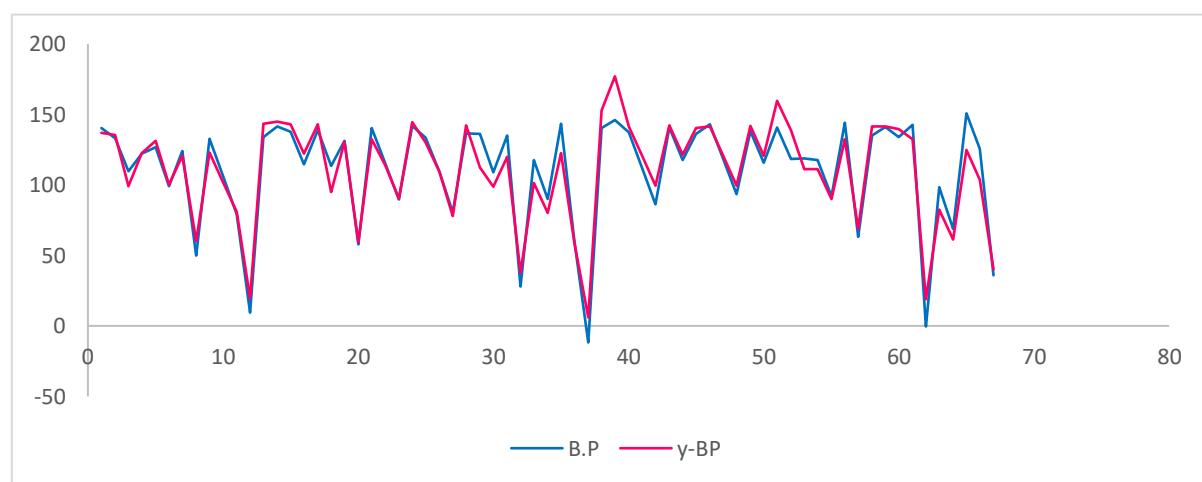


Figure 1. Curves for practical and Theoretical values of BP of 67 Alkanes with a double regression model of the ${}_{2}R$ and ${}_{2}SCI$ having $r = 0.956328$.

Also, we obtained a promising, powerful correlation of 0.974126 between CT and ${}_{2}R2$, ${}_{2}SGO$ of Alkanes. Their practical and theoretical curves are plotted in Figure 2.

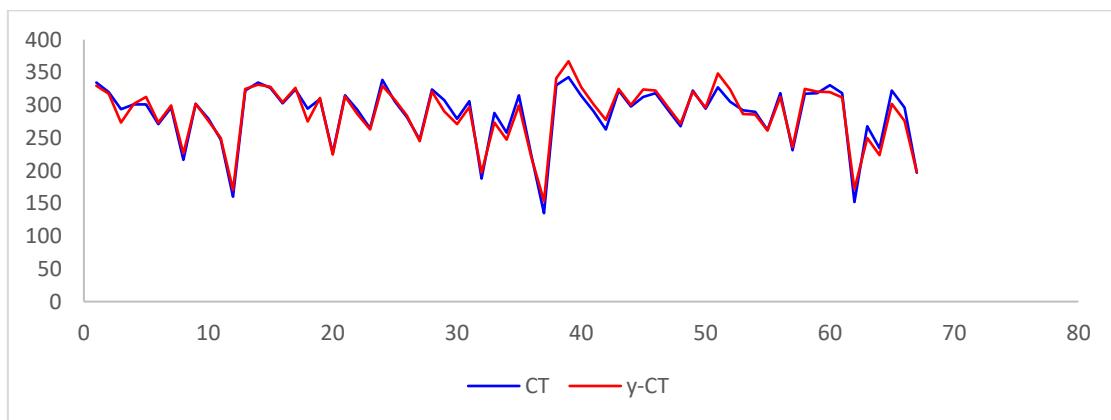


Figure 2. Curves for practical and Theoretical values of CT of 67 Alkanes with a double regression model of the ${}_2R$ and ${}_2SCI$ having $r = 0.974126$.

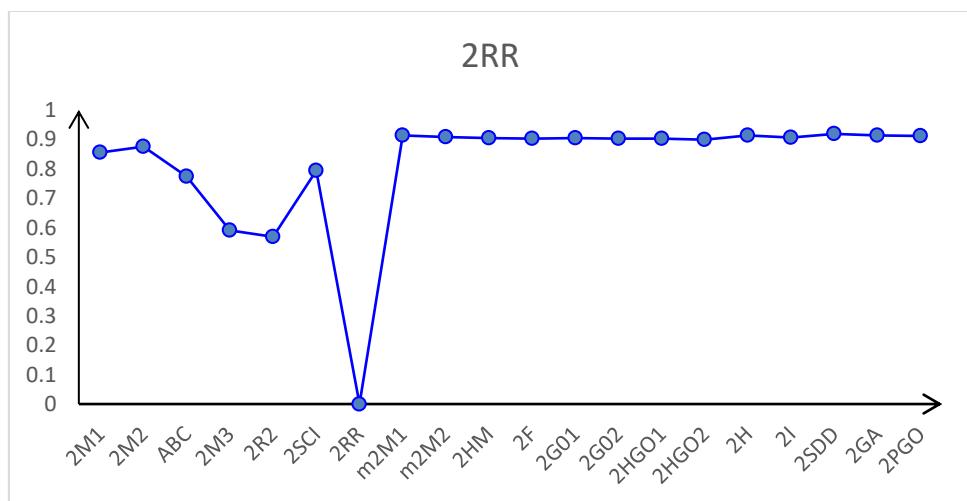


Figure 3. The correlation coefficient of Double regression model of B.P against ${}_2RR$ with different Tis.

4. Conclusions

In this paper, we investigated the linear and double regression models of some of the properties of alkane groups considering 67 alkanes. The comprehensive study reveals that the linear regression models correlate at most 0.9193.

In contrast to linear regression, double regression of the proposed indices fits well and correlates strongly with all of the alkane properties investigated. Most of the investigated properties are well modeled ($r > 0.9$). Figure 3 shows the curve of the correlation coefficient against the double regression of ${}_2RR$ with the remaining all the considered indices. It can be observed from the above figure that the double regression of ${}_2RR$ except with ${}_2M_3$ and ${}_2SCI$ correlates well with all the considered TIs for the boiling point of the alkanes. All the results of this paper promise to be a useful parameter in the QSPR/QSAR studies of alkanes.

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Conflicts of Interest

The authors declare no conflict of interest.

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