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QSPR analysis on graph energies of chemical graphs

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Chemical graph theory is a bridge between Chemistry and Graph theory. Graph energies are important tools for QSPR researches. Thus, this study aims to relate several energies with the QSPR analysis of 67 alkanes. We compare these results with the Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy. Our study reveals some interesting results based on the predicting power of these graph energies.
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KEYWORDS

QSPR-analysis; octane isomers; Maximum Degree Energy; Minimum Degree Energy; Second Zagreb Energy.

Introduction

Graph theory is not only the study of different properties of objects, but also speaks about the objects with the same properties. Graph theory is used to investigate the properties through Quantitative Structure- Activity Relationship (QSAR) and Quantitative Structure- Property Relationship (QSPR) models through graph invariants such as topological indices. The concept of topological index while working on boiling point was firstly introduced by Wiener in 1947. The topological indices have found applications in different areas of mathematics, physics, biology, chemistry, informatics, etc. [6,10,23], but their most important use is in the non-empirical and Quantitative Structure -Activity Relationships (QSAR), and Quantitative Structure- Property Relationships (QSPR) [1,2,3,8,12,13,15,16,21,22,24].

Octane isomers

Octane isomers are the important set of organic molecules to test the applicability of various topological parameters in quantitative structure-property/activity relationships (QSPR/QSAR). These compounds structurally differ enough to yield considerable variation in shape, branching, and non-polarity [19]. In a comprehensive study of numerous properties of octane isomers, Randic *et al.* [17,18,19] have used single molecular descriptors and concluded that different physicochemical properties depend on different descriptors.

In a molecular graph, chemical bond between them and carbon atoms in a hydrocarbon system represent edges and vertices, respectively. A plenty of work has been done on chemical graph theory and graph energies. Certain elementary results on the graph's energy are described in the thesis of Siraj [20].

Let G be a finite, simple, and undirected graph and its vertex set and edge set are given by $V(G) = \{v_1, v_2, v_3, \ldots, v_p\}$ *and* $E(G) = \{e_1, e_2, e_3, \ldots, e_q\}$, respectively. In 1978, Ivan Gutman innovated a novel graph spectral quantity which he named graph energy [9]. Let G be a simple graph of order *n*. Let A(G) be its adjacency matrix. The eigenvalues of A(G), denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$ form the spectrum of G [7].

Definition: The sum of the absolute values of all eigenvalues of the graph G is called the energy of the graph G and is given as $E(G) = \sum_{i=1}^{n} |\lambda_i|$

The following graph energies are considered for the QSPR study.

Maximum Degree Energy

In [4], the maximum degree energy E_M of a simple connected graph G is the sum of the absolute values of eigen values of the maximum degree matrix $M(G)$ of a graph G.

Then, $M(G) = [M_{ij}]$ where,

$$M_{ij} = \begin{cases} \max(d_i, d_j), & if\ v_i, v_j \epsilon E(G) \\ 0, & otherwise \end{cases}$$

Where, $d_i\ and\ d_j$ are the degrees of vertices $v_i\ and\ v_{j,}$, respectively.

Minimum Degree Energy

In [5], the minimum degree energy E_m of a simple connected graph G is the sum of the absolute values of eigenvalues of the minimum degree matrix $m(G)$ of a graph G.

Then, $m(G) = [m_{ij}]$ where,

$$m_{ij} = \begin{cases} \min(d_i, d_j), & if\ v_i, v_j \epsilon E(G) \\ 0, & otherwise \end{cases}$$

Where, $d_i\ and\ d_j$ are the degrees of vertices $v_i\ and\ v_{j,}$, respectively.

Second Zagreb Energy

In [14], the Second Zagreb energy ZE_2 of a simple connected graph G is the sum of the absolute values of eigenvalues of the second Zagreb matrix $Z^{(2)}$ (G) of G.

Then, $Z^{(2)}$ (G) = $[Z_{ij}^{(2)}]$ where,

$$Z_{ij}^{(2)} = \begin{cases} d_i d_j, & if\ v_i, v_j \in E(G) \\ 0 & otherwise \end{cases}$$

Where, $d_i\ and\ d_j$ are the degrees of vertices $v_i\ and\ v_{j,}$, respectively.

The use of selected graph energies in QSPR studies

We have used three energies. M_{ij}, m_{ij}, Z_{ij}^2 for eight representative physical properties molar volumes (mv) at 20^0C, molar refractions (mr) at 20^0C, boiling points (bp), surface tensions (st) at 20^0C, melting points (mp), critical temperature (ct), critical Pressure (cp) and heats of vaporization (hv) at 25 ^{0}C of the 67 alkanes from n-butanes to nonanes are listed in Table 1 and values for these properties were taken from [11].

TABLE 1

Sl No.	Alkane	$bp(^\circ C)$	$mv(cm^3)$	$mr(cm^3)$	$hv(kJ)$	$ct(^\circ C)$	$cp(atm)$	$st(\frac{dyne}{cm})$	$mp(^\circ C)$
1	Butane	-0.5				152.01	37.47		-138.35
2	2-methyl propane	-11.73				134.98	36		-159.6
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16	-129.72
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.7	32.9	15	-159.9
5	2,2 dimethylpropane	9.503	112.074	25.7243	21.78	160.6	31.57		-16.55
6	Hexane	68.74	130.688	29.9066	31.55	234.7	29.92	18.42	-95.35
7	2-methylpentane	60.271	131.933	29.9459	29.86	224.9	29.95	17.38	-153.67
8	3-methyalpentane	63.282	129.717	30	30.27	231.2	30.83	18.12	-118
9	2,2-methylbutane	49.741	132.744	29.9347	27.69	216.2	30.67	16.3	-99.87
10	2,3-dimethylbutane	57.988	130.24	29.8104	29.12	227.1	30.99	17.37	-128.54
11	Heptanes	98.427	146.54	34.5504	36.55	267.55	27.01	20.26	-90.61
12	2-methylhexane	90.052	147.656	34.5908	34.8	257.9	27.2	19.29	-118.28
13	3-methylhexane	91.85	145.821	34.4597	35.08	262.4	28.1	19.79	-119.4
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.6	28.6	20.44	-118.6
15	2,2-dimethylpentane	79.197	148.695	34.6166	32.43	247.7	28.4	18.02	-123.81

16	2,3-dimethylpentane	89.784	144.153	34.3237	34.24	264.6	29.2	19.96	-119.24
17	2,4-dimethylpentane	80.5	148.949	34.6192	32.88	247.1	27.4	18.15	-119.24
18	3,3-dimethylpentane	86.064	144.53	34.3323	33.02	263	30	19.59	-134.46
19	Octane	125.665	162.592	39.1922	41.48	296.2	24.64	21.76	-56.79
20	2-methylheptane	117.647	163.663	39.2316	39.68	288	24.8	20.6	-109.04
21	3-methylheptane	118.925	161.832	39.1001	39.83	292	25.6	21.17	-120.5
22	4-methylheptane	117.709	162.105	39.1174	39.67	290	25.6	21	-120.95
23	3-ethylhexane	118.53	160.07	38.94	39.4	292	25.74	21.51	
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279	25.6	19.6	-121.18
25	2,3-dimethylhexane	115.607	160.39	38.98	38.79	293	26.6	20.99	
26	2,4-dimethylhexane	109.42	163.09	39.13	37.76	282	25.8	20.05	-137.5
27	2,5-dimethylhexane	109.1	164.69	39.25	37.86	279	25	19.73	-91.2
28	3,3-dimethylhexane	111.96	160.87	39	37.93	290.84	27.2	20.63	-126.1
29	3,4-dimethylhexane	117.72	158.81	38.84	39.02	298	27.4	21.64	
30	3-ethyl-2-thylpentane	115.65	158.79	38.83	38.52	295	27.4	21.52	-114.96
31	3-ethyl-3-thylpentane	118.25	157.02	38.71	37.99	305	28.9	21.99	-90.87
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294	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	29	21.56	-100.7
35	2,3,4-trimethylpentane	113.46	158.85	38.56	37.61	295	27.6	21.14	-109.21
36	Nonane	150.79	178.71	43.84	46.44	322	22.74	22.92	-53.52
37	2-methyloctane	143.26	179.77	43.87	44.65	315	23.6	21.88	-80.4
38	3-methyloctane	144.18	177.95	43.72	44.75	318	23.7	22.34	-107.64
39	4-methyloctane	142.48	178.15	43.76	44.75	318.3	23.06	22.34	-113.2
40	3-ethylheptane	143	176.41	43.64	44.81	318	23.98	22.81	-114.9
41	4-ethylheptane	141.20	175.68	43.49	44.81	318.3	23.98	22.81	
42	2,2-dimethylheptane	132.69	180.5	43.91	42.28	302	22.8	20.8	-113
43	2,3-dimethylheptane	140.5	176.65	43.63	43.79	315	23.79	22.34	-116
44	2,4-dimethylheptane	133.5	179.12	43.73	42.87	306	22.7	23.3	
45	2,5-dimethylheptane	136	179.37	43.84	43.87	307.8	22.7	21.3	
46	2,6-dimethylheptane	135.21	180.91	43.92	42.82	306	23.7	20.83	-102.9
47	3,3-dimethylheptane	137.3	176.897	43.687	42.66	314	24.19	22.01	
48	3,4-dimethylheptane	140.6	175.349	43.5473	43.84	322.7	24.77	22.8	
49	3,5-dimethylheptane	136	177.386	43.6379	42.98	312.3	23.59	21.77	
50	4,4-dimethylheptane	135.2	176.897	43.6022	42.66	317.8	24.18	22.01	
51	3-ethyl-2-ethylhexane	138	175.445	43.655	43.84	322.7	24.77	22.8	
52	4-ethyl-2-ethylhexane	133.8	177.386	43.6472	42.98	330.3	25.56	21.77	
53	3-ethyl-3-ethylhexane	140.6	173.077	43.268	44.04	327.2	25.66	23.22	

54	2,2,4-trimethylhexane	126.54	179.22	43.7638	40.57	301	23.39	20.51	-120
55	2,2,5-trimethylhexane	124.084	181.346	43.9356	40.17	296.6	22.41	20.04	-105.78
56	2,3,3-trimethylhexane	137.68	173.78	43.4347	42.23	326.1	25.56	22.41	-116.8
57	2,3,4-trimethylhexane	139	173.498	43.4917	42.93	324.2	25.46	22.8	
58	2,3,5-trimethylhexane	131.34	177.656	43.6474	41.42	309.4	23.49	21.27	-127.8
59	3,3,4-trimethylhexane	140.46	172.055	43.3407	42.28	330.6	26.45	23.27	-101.2
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.8	26.94	23.75	-33.11
61	2,2-dimethyl-3-ethylpentane	133.83	174.537	43.4571	42.02	322.6	25.96	22.38	-99.2
62	2,3-dimethyl-3-ethylpentane	142	170.093	42.9542	42.55	338.6	26.94	23.87	
63	2,4-dimethyl-3-ethylpentane	136.73	173.804	43.4037	42.93	324.2	25.46	22.8	-122.2
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41	334.5	27.04	23.38	-99
65	2,2,3,4-tetramethylpentane	133.016	173.557	43.4359	41	319.6	25.66	21.98	-121.09
66	2,2,4,4-tetramethylpentane	122.284	178.256	43.8747	38.1	301.6	24.58	20.37	-66.54
67	2,3,3,4-tetramethylpentane	141.551	169.928	43.2016	41.75	334.5	26.85	23.31	-102.12

TABLE 2

	Alkanes	M_{ij}	m_{ij}	Z_{ij}^2
1	Butane	0.894	5.656	11.313
2	2-methyl propane	10.392	3.461	10.392
3	Pentane	10.928	8	16
4	2-methyl butane	15.7006	6.269	17.316
5	2,2 dimethylpropane	16	4	16
6	Hexane	13.976	10.724	22.976
7	2-methylpentane	15.726	8.598	21.808
8	3-methyalpentane	17.114	7.656	23.697
9	2,2-methylbutane	19.566	6.771	23.975
10	2,3-dimethylbutane	18	8.246	24.738
11	Heptanes	16.109	14.393	26.221
12	2-methylhexane	16.58	10.724	27.362
13	3-methylhexane	19.098	11.328	28.386
14	3-ethylpentane	18.582	11.211	29.166
15	2,2-dimethylpentane	21.385	9.103	28.407
16	2,3-dimethylpentane	21.214	10.81	26.832
17	2,4-dimethylpentane	20.485	9.152	27.458
18	3,3-dimethylpentane	23.039	9.437	31.322
19	Octane	19.036	15.81	30.539
20	2-methylheptane	19.566	13.708	32.056
21	3-methylheptane	18.624	11.206	32.852
22	4-methylheptane	21.018	13.931	32.681
23	3-ethylhexane	22.128	14.606	37.789
24	2,2-dimethylhexane	24.564	11.864	33.987
25	2,3-dimethylhexane	23.22	13.24	35.594
26	2,4-dimethylhexane	21.83	11.328	32.471
27	2,5-dimethylhexane	23.466	11.232	30.802
28	3,3-dimethylhexane	24.906	11.814	33.25
29	3,4-dimethylhexane	20.39	11.972	33.374

30	3-ethyl-2-methylpentane	23.033	13.025	34.395
31	3-ethyl-3-methylpentane	26.33	11.999	34.862
32	2,2,3-trimethylpentane	25.518	9.12	21.349
33	2,2,4-trimethylpentane	26.122	9.632	33.963
34	2,3,3-trimethylpentane	27.176	19.653	39.74
35	2,3,4-trimethylpentane	25.276	12.662	40.521
36	Nonane	19.034	15.269	36.427
37	2-methyloctane	23.913	15.788	37.525
38	3-methyloctane	24.28	15.678	38.599
39	4-methyloctane	24.121	15.179	38.483
40	3-ethylheptane	24.302	15.9708	37.557
41	4-ethylheptane	24.255	16.209	39.281
42	2,2-dimethylheptane	26.611	14.21	38.659
43	2,3-dimethylheptane	26.256	15.932	41.015
44	2,4-dimethylheptane	25.788	14.235	38.658
45	2,5-dimethylheptane	27.038	14.681	39.76
46	2,6-dimethylheptane	25.754	13.1104	36.196
47	3,3-dimethylheptane	28.047	14.547	55.819
48	3,4-dimethylheptane	26.435	15.266	41.836
49	3,5-dimethylheptane	20.428	14.6008	40.68
50	4,4-dimethylheptane	17.906	14.166	40.432
51	3-ethyl-2-methylhexane	26.168	15.283	41.51
52	4-ethyl-2-methylhexane	24.842	13.412	37.681
53	3-ethyl-3-methylhexane	28.297	13.723	42.937
54	2,2,4- trimethyl hexane	29.535	11.377	40.637
55	2,2,5- trimethyl hexane	29.465	12.523	39.963
56	2,3,3- trimethyl hexane	29.052	12.648	44.383
57	2,3,4- trimethyl hexane	28.5006	15.231	44.165
58	2,3,5- trimethyl hexane	28.005	12.802	39.717
59	3,3,4- trimethyl hexane	30.387	13.347	45.948
60	3,3-diethylpentane	24.92	12.246	44.249
61	2,2-dimethyl-3-thylpentane	28.733	13.488	39.798
62	2,3-dimethyl-3-thylpentane	28.5106	13.655	42.126
63	2,4-dimethyl-3-thylpentane	26.813	17.376	42.776
64	2,2,3,3-tetramethylpentane	32.278	12.408	49.07
65	2,2,3,4-tetramethylpentane	30.993	12.484	45.548
66	2,2,4,4-tetramethylpentane	31.744	10.097	40.389
67	2,3,3,4-tetramethylpentane	31.288	12.305	47.778

Regression Models: The following statistical models have been used for the study:

1) Linear Model:

$P = A + B(TI)$

2) Quadratic model:

$P = A + B(TI) + C(TI)^2$

Where, P is a physical property, TI is a topological index and A, B, and C are constants. The followings are different regression models for each topological index, which are listed below.

Linear Model:

1) Maximum degree energy $M_{ij}(G)$:

$bp = -6.7005 + [M_{ij}(G)]\ 5.0387$

$mv = 97.1519 + [M_{ij}(G)]\ 2.7632$

$mr = 19.1559 + [M_{ij}(G)]\ 0.8593$

$hv = 22.0944 + [M_{ij}(G)]\ 0.7079$

$ct = 137.4623 + [M_{ij}(G)]\ 6.4755$

$cp = 35.2045 - [M_{ij}(G)]\ 0.3719$

$St = 14.6962 + [M_{ij}(G)] 0.2643$

$mp = -130.4421 + [M_{ij}(G)]\ 0.9453$

2) Minimum degree energy $m_{ij}(G)$:

$bp = -18.0655 + [m_{ij}(G)]\ 10.3757$

$mv = 103.6366 + [m_{ij}(G)]\ 4.6826$

$mr = 21.7496 + [m_{ij}(G)]\ 1.4101$

$hv = 18.4233 + [m_{ij}(G)]\ 1.6262$

ct = 136.386+ $[m_{ij}(G)]$ 12.2311
cp = 36.0431-$[m_{ij}(G)]$ 0.7657
St = 13.5881 + $[m_{ij}(G)]$0.5825
mp = -131.2434+ $[m_{ij}(G)]$1.8894

3) Second Zagreb energy $Z_{ij}^{(2)}(G)$:

$bp = -18.6006 + [Z_{ij}^{(2)}(G)]\ 3.7007$

$mv = 97.2123 + [Z_{ij}^{(2)}(G)]\ 1.8425$
$mr = 19.2455 + [Z_{ij}^{(2)}(G)]\ 0.571$
$hv = 19.3908 + [Z_{ij}^{(2)}(G)]0.5491$
ct = 128.3849 + $[Z_{ij}^{(2)}(G)]$ 4.5759
cp =35.7149 - $[Z_{ij}^{(2)}(G)]$ 0.2625
St = 13.6247 + $[Z_{ij}^{(2)}(G)]$ 0.2059
mp = -134.2955+ $[Z_{ij}^{(2)}(G)]$0.767

Note: In tables 3 to 8, N is the total number of chemical structures used for estimation during analysis, *r* is the correlation coefficient, *s* is the standard error of estimate, and F (Fisher statistic) is the statistical test to know the goodness of fit for regression analysis.

TABLE 3 Statistical parameters for the linear QSPR model for the Maximum degree energy $M_{ij}(G)$

Physical Properties	N	A	B	r	s	F
Boiling point	67	-6.7005	5.0387	0.7348	26.9921	74.907
Molar volume	65	97.1519	2.7632	0.7483	11.9547	79.268
Molar refraction	65	19.1559	0.8593	0.78102	3.3316	98.710
Heats of vapourization	65	22.0944	0.7079	0.6244	4.2651	40.868
Critical temperature	67	137.4623	6.4755	0.8062	27.0638	123.064
Critical pressure	67	35.2045	-0.3719	0.6782	2.3242	55.029
Surface tension	64	14.6962	0.2643	0.6403	1.5236	42.930
Melting point	52	-130.4421	0.9453	0.2144	26.6437	2.429

TABLE 4 Statistical parameters for the linear QSPR model for the Minimum degree energy $m_{ij}(G)$

Physical Properties	N	A	B	r	S	F
Boiling point	67	-18.0655	10.3757	0.8246	22.3494	139.070
Molar volume	65	103.6366	4.6826	0.7483	11.8987	80.612
Molar refraction	65	21.7496	1.4101	0.7615	3.4732	85.789
Heats of vapourization	65	18.4233	1.6262	0.8544	2.8538	168.998
Critical temperature	67	136.386	12.2311	0.8366	25.1815	152.229
Critical pressure	67	36.0431	-0.7657	0.7615	2.0382	91.073
Surface tension	64	13.5881	0.5825	0.7874	1.2171	102.433
Melting point	52	-131.2434	1.8894	0.2302	26.556	2.776

TABLE 5 Statistical parameters for the linear QSPR model for the Second Zagreb energy $Z_{ij}^{(2)}(G)$

Physical Properties	N	A	B	r	s	F
Boiling point	67	-18.6006	3.7007	0.8544	65.4314	147.362
Molar volume	65	97.2123	1.8425	0.8485	9.5194	161.372
Molar refraction	65	19.2455	0.571	0.8831	2.4897	226.554
Heats of vapourization	65	19.3908	0.5491	0.8306	3.0618	138.560
Critical temperature	67	128.3849	4.5759	0.91104	18.9544	318.408
Critical pressure	67	35.7149	-0.2625	0.7615	2.0457	89.928
Surface tension	64	13.6247	0.2059	0.8246	1.1133	134.520
Melting point	52	-134.2955	0.767	0.2626	26.3276	3.696

Quadratic Model:

1) Maximum degree energy $M_{ij}(G)$:

$bp = -39.7869 + 8.7194\ [M_{ij}(G)]$-0.0919 $[M_{ij}(G)]^{\ 2}$
$mv = 8.6035 + 10.92508\ [M_{ij}(G)]$ - 0.1793 $[M_{ij}(G)]^{\ 2}$

$mr = -3.8685 + 2.9815\,[M_{ij}(G)] - 0.0466\,[M_{ij}(G)]^2$

$hv = -6.4955 + 3.3431\,[M_{ij}(G)] - 0.0579\,[M_{ij}(G)]^2$

$ct = 103.64006 + 10.23808\,[M_{ij}(G)] - 0.0939\,[M_{ij}(G)]^2$

$cp = 41.0006 + 1.0166\,[M_{ij}(G)] - 0.0161\,[M_{ij}(G)]^2$

$St = 7.4714 + 0.9278\,[M_{ij}(G)] - 0.0145\,[M_{ij}(G)]^2$

$mp = -145.7607 + 2.6914\,[M_{ij}(G)] - 0.0441\,[M_{ij}(G)]^2$

2) **Minimum degree energy $m_{ij}(G)$:**

$bp = -116.3074 + 29.4347\,[m_{ij}(G)] - 0.8466\,[m_{ij}(G)]^2$

$mv = 37.7159 + 16.5487\,[m_{ij}(G)] - 0.5016\,[m_{ij}(G)]^2$

$mr = 3.1433 + 4.7593\,[m_{ij}(G)] - 0.1416\,[m_{ij}(G)]^2$

$hv = -0.6825 + 5.0653\,[m_{ij}(G)] - 0.1454\,[m_{ij}(G)]^2$

$ct = 1.5489 + 38.3896\,[m_{ij}(G)] - 0.16208\,[m_{ij}(G)]^2$

$cp = 44.3739 - 2.3819\,[m_{ij}(G)] + 0.0717\,[m_{ij}(G)]^2$

$St = 2.93306 + 2.3942\,[m_{ij}(G)] - 0.0734\,[m_{ij}(G)]^2$

$mp = -116.595008 - 0.9876\,[m_{ij}(G)] + 0.1289\,[m_{ij}(G)]^2$

3) **Second Zagreb energy $Z_{ij}^{(2)}(G)$:**

$bp = -100.9841 + 9.4004[Z_{ij}^{(2)}(G)] - 0.0898\,[Z_{ij}^{(2)}(G)]^2$

$mv = 28.2939 + 6.1975[Z_{ij}^{(2)}(G)] - 0.06463\,[Z_{ij}^{(2)}(G)]^2$

$mr = 1.5094 + 1.6917\left[Z_{ij}^{(2)}(G)\right] - 0.0166\,[Z_{ij}^{(2)}(G)]^2$

$hv = -1.1473 + 1.8469\left[Z_{ij}^{(2)}(G)\right] - 0.0192\left[Z_{ij}^{(2)}(G)\right]^2$

$ct = 28.3231 + 11.4987\left[Z_{ij}^{(2)}(G)\right] - 0.1091\,[Z_{ij}^{(2)}(G)]^2$

$cp = 45.82906 - 0.9622\left[Z_{ij}^{(2)}(G)\right] + 0.01102\left[Z_{ij}^{(2)}(G)\right]^2$

$St = 7.7847 + 0.5657\left[Z_{ij}^{(2)}(G)\right] - 0.0052\left[Z_{ij}^{(2)}(G)\right]^2$

$mp = -145.02 + 1.5465\left[Z_{ij}^{(2)}(G)\right] - 0.0128\left[Z_{ij}^{(2)}(G)\right]^2$

TABLE 6 Statistical parameters for the quadratic QSPR model for the Maximum degree energy $M_{ij}(G)$

Physical Properties	N	A	B	C	r	s	F
Boiling point	67	−39.7869	8.7194	- 0.0919	0.7429	26.713	39.423
Molar volume	65	8.6035	10.92508	- 0.1793	0.7936	11.018	52.745
Molar refraction	65	−3.8685	2.9815	- 0.0466	0.8161	3.109	61.830
Heats of vaporization	65	-6.4955	3.3431	-0.0579	0.6891	4	28.043
Critical temperature	67	103.64006	10.23808	-0.0939	0.8168	26.764	64.148
Critical pressure	67	41.0006	-1.0166	0.0161	0.7337	2.163	37.319
Surface tension	64	7.4714	0.9278	-0.0145	0.6697	1.484	24.810
Melting point	52	-145.7607	2.6914	-0.0441	0.237	26.775	1.458

TABLE 7 Statistical parameters for the quadratic QSPR model for the Minimum degree energy $m_{ij}(G)$

Physical Properties	N	A	B	C	r	s	F
Boiling point	67	−116.307	29.4347	- 0.8466	0.8789	19.037	108.639
Molar volume	65	37.7159	16.5487	- 0.5016	0.822	10.312	64.598
Molar refraction	65	3.1433	4.7593	- 0.1416	0.8245	3.045	65.822
Heats of vaporization	65	-0.6825	5.0653	-0.1454	0.912	2.264	153.367
Critical temperature	67	1.5489	38.3896	-1.162	0.9097	19.262	153.624
Critical pressure	67	44.3739	-2.3819	0.0717	0.8284	1.783	70.035
Surface tension	64	2.933	2.3942	-0.0734	0.8686	0.99	93.796
Melting point	52	-116.595	-0.9876	0.1289	0.2421	26.751	1.505

TABLE 8 Statistical parameters for the quadratic QSPR model for the Second Zagreb energy $Z_{ij}^{(2)}(G)$

Physical Properties	N	A	B	C	r	s	F
Boiling point	67	-100.9841	9.4004	-0.0898	0.8945	17.841	128.114
Molar volume	65	28.2939	6.1975	-0.0646	0.9089	7.55	147.354
Molar refraction	65	1.5094	1.6917	-0.0166	0.9288	1.994	194.742
Heats of vapourization	65	-1.1473	1.8469	-0.01926	0.8886	2.532	116.382
Critical temperature	67	28.3231	11.4987	-0.1091	0.95008	14.474	296.762
Critical pressure	67	45.829	-0.9622	0.01102	0.8585	1.632	89.745
Surface tension	64	7.7847	0.5657	-0.0052	0.8578	1.027	84.995
Melting point	52	-145.02	1.5465	-0.0128	0.2668	26.561	1.878

Discussion and concluding remarks

We have tested the model described in Table 1 for 67 alkanes from n-butanes to nonanes for linear and quadratic regression models of graph energies.

By inspection of the data given in Tables 3 to 8 as a result of QSPR analysis, it is desirable to extract the number of conclusions for the graph energies.

First, the Maximum Degree Energy is correlated, to predict physical properties of alkanes. In linear regression model, we can see that the correlation coefficient value ranges from 0.2144 to 0.8062. It is good in Critical temperature(ct) of alkanes with correlation coefficient r=0.806. It is poor in other physical properties.

In linear model of the Minimum Degree Energy, we can see that correlation coefficient value ranges from 0.2302 to 0.8544. It is good especially in Boiling point(Bp), Heat of vaporization(hv), and Critical temperature(ct) of alkanes with correlation coefficient r=0.8246, 0.8544, and 0.8366, respectively. The correlation is poor for other physical properties.

In linear regression model of the Second Zagreb Energy, we can see that the correlation coefficient value ranges from 0.2626 to 0.911. It is high especially in Critical temperature(ct) with r= 0.911. We can use the Second Zagreb Energy as a tool for predicting physical properties of alkanes.

In quadratic model, we can see that correlation coefficient value varies from 0.237 to 0.8168. It is good especially in Molar refraction(mr) and Critical temperature(ct) of alkanes with correlation coefficient r=0.8161 and 0.8168 respectively. The correlation is poor for other physical properties.

In quadratic model, we can see that correlation coefficient value varies from 0.2421 to 0.912. However, it is very high in Heat of vaporization (hv) and Critical temperature(ct) with r= 0.912 and 0.9097, we can use Minimum Degree Energy as a tool to predict the physical properties of alkanes.

In quadratic model, we can see that the correlation coefficient value varies from 0.2668 to 0.9288. It is high especially in Molar volume (mv), Molar refraction(mr), and Boiling point(Bp) of alkanes. The correlation is

poor for melting points of alkanes, with correlation coefficient value of r = 0.2668.

However, in comparision with linear and quadratic models, the correlation is high in quadratic model for all physical properties and weak correlation to Melting point (mp) in linear and quadratic models.

If the absolute values of correlation coefficient are less than 0.8 can be characterized as useless, from the practical point of view graph energies.

Future scope

The QSPR study has revealed that the molecular descriptors are best to predict the physicochemical properties of alkanes from n-butanes to nonane. The chemical people can use these topological indices for experimental data verification or they can reduce time by using these results directly in their experimentation. These graph energies will lead to many new applications in the chemical fields.

Correlation of graph energies with physico-chemical properties of 67 alkanes

In the following Figures, the correlation of Graph energies with physical properties of alkanes are demonstrated.

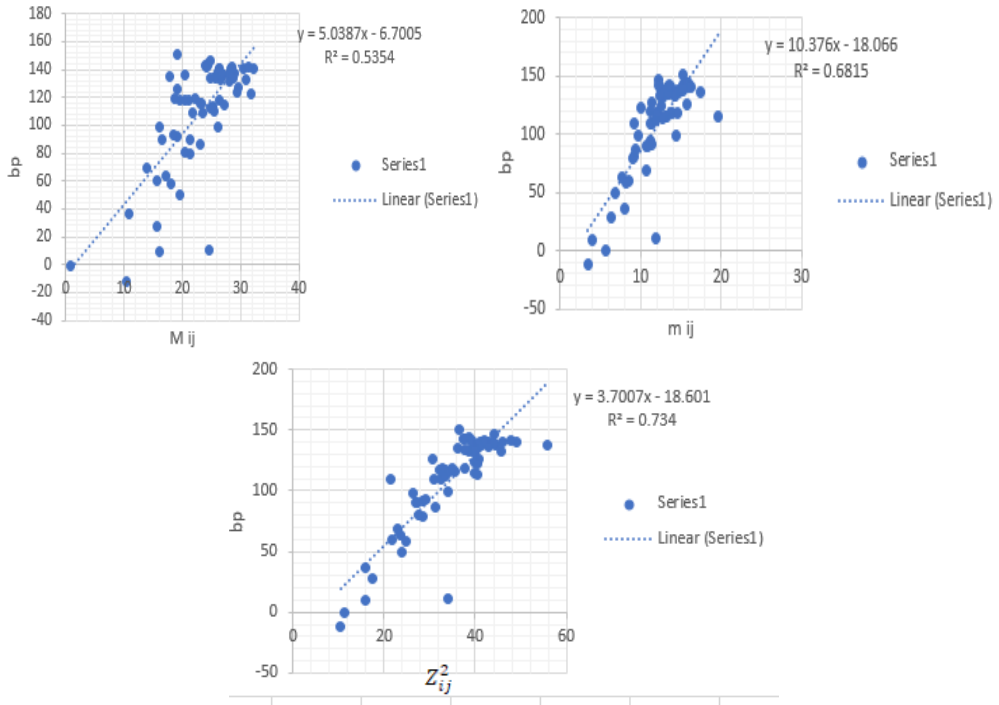

FIGURE 1 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (bp) with physical properties of 67 alkanes in linear model

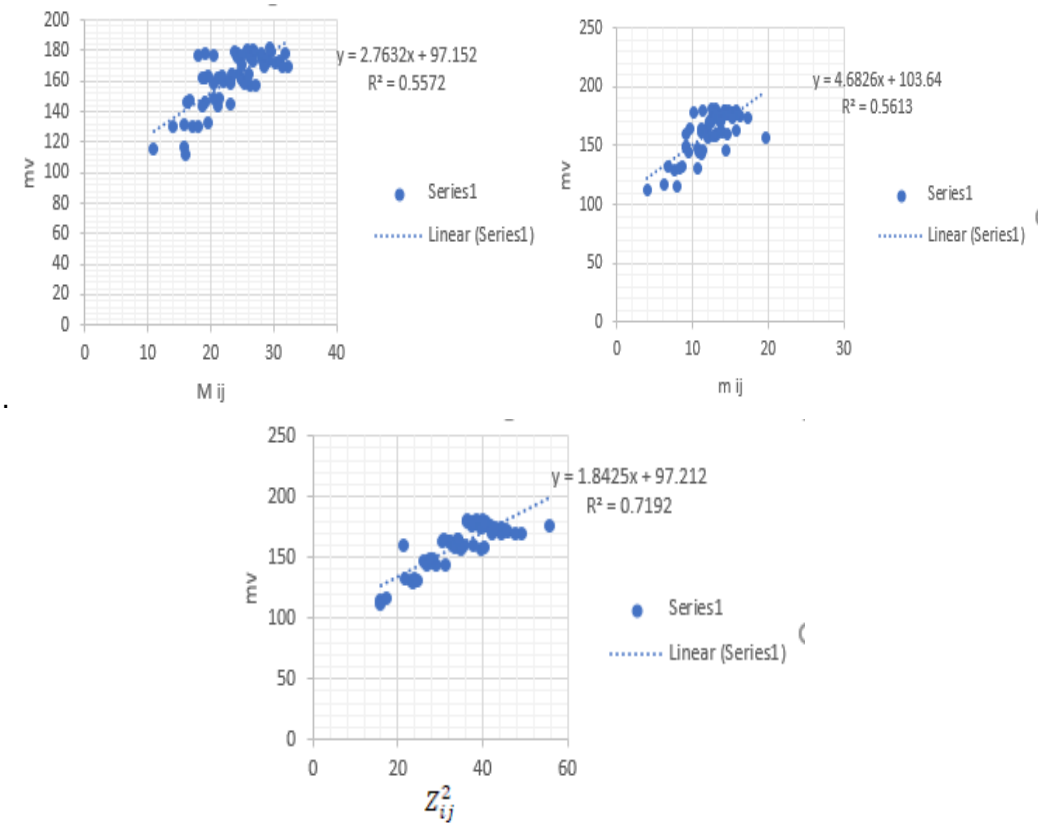

FIGURE 2 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (mv) with physical properties of 67 alkanes in linear model

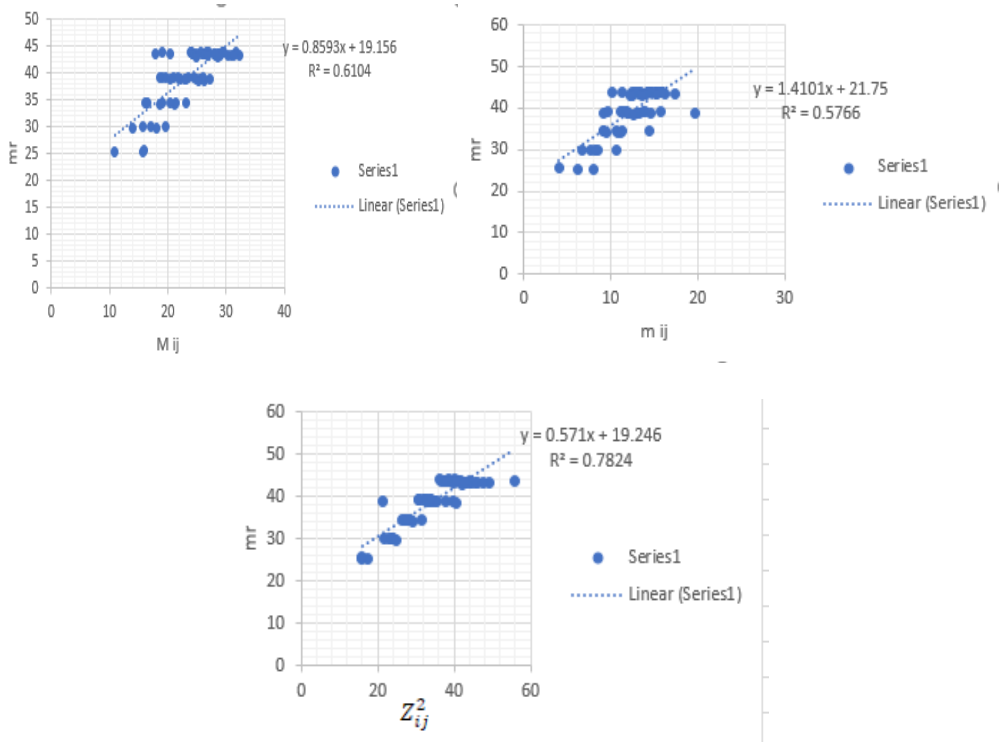

FIGURE 3 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (mr) with physical properties of 67 alkanes in linear model

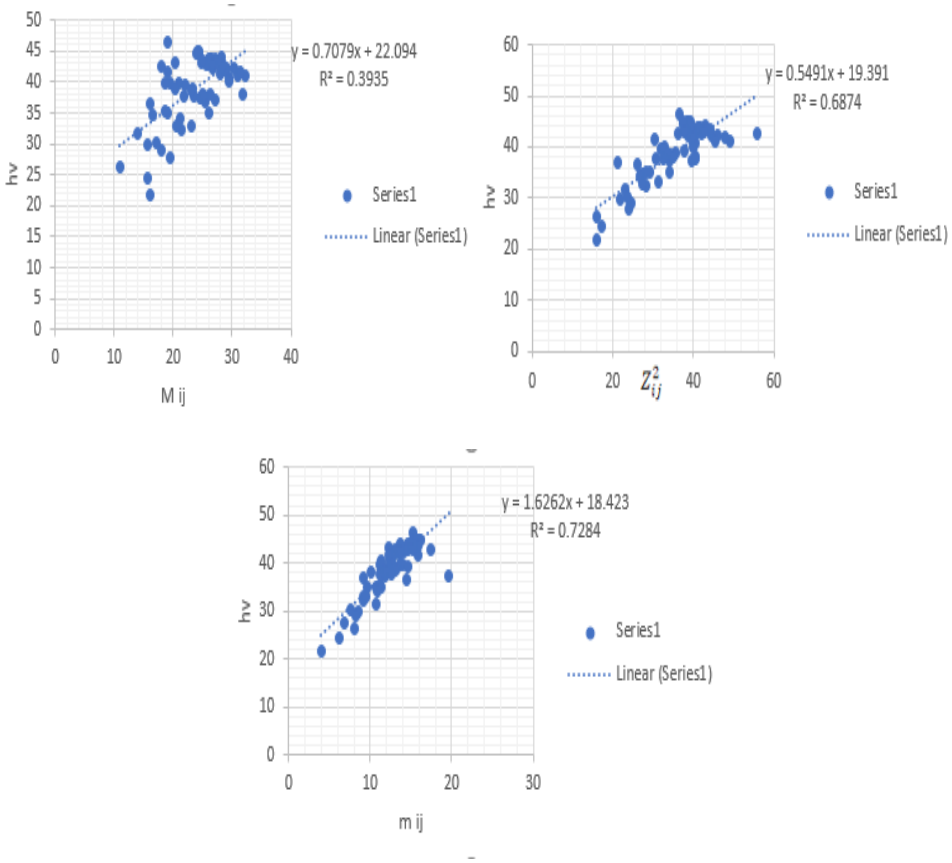

FIGURE 4 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (hv) with physical properties of 67 alkanes in linear model

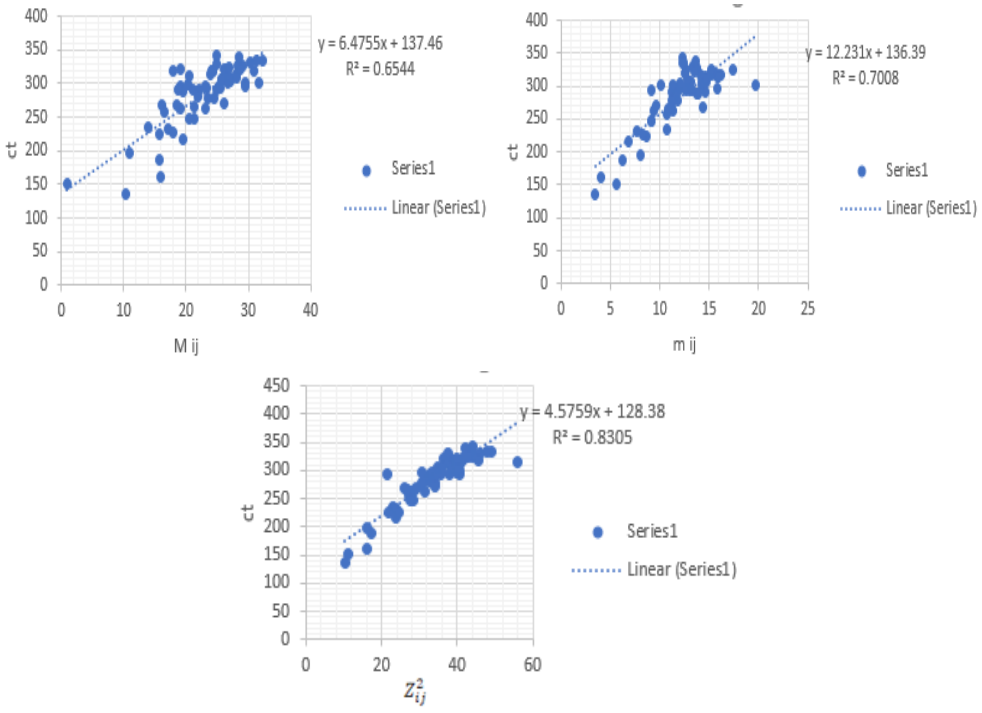

FIGURE 5 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (ct) with physical properties of 67 alkanes in linear model

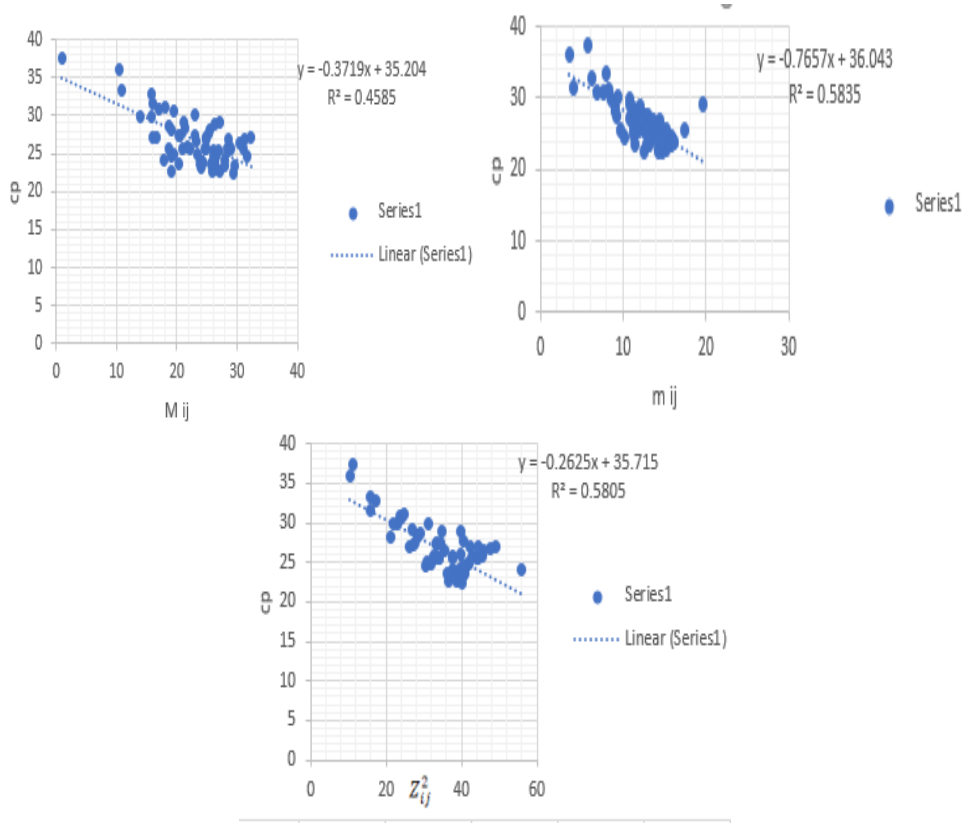

FIGURE 6 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (cp) with physical properties of 67 alkanes in linear model

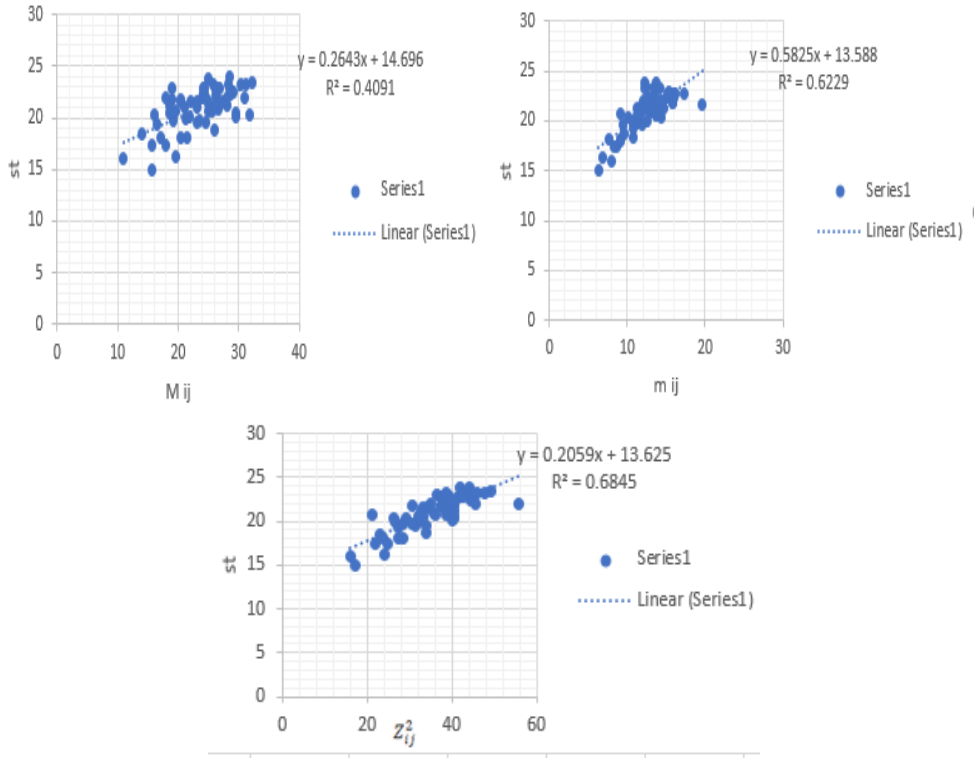

FIGURE 7 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (st) with physical properties of 67 alkanes in linear model

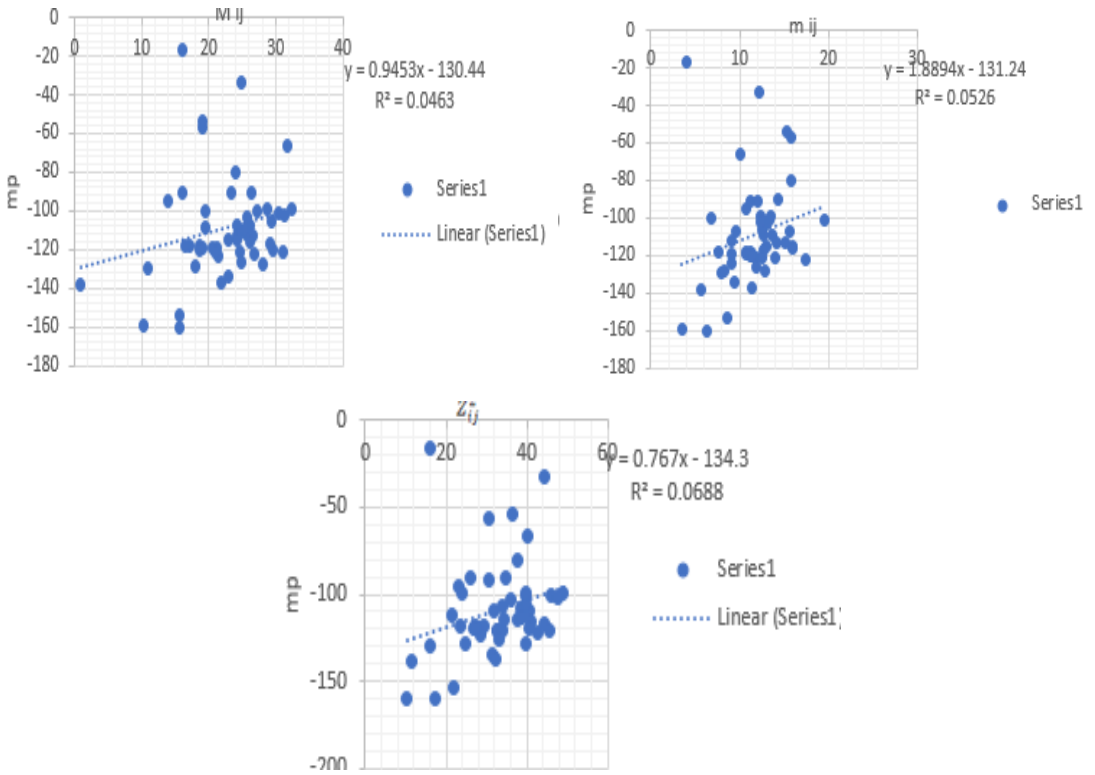

FIGURE 8 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (mp) with physical properties of 67 alkanes in linear model

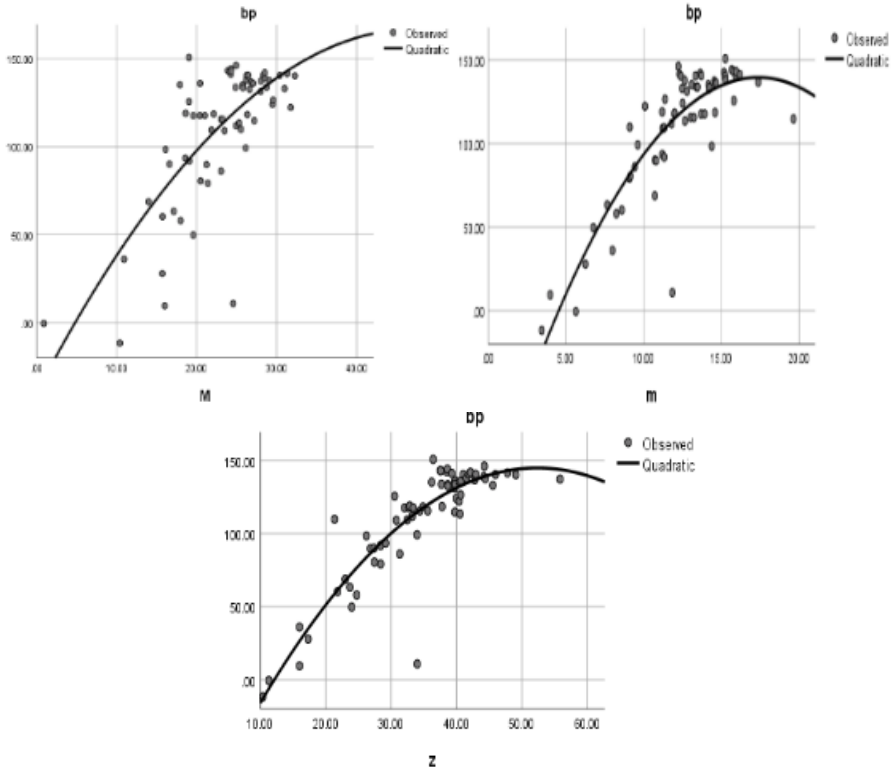

FIGURE 9 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (bp) with physical properties of 67 alkanes in Quadratic model

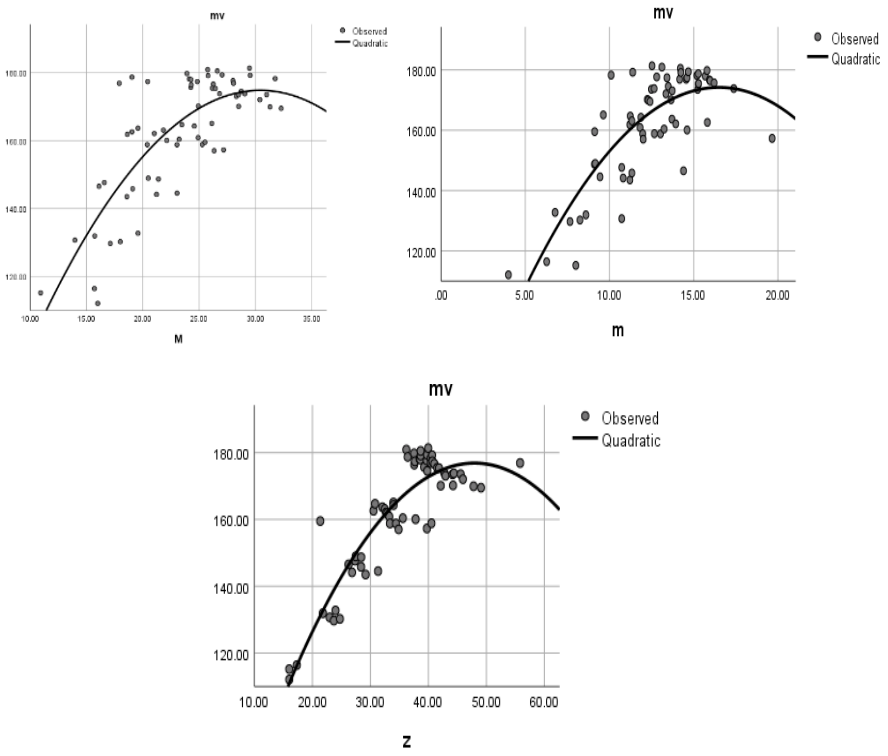

FIGURE 10 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (mv) with physical properties of 67 alkanes in Quadratic model

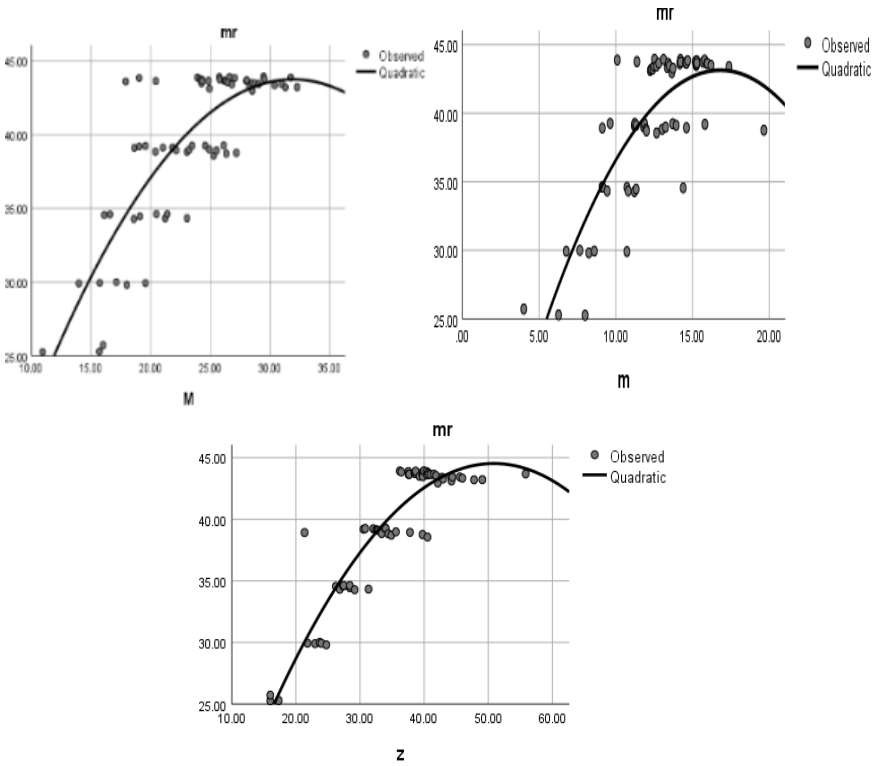

FIGURE 11 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (mr) with physical properties of 67 alkanes in Quadratic model

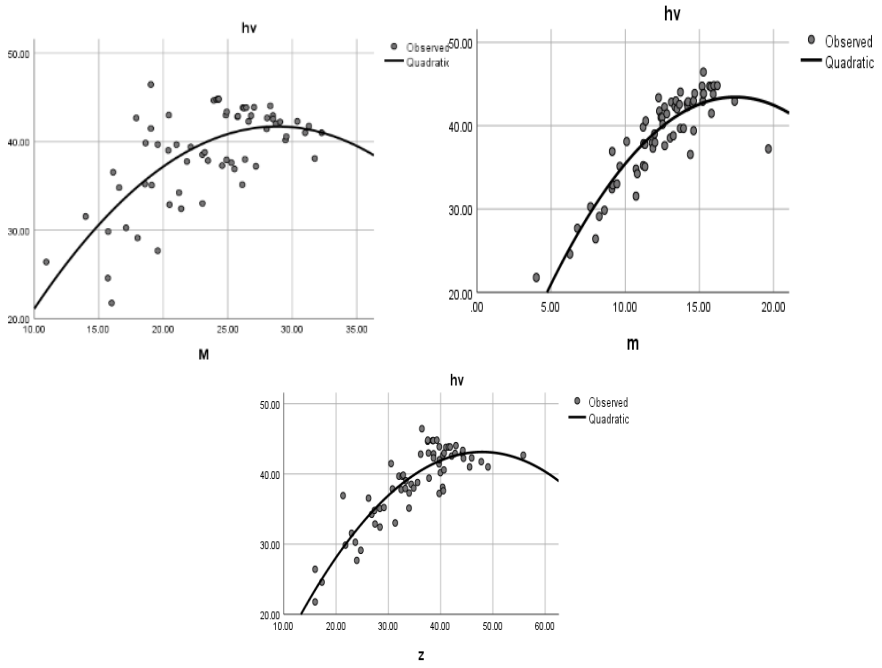

FIGURE 12 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (hv) with physical properties of 67 alkanes in Quadratic model

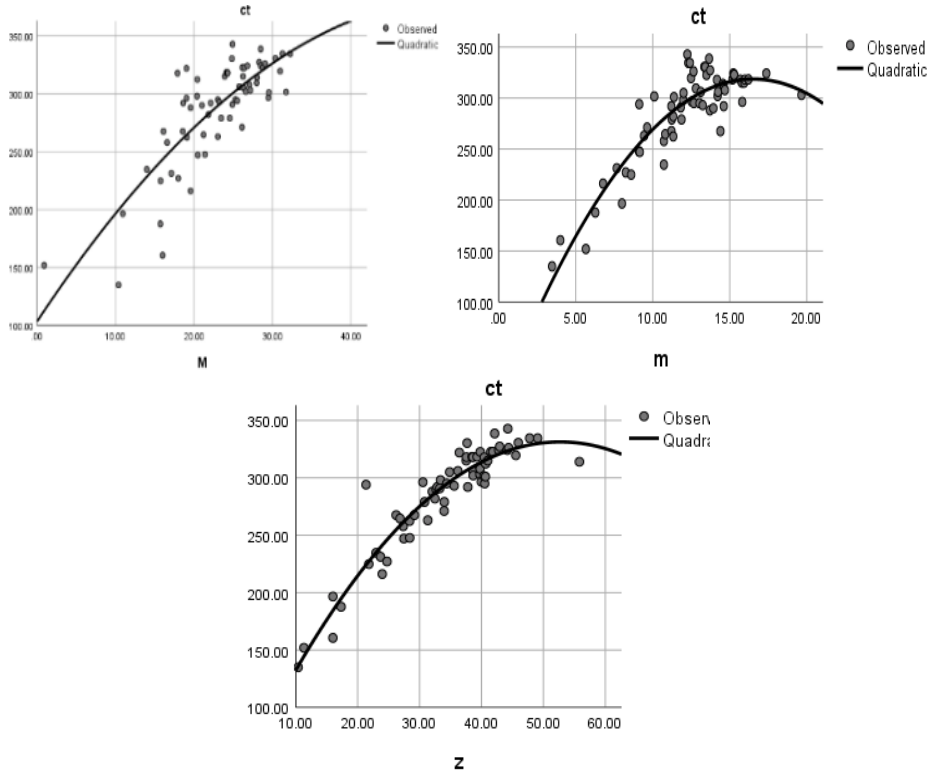

FIGURE 13 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (ct) with physical properties of 67 alkanes in Quadratic model

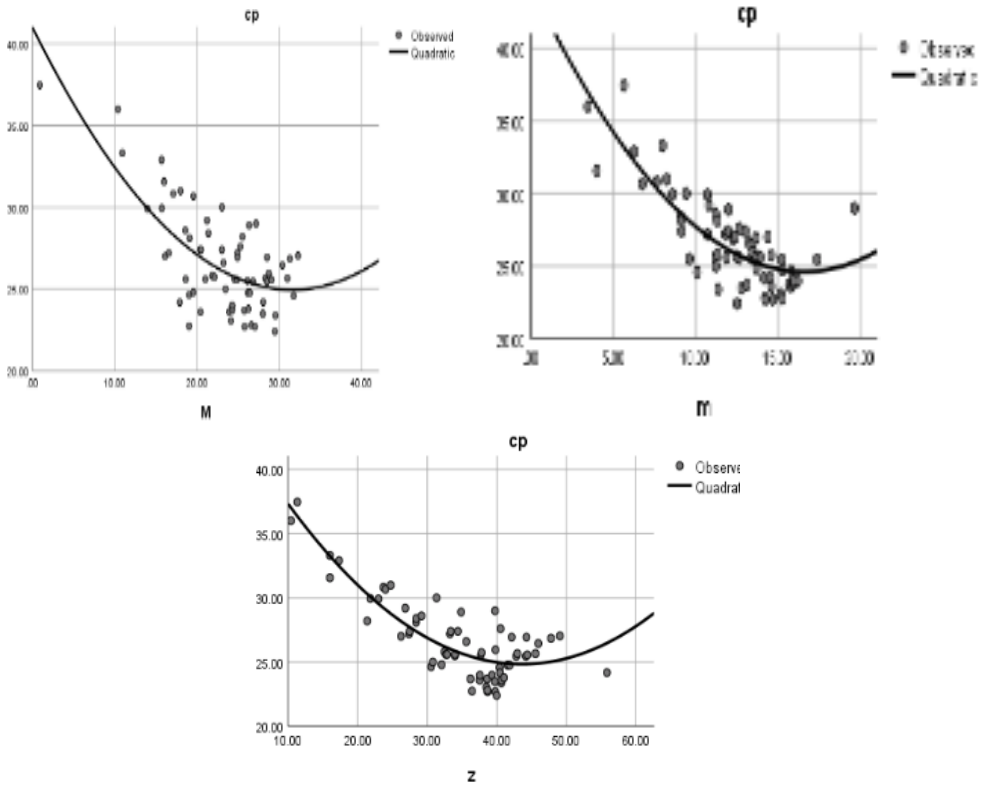

FIGURE 14 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (cp) with physical properties of 67 alkanes in Quadratic model

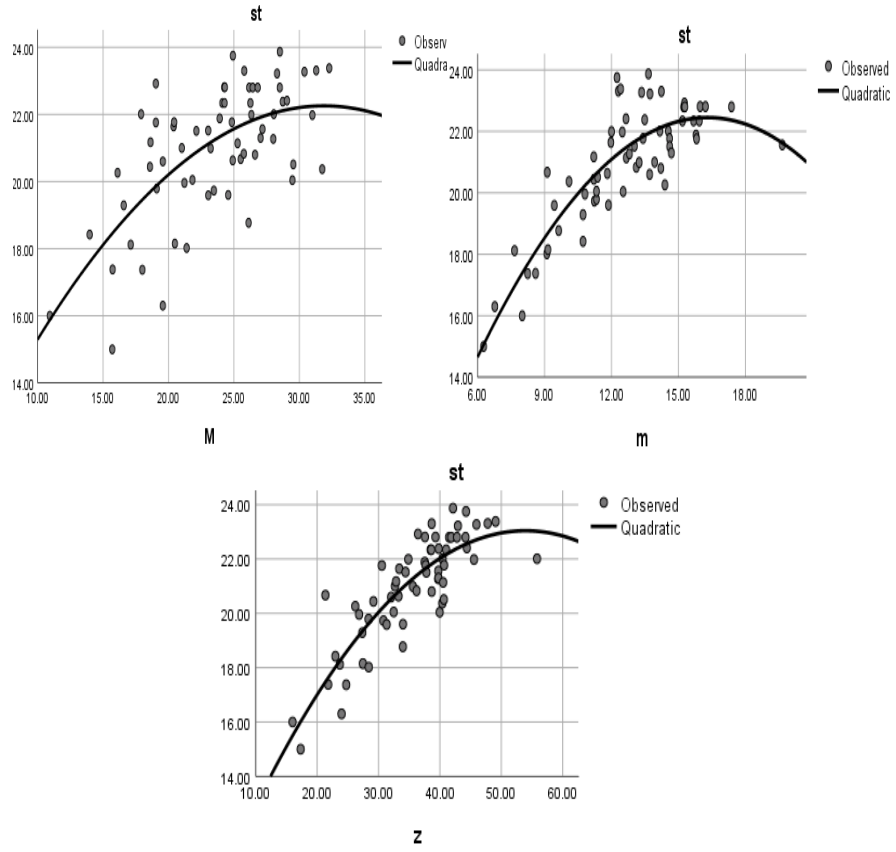

FIGURE 15 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (st) with physical properties of 67 alkanes in linear model

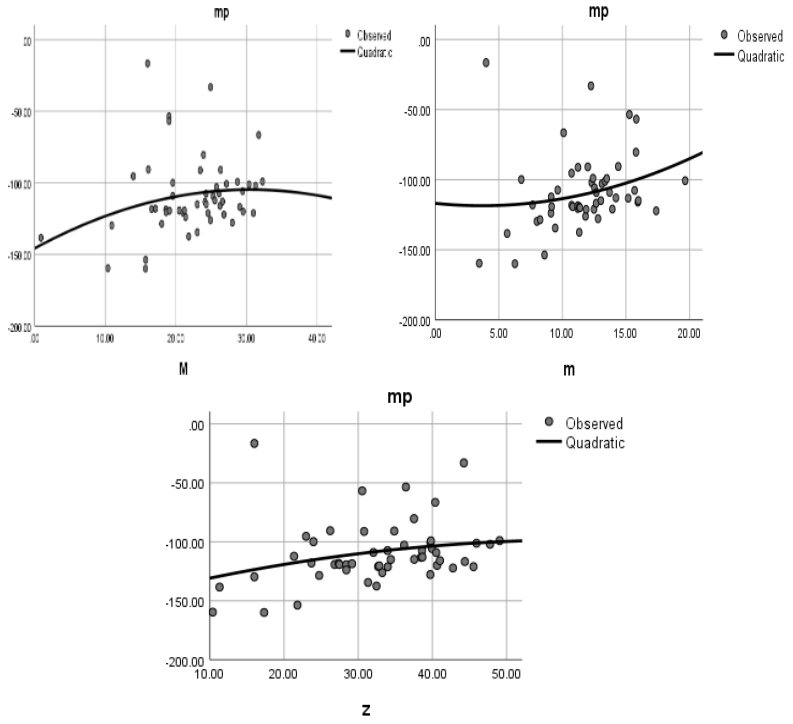

FIGURE 16 Correlation between Maximum Degree Energy, Minimum Degree Energy, and Second Zagreb Energy (mp) with physical properties of 67 alkanes in Quadratic model

Conclusion

The correlation coefficient (r) shows the eligibility level of the topological index as a tool to predict the physico-chemical properties of chemical compounds in the QSPR analysis. The results of QSPR studies reveals that the regression model is the most significant model to predict the physico-chemical properties of chemical compounds.

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Conflict of interest

There are no conflicts of interests.

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