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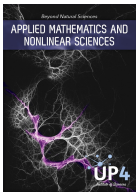

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QSPR Analysis of Certain Graph Theocratical Matrices and Their Corresponding Energy

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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 certain graph theocratical matrices and their corresponding energy. Our study reveals some important results which helps to characterize the useful topological indices based on their predicting power.

Keywords: Elastohydrodynamic lubrication, Line contact, Multigrid, Multilevel technique, Bio-based oil
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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.

The numerical invariants of chemical graphs are increasingly being used for a single number characterization of the corresponding chemical compounds [5]. These invariants are named in the chemical literature as topological indices [1, 2] or graph-theocratical indices [29]. The former term is the more common of the two. Topological indices have found application in various areas of chemistry, physics, mathematics, informatics, biology, etc [29], but their most important use to date is in the non-empirical Quantitative Structure- Property Relationships (QSPR) and Quantitative Structure -Activity Relationships (QSAR) [4, 24, 26, 27].

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2 Survey on Graph Theocratical Matrices

1. **Vertex Adjacency Matrix:** The term vertex adjacency matrix was first introduced in chemical graph theory by Mallion in his interesting paper [20] on graph theocratical aspects of the ring current theory. Below we give the vertex adjacency matrix of the vertex labeled graph G.
et $G=(V,E)$ be a grapLh where $V=\{1,2,3,\cdots,n\}$ the vertex adjacency matrix of a graph with vertex set $V=\{1,2,3,\cdots,n\}$ is the $n\times n$ matrix in which $a_{ij}=1$ if and only if there is an adjacency from vertex i to vertex j. Each diagonal entry in the adjacency matrix of a graph is zero. i.e.,

$$a_{ij}=\begin{cases}1, \text{ if } v_i \text{ is adjacent to } v_j;\\ 0, \text{ otherwise.}\end{cases}$$

2. **Vertex Zagreb Adjacency Matrix:** Motivated by Zagreb matrix [10] we define new adjacency matrix based on the vertex degrees which is as follows:
let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the vertex Zagreb adjacency matrix $Z_1(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases}1, & \text{if } v_i \text{ is adjacent to } v_j;\\ deg(v_i)^2 & \text{if } v_i=v_j;\\ 0, & \text{otherwise.}\end{cases}$$

3. **Forgotten Adjacency Matrix:** Recently, Gutman and Furtula [7] have studied the forgotten topological index $F(G)$ of a molecular graph G. Based on the definition of adjacency matrix and vertex degrees of a graph G, we define the forgotten adjacency matrix as follows:
let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the forgotten adjacency matrix $F(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases}1, & \text{if } v_i \text{ is adjacent to } v_j;\\ deg(v_i)^3 & \text{if } v_i=v_j;\\ 0, & \text{otherwise.}\end{cases}$$

4. **Harmonic Matrix:** Motivated by Harmonic index [6] of a molecular graph G, the harmonic matrix is defined as follows:

let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the harmonic matrix $H(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases}\frac{2}{deg(v_i)+deg(v_j)}, \text{ if } v_i \text{ is adjacent to } v_j;\\ 0, \text{ otherwise.}\end{cases}$$

5. **Geometric-Airthmetic Matrix:** Again on the same lines of harmonic index, we define GA- matrix [28] based on a GA-index of a molecular graph G as:

let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the harmonic matrix $H(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases}\frac{2\sqrt{deg(v_i)deg(v_j)}}{deg(v_i)+deg(v_j)}, \text{ if } v_i \text{ is adjacent to } v_j;\\ 0, \text{ otherwise.}\end{cases}$$

6. **Degree-Sum Matrix:** Ramane et. al [22] have introduced degree-sum matrix associated with a graph and obtained some upper and lower bounds for its eigenvalues.

let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the degree-sum matrix $H(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases} deg(v_i)+deg(v_j), & \text{if } v_i \neq v_j; \\ 0, & \text{otherwise.} \end{cases}$$

7. **Laplacian Matrix:** In [11] Gutman and Zhou have put forward the Laplacian matrix. The Laplacian matrix sometimes also called a Kirchoff matrix [3] due to its role in matrix tree theorem, Implicitin the electrical network work of Kirchoff in his paper Kirchoff also introduced the concept of the spanning tree.

   let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the Laplacian matrix $L(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases} -1, & \text{if } v_i \neq v_j \text{ and } v_i \text{ is adjacent to } v_j; \\ 0 & \text{if } v_i \neq v_j \text{ and } v_i \text{ is not adjacent to } v_j; \\ degv_i, & v_i = v_j. \end{cases}$$

8. **Sum-Connectivity Matrix:** The sum-connectivity matrix denoted by SC_{ij} was introduced independently by Zhou and Trianjstic [34] it is defined as follows:

   let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the harmonic matrix $SC_{ij}(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases} \frac{1}{\sqrt{deg(v_i)+deg(v_j)}}, & \text{if } v_i \text{ is adjacent to } v_j; \\ 0, & \text{otherwise.} \end{cases}$$

9. **Vertex Randić Matrix:** The vertex-connectivity matrix denoted by Rij introduced by Randic [23]. It can be regarded as edge-weighted matrix of the graph defined as:

   let $G=(V,E)$ be a graph where $V=\{1,2,3,\cdots,n\}$ then the harmonic matrix $R(G)$ of a graph G is defined as follows i.e.,

$$a_{ij}=\begin{cases} \frac{1}{\sqrt{deg(v_i)deg(v_j)}}, & \text{if } v_i \text{ is adjacent to } v_j; \\ 0, & \text{otherwise.} \end{cases}$$

3 The characteristic polynomial and corresponding energy

1. **Vertex Adjacency Energy.** The characteristic polynomial of $A(G)$ is denoted by

$$f_n(G,a)=det(aI-A(G)).$$

   Since $A(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$a_1 \geq a_2 \geq a_3 \geq \cdots, \geq a_n.$$

   The energy of G is then defined as

$$E(G)=\sum_{i=1}^{n}|a_i|.$$

2. **Vertex Zagreb Adjacency Energy.** The characteristic polynomial of $Z_1(G)$ is denoted by

$$f_n(G,z) = det(zI - Z_1(G)).$$

Since $Z_1(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$z_1 \geq z_2 \geq z_3 \geq \cdots, \geq z_n.$$

The vertex Zagreb energy of G is then defined as

$$Z_1E(G) = \sum_{i=1}^{n} |z_i|.$$

3. **Forgotten Energy.** The characteristic polynomial of $F(G)$ is denoted by

$$f_n(G,f) = det(fI - F(G)).$$

Since $F(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$f_1 \geq f_2 \geq f_3 \geq \cdots, \geq f_n.$$

The forgotten energy of G is then defined as

$$FE(G) = \sum_{i=1}^{n} |f_i|.$$

4. **Harmonic Energy.** The characteristic polynomial of $H(G)$ is denoted by

$$f_n(G,h) = det(hI - H(G)).$$

Since $H(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$h_1 \geq h_2 \geq h_3 \geq \cdots, \geq h_n.$$

The harmonic energy of G is then defined as

$$HE(G) = \sum_{i=1}^{n} |h_i|.$$

5. **Geometric-Airthmetic Energy.** The characteristic polynomial of $GA(G)$ is denoted by

$$f_n(G,g) = det(gI - GA(G)).$$

Since $GA(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$g_1 \geq g_2 \geq g_3 \geq \cdots, \geq g_n.$$

The Geometric-Airthmetic energy of G is then defined as

$$GAE(G) = \sum_{i=1}^{n} |g_i|.$$

6. **Degree-Sum Energy.** The characteristic polynomial of $DS(G)$ is denoted by

$$f_n(G,d) = det(dI - DS(G)).$$

Since $DS(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$d_1 \geq d_2 \geq d_3 \geq \cdots, \geq d_n.$$

The Degree-Sum energy of G is then defined as

$$DSE(G) = \sum_{i=1}^{n} |d_i|.$$

7. **Laplacian Energy.** The characteristic polynomial of $L(G)$ is denoted by

$$f_n(G,\lambda) = det(\lambda I - L(G)).$$

Since $L(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots, \geq \lambda_n.$$

The Laplacian energy of G is then defined as

$$LE(G) = \sum_{i=1}^{n} |\lambda_i|.$$

8. **Sum-Connectivity Energy.** The characteristic polynomial of $SC(G)$ is denoted by

$$f_n(G,\mu) = det(\mu I - SC(G)).$$

Since $SC(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$\mu_1 \geq \mu_2 \geq \mu_3 \geq \cdots, \geq \mu_n.$$

The Sum-Connectivity energy of G is then defined as

$$SCE(G) = \sum_{i=1}^{n} |\mu_i|.$$

9. **Vertex Randić Energy.** The characteristic polynomial of $R(G)$ is denoted by

$$f_n(G,r) = det(rI - R(G)).$$

Since $R(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as follows:

$$r_1 \geq r_2 \geq r_3 \geq \cdots, \geq r_n.$$

The Vertex Randić Energy of G is then defined as

$$RE(G) = \sum_{i=1}^{n} |r_i|.$$

4 The Use of Graph Theoretical Matrices in QSPR Studies

We have used nine Graph Theoretical Matrices viz, vertex-adjacency matrix, vertex Zagreb adjacency Matrix, forgotten adjacency matrix, harmonic matrix, geometric-airthmetic matrix, degree-sum matrix, laplacian matrix, sum-connectivity matrix and vertex Randić matrix respectively 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 68 alkanes from n-butanes to nonanes. Values for these property were taken from Dejan Plavsić et. al [21]. The corresponding energy of the above said matrices and the experimental values for the physical properties of 68 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

S.No.	Alkane	bp($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
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	2,2, 3,3-tetramethylbutane	106.470				270.8	24.5		
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

S.No.	Alkane	bp($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
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	
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	$E(G)$	$Z_1E(G)$	$F_E(G)$	$HE(G)$	$GA_E(G)$	$DS_E(G)$	$L_E(G)$	$SC_E(G)$	$R_E(G)$
1	Butane	2.828	10	18	2.844	4.268	18.166	6	2.516	3
2	2-methyl propane	2.828	11.243	30	1.732	3	18.422	6	1.732	2
3	Pentane	4.472	14.001	25.999	3.274	5.286	25.874	8	2.98	3.414
4	2-methyl butane	5.226	16	38	2.86	4.758	26.253	8	2.72	3.154
5	2,2 dimethylpropane	4	20	68	1.6	3.2	26.88	8	1.788	2
6	Hexane	6.988	17.99	34	4.086	6.788	33.698	10	3.768	4.236
7	2-methylpentane	6.064	14.999	46	3.254	5.722	34.168	10	3.15	3.528
8	3-methyalpentane	6.9	20	46	3.924	6.442	34.168	10	3.652	4.23
9	2,2-methylbutane	5.818	23.992	76.001	2.798	5.024	34.485	10	2.824	3.224
10	2,3-dimethylbutane	6.004	22	58	2.906	5.292	34.628	10	2.944	3.334
11	Heptanes	8.054	21.999	41.98	4.59	7.868	41.58	12	4.284	4.732
12	2-methylhexane	7.728	24.001	53.991	4.282	7.266	42.12	11.999	4.17	4.376
13	3-methylhexane	7.88	24	54	4.376	7.456	43.058	11.999	4.112	4.632
15	3-ethylpentane	6.9	20	56	4.586	7.654	38.08	10	4.24	4.828
16	2,2-dimethylpentane	6.72	27.999	83.999	3.176	5.966	43.06	12.001	3.24	3.582
17	2,3-dimethylpentane	7.664	24.999	65.999	3.966	6.92	42.648	12.001	3.872	4.404
18	2,4-dimethylpentane	6.156	20	46	3.226	6.148	43.015	10	3.312	3.632
19	3,3-dimethylpentane	6.596	28	83.999	3.944	6.802	43.266	12	3.666	5.74
20	Octane	9.516	26	50	5.324	9.312	49.496	14	4.76	5.468
21	2-methylheptane	8.764	28	62	4.792	8.294	50.09	14	4.33	4.82
22	3-methylheptane	9.408	27.999	62	5.138	8.924	49.996	14	4.608	5.41
23	4-methylheptane	8.828	27.999	62	4.734	8.402	50.09	14	4.298	4.974

S.No.	Alkane	$E(G)$	$Z_1E(G)$	$F_E(G)$	$HE(G)$	$GA_E(G)$	$DS_E(G)$	$L_E(G)$	$SC_E(G)$	$R_E(G)$
24	3-ethylhexane	7.88	24	54	5.282	9.034	50.09	11.999	4.536	5.502
25	2,2-dimethylhexane	8.312	31.999	91.999	4.008	7.522	51.14	14	3.892	4.424
26	2,3-dimethylhexane	8.646	30.001	73.999	4.376	7.95	50.671	15	4.198	4.792
27	2,4-dimethylhexane	8.564	30	74	4.314	7.862	49.825	14.001	4.114	4.678
28	2,5-dimethylhexane	8.472	30	74	3.714	7.095	50.671	14	3.761	4.468
29	3,3-dimethylhexane	8.52	31.998	92	4.334	7.772	51.14	14	3.968	4.752
30	3,4-dimethylhexane	9.332	30	74	5.002	8.584	50.413	14.001	4.5	5.41
31	3-ethyl-2-methylpentane	7.664	29	70	4.588	4.51	51.016	14	4.16	4.916
32	3-ethyl-3-methylpentane	7.596	32	91.246	5.048	8.526	51.14	14	4.336	5.488
33	2,2,3-trimethylpentane	7.3	34.001	104	3.902	7.228	51.876	16	3.808	4.448
34	2,2,4-trimethylpentane	7.384	33.999	104	3.1444	6.386	51.701	14	3.056	3.684
35	2,3,3-trimethylpentane	8.054	34	104.001	4.026	7.374	47.686	14	4.068	4.6
36	2,3,4-trimethylpentane	8.424	32	86.001	4.002	7.5	51.24	14	4.09	4.574
36	2,2,3,3-tetramethylbutane	7.212	38	134	2.816	5.892	52.698	15.998	3.179	3.5
37	Nonane	10.628	30	58.001	5.884	10.432	57.432	16	5.574	6.028
38	2-methyloctane	10.252	32	70.001	5.342	9.792	58.07	16	5.22	5.22
39	3-methyloctane	10.472	32	69.998	5.662	10.042	58.07	15.999	5.418	5.954
40	4-methyloctane	10.384	32	70.001	5.58	9.97	58.07	16	5.354	5.858
41	3-ethylheptane	10.564	28.126	69.999	5.864	10.214	58.07	15.999	5.039	5.49
42	4-ethylheptane	10.492	32	70	5.79	10.138	57.842	16	5.3	5.902
43	2,2-dimethylheptane	9.336	35.999	99.999	4.502	8.754	59.21	16	4.355	4.916
44	2,3-dimethylheptane	10.176	34.001	81.999	5.202	9.49	58.694	16	5.118	5.632
45	2,4-dimethylheptane	9.508	34	81.999	4.728	8.866	58.694	16	4.718	5.132
46	2,5-dimethylheptane	10.152	34	81.999	5.162	9.438	58.694	16	5.092	5.598
47	2,6- dimethylheptane	10.096	35.999	99.999	4.564	8.536	59.21	15.999	4.64	4.98

S.No.	Alkane	$E(G)$	$Z_1E(G)$	$F_E(G)$	$HE(G)$	$GA_E(G)$	$DS_E(G)$	$L_E(G)$	$SC_E(G)$	$R_E(G)$
48	3,3- dimethylheptane	9.464	33.999	82	5.194	9.324	58.694	16	5.072	5.632
49	3,4- dimethylheptane	10.312	34	81.999	5.45	9.672	59.079	15.999	5.262	3.939
50	3,5- dimethylheptane	10.29	33.999	82.001	5.418	9.628	58.978	16	5.24	5.85
51	4,4- dimethylheptane	9.43	36.001	99.999	4.744	8.73	59.588	16	4.684	5.146
52	3-ethyl-2-methylhexane	10.198	33.999	81.999	5.35	9.606	58.694	16	5.184	5.73
53	4-ethyl-2-methylhexane	10.176	34.001	81.999	5.308	9.55	58.694	15.91	5.158	5.698
54	3-ethyl-3-methylhexane	10.262	36	99.999	5.504	9.56	59.21	15	5.252	5.952
55	2,2,4- trimethylhexane	9.13	38	111.999	4.242	8.134	59.814	15.999	4.372	4.796
56	2,2,5- trimethylhexane	9.06	37.993	112	4.022	8.012	59.814	16	4.256	4.582
57	2,3,3- trimethylhexane	9.3	37.999	112	4.418	8.34	59.814	16.176	4.496	4.97
58	2,3,4- trimethylhexane	10.096	36	93.999	5.068	9.184	59.307	16.001	5.02	5.648
59	2,3,5- trimethylhexane	9.336	36.017	94	4.366	8.428	59.307	15.999	4.5	4.918
60	3,3,4- trimethylhexane	10.036	44	112.002	5.086	9.052	59.814	16	4.994	5.67
61	3,3-diethylpentane	10.472	36	100	5.793	7.736	59.21	15.55	4.903	3.042
62	2,2-dimethyl-3-ethylpentane	9.3	37.999	59.814	4.528	6.954	112.003	16	4.476	4.498
63	2,3-dimethyl-3-ethylpentane	10.062	38.001	61.877	5.116	8.43	112.001	16.001	3.976	4.376
64	2,4-dimethyl-3-ethylpentane	8.884	31	57.368	5.088	8.78	74.999	14	4.818	5.582
65	2,2,3,3-tetramethylpentane	8.98	42	60.9	4.24	7.35	142	15.998	4.122	4.672
66	2,2,3,4- tetramethylpentane	9.02	40	60.408	3.93	7.75	124	16.001	4.168	4.614
67	2,2,4,4- tetramethylpentane	7.936	42	60.9	3.056	6.61	142	16	4.44	3.726
68	2,3,3,4- tetramethylpentane	9.152	39.243	57.278	4.14	7.96	124	14.999	4.992	4.74

5 Regression Models

We have tested the following linear regression model

$$P = A + B(TI) \tag{1}$$

where P = physical property, TI = topological index .

Using (3.1), we have obtained the following different linear models for each degree based topological index, which are listed below.

1. **Vertex adjacency energy $E(G)$:**

$$bp = -51.397 + [E(G)]19.268 \tag{2}$$
$$mv = 75.5727 + [E(G)]10.1894 \tag{3}$$
$$mr = 13.1325 + [E(G)]3.0530 \tag{4}$$
$$hv = 10.0231 + [E(G)]3.3206 \tag{5}$$
$$ct = 91.9103 + [E(G)]23.1023 \tag{6}$$
$$cp = 28.9043 + [E(G)]0.0858 \tag{7}$$
$$st = 11.0052 + [E(G)]1.1474 \tag{8}$$
$$mp = -145.3088 + [E(G)]4.4911 \tag{9}$$

2. **Vertex Zagreb adjacency energy $Z_1E(G)$:**

$$bp = -13.358 + [Z_1E(G)]4.1092 \tag{10}$$
$$mv = 94.7149 + [Z_1E(G)]2.2017 \tag{11}$$
$$mr = 18.6119 + [Z_1E(G)]0.6778 \tag{12}$$
$$hv = 14.0714 + [Z_1E(G)]0.7822 \tag{13}$$
$$ct = 211.4016 + [Z_1E(G)]1.0167 \tag{14}$$
$$cp = 32.606 - [Z_1E(G)]0.0988 \tag{15}$$
$$st = 14.4576 + [Z_1E(G)]0.2108 \tag{16}$$
$$mp = -139.2218 + [Z_1E(G)]1.0322 \tag{17}$$

3. **Forgotten adjacency energy $FE(G)$:**

$$bp = 49.581 + [FE(G)]0.829 \tag{18}$$
$$mv = 127.4698 + [FE(G)]0.4683 \tag{19}$$
$$mr = 29.0759 + [FE(G)]0.1390 \tag{20}$$
$$hv = 490.0581 - [FE(G)]5.8696 \tag{21}$$
$$ct = 131.1926 + [FE(G)]5.1377 \tag{22}$$
$$cp = 31.4563 - [FE(G)]0.0249 \tag{23}$$
$$st = 18.4178 + [FE(G)]0.034156 \tag{24}$$
$$mp = -123.9450 + [FE(G)]0.2094 \tag{25}$$

4. **harmonic energy** $HE(G)$**:**

$$bp = -29.71 + [HE(G)]32.08 \quad (26)$$
$$mv = 100.054 + [HE(G)]13.9260 \quad (27)$$
$$mr = 20.4799 + [HE(G)]4.2371 \quad (28)$$
$$hv = 31.9676 + [HE(G)]1.4827 \quad (29)$$
$$ct = 118.2041 + [HE(G)]38.4066 \quad (30)$$
$$cp = 27.5611 + [HE(G)]0.4722 \quad (31)$$
$$st = 12.1028 + [HE(G)]1.9642 \quad (32)$$
$$mp = -137.1760 + [HE(G)]6.6745 \quad (33)$$

5. **Geometric-Arithmetic energy** $GAE(G)$**:**

$$bp = -36.99 + [GAE(G)]18.984 \quad (34)$$
$$mv = 90.04705 + [GAE(G)]9.0967 \quad (35)$$
$$mr = 18.0357 + [GAE(G)]2.6920 \quad (36)$$
$$hv = 34.6289 + [GAE(G)]0.5068 \quad (37)$$
$$ct = 113.4305 + [GAE(G)]22.2200 \quad (38)$$
$$cp = 27.3753 + [GAE(G)]0.2895 \quad (39)$$
$$st = 12.6092 + [GAE(G)]1.0425 \quad (40)$$
$$mp = -133.5245 + [GAE(G)]3.28 \quad (41)$$

6. **Degree sum energy** $DSE(G)$**:**

$$bp = 59.931 + [DSE(G)]0.897 \quad (42)$$
$$mv = 138.925 + [DSE(G)]0.402892 \quad (43)$$
$$mr = 31.1877 + [DSE(G)]0.1300 \quad (44)$$
$$hv = 32.5560 + [DSE(G)]0.1074 \quad (45)$$
$$ct = 219.9439 + [DSE(G)]1.1727 \quad (46)$$
$$cp = 32.1358 - [DSE(G)]0.04447 \quad (47)$$
$$st = 18.4122 + [DSE(G)]0.04367 \quad (48)$$
$$mp = -122.6285 + [DSE(G)]0.2430 \quad (49)$$

7. **Laplacian energy** $LE(G)$**:**

$$bp = 105.998 + [LE(G)]0.795 \quad (50)$$
$$mv = 61.7923 + [LE(G)]7.1569 \quad (51)$$
$$mr = 9.2778 + [LE(G)]2.1462 \quad (52)$$
$$hv = 28.1626 + [LE(G)]0.7323 \quad (53)$$
$$ct = 71.1141 + [LE(G)]15.5601 \quad (54)$$
$$cp = 31.3140 - [LE(G)]0.1221 \quad (55)$$
$$st = 10.9055 + [LE(G)]0.755115 \quad (56)$$
$$mp = -146.7815 + [LE(G)]2.8215 \quad (57)$$

8. **Sum connectivity energy** $SCE(G)$**:**

$$bp = -57.214 + [SCE(G)]39.634 \quad (58)$$
$$mv = 79.5397 + [SCE(G)]19.1531 \quad (59)$$
$$mr = 14.5174 + [SCE(G)]5.762765 \quad (60)$$
$$hv = 32.3464 + [SCE(G)]1.4459 \quad (61)$$
$$ct = 86.5805 + [SCE(G)]47.1321 \quad (62)$$
$$cp = 26.5275 + [SCE(G)]0.7319 \quad (63)$$
$$st = 0.7399 + [SCE(G)]2.3432 \quad (64)$$
$$mp = -144.7607 + [SCE(G)]8.7341 \quad (65)$$

9. **Vertex Randic energy** $RE(G)$**:**

$$bp = -33.08 + [RE(G)]30.673 \quad (66)$$
$$mv = 4740.533522 - [RE(G)]960.1500 \quad (67)$$
$$mr = 20.0386 + [RE(G)]4.0559 \quad (68)$$
$$hv = 24.5656 + [RE(G)]2.8952 \quad (69)$$
$$ct = 116.5371 + [RE(G)]36.2135 \quad (70)$$
$$cp = 25.3061 + [RE(G)]0.9224 \quad (71)$$
$$st = 13.07611 + [RE(G)]1.6338 \quad (72)$$
$$mp = -113.7685 + [RE(G)]1.0137 \quad (73)$$

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

Physical Properties	N	a	b	r	s	F
Boiling point	68	-51.397	19.268	0.959	10.54257	763.634
Molar volume	65	75.5727	10.1894	0.905	7.62675	286.565
Molar refraction	65	13.1325	3.0530	0.912	2.19071	311.823
Heats of vaporization	65	10.0231	3.3206	0.968	1.3755	935.676
Critical temperature	68	91.9103	23.1023	0.936	16.0513	496.344
Critical Pressure	68	28.9043	0.0858	0.006	565.769	0.003
Surface tension	64	11.0052	1.1474	0.871	0.9705	194.411
Melting point	52	-145.3088	4.4911	0.316	25.8886	5.528

Table 4. Statical parameters for the linear QSPR model for $Z_1E(G)$.

Physical Properties	N	a	b	r	s	F
Boiling point	68	-13.358	4.1092	0.837	20.46726	154.120
Molar volume	65	94.714914	2.201775	0.843	9.6547	155.135
Molar refraction	65	18.6119	0.6778	o.873	2.6070	201.663
Heats of vaporization	65	14.0714	0.7822	0.736	3.7075	74.461
Critical temperature	68	211.4016	1.0167	0.855	23.6776	180.025
Critical Pressure	68	32.606	-0.0988	0.030	119.570	5.061
Surface tension	64	14.4576	0.2108	0.727	1.35607	69.337
Melting point	52	-137.1762	6.6745	0.312	25.9224	5.383

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

Physical Properties	N	a	b	r	s	F
Boiling point	68	49.581	0.829	0.524	31.8288	25.020
Molar volume	65	127.4698	0.4683	0.551	14.9892	27.500
Molar refraction	65	29.0759	0.1390	0.55	4.4616	27.365
Heats of vaporization	65	490.0581	-5.8696	0.410	4.9948	12.738
Critical temperature	68	131.1926	5.1377	0.525	38.8983	25.158
Critical Pressure	68	31.4563	-0.0249	0.024	135.575	0.038
Surface tension	64	18.4178	0.0341	0.369	1.83471	9.750
Melting point	52	-123.9450	0.2094	0.187	26.7987	1.821

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

Physical Properties	N	a	b	r	s	F
Boiling point	68	-29.71	32.08	0.825	21.1104	140.91
Molar volume	65	100.054	13.9260	0.682	13.1375	54.809
Molar refraction	65	20.4799	4.2371	0.698	3.8278	59.766
Heats of vaporization	65	31.9676	1.4827	0.856	2.8351	172.070
Critical temperature	67	118.2041	38.4066	0.808	26.9494	123.915
Critical Pressure	68	27.5611	0.4722	0.018	24.6671	0.022
Surface tension	64	12.1028	1.9642	0.804	1.1734	113.396
Melting point	52	-137.1762	6.6745	0.239	26.4944	3.018

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

Physical Properties	**N**	**a**	**b**	**r**	**s**	**F**
Boiling point	68	-36.99	18.984	0.870	18.4148	205.922
Molar volume	65	90.0410	9.0967	0.791	11.0019	104.98
Molar refraction	65	18.0357	2.6920	0.787	3.2997	102.211
Heats of vaporization	65	34.6289	0.5068	0.89	2.4722	246.160
Critical temperature	68	113.4305	22.2200	0.833	25.3083	149.343
Critical Pressure	68	27.3753	0.2895	0.020	24.661	0.027
Surface tension	64	12.6092	1.0425	0.767	1.2654	88.825
Melting point	52	-132.52	3.28	0.208	26.6869	2.256

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

Physical Properties	**N**	**a**	**b**	**r**	**s**	**F**
Boiling point	68	59.931	0.897	0.597	29.9848	36.560
Molar volume	65	138.935	0.4028	0.549	15.0099	27.250
Molar refraction	65	31.1877	0.1300	0.596	4.2888	34.79
Heats of vaporization	65	32.5560	0.1074	0.481	4.8027	18.918
Critical temperature	68	219.9439	1.1727	0.638	35.1156	45.347
Critical Pressure	68	32.1358	-0.0444	0.045	81.216	0.133
Surface tension	64	18.4122	0.0436	0.540	1.6617	25.459
Melting point	52	-122.628	0.2430	0.244	26.4571	3.164

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

Physical Properties	**N**	**a**	**b**	**r**	**s**	**F**
Boiling point	68	105.998	0.795	0.951	11.6074	618.389
Molar volume	65	61.7923	7.1569	0.964	4.7915	822.621
Molar refraction	65	9.2778	2.1462	0.972	1.2624	1065.626
Heats of vaporization	65	28.1626	0.7323	0.924	2.0990	365.873
Critical temperature	68	71.1141	15.5601	0.935	16.1580	462.301
Critical Pressure	68	31.3140	-0.1221	0.014	24.6698	0.012
Surface tension	64	10.9055	0.7551	0.834	1.0888	141.725
Melting point	52	-146.7815	2.8215	0.301	26.0151	4.989

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

Physical Properties	**N**	**a**	**b**	**r**	**s**	**F**
Boiling point	68	-57.214	39.635	0.907	15.7086	307.683
Molar volume	65	79.5397	19.1531	0.823	10.1925	132.724
Molar refraction	65	14.5174	5.7627	0.833	2.9563	142.822
Heats of vaporization	65	32.3464	1.44459	0.931	1.9928	412.801
Critical temperature	68	86.5805	47.321	0.883	21.4546	233.650
Critical Pressure	68	26.5275	0.7319	0.025	24.6642	0.043
Surface tension	64	0.7399	2.3432	0.847	1.0489	157.493
Melting point	52	-144.7607	8.7341	0.278	26.2084	4.181

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

Physical Properties	N	a	b	r	s	F
Boiling point	68	-33.08	30.673	0.776	23.5965	99.608
Molar volume	65	4740.5335	-960.1500	0.655	13.5743	47.350
Molar refraction	65	20.0386	4.0559	0.656	4.0335	47.567
Heats of vaporization	65	24.5656	2.8952	0.764	3.53619	88.107
Critical temperature	68	116.5371	36.2135	0.749	30.3071	84.165
Critical Pressure	68	25.3061	0.9224	0.035	29.00	0.083
Surface tension	64	13.0761	1.6338	0.667	1.46987	49.788
Melting point	52	-113.7685	1.0137	0.035	27.2655	0.061

6 Discussion and Concluding Remarks

By inspection of the data in Tables 3 to 11, it is possible to draw a number of conclusions for the given energy like invariants.

First, the famous and much studied invariant, energy of a graph found more suitable tool to predict physical property of alkane, especially Boiling points, Molar volume, Surface tension, Critical temperature, Heats of vaporization and Molar refractions of alkanes with correlation coefficient values $r = 0.959, 0.905, 0.871, 0.968$ and 0.912 respectively.

Motivated by vertex Zagreb energy. Here we introduced a new topological invariant namely, vertex Zagreb adjacency energy. The QSPR study of vertex Zagreb energy reveals that Z1E(G) can be useful in predicting the Boiling points, Critical temperatures, Molar volumes and Molar refraction of alkanes also from Table 4,we can see that the correlation coefficient value of $Z_1E(G)$ with physical properties of alkanes lies between 0.030 to 0.873.

In addition by using the recently advocated idea of using Forgotten index in QSPR studies, we introduced Forgotten adjacency energy. The QSPR study of $FE(G)$ shows that the idea of using $FE(G)$ in QSPR study does not make sense. Since the correlation coefficient values FE(G) with physical properties of alkanes lies between 0.024 to 0.551.

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. The Table 6 reveals that harmonic energy is also useful tool in predicting the Boiling point, Heats of vaporization, Surface tensions and Critical temperature of alkanes with correlation coefficient values $r = 0.825, 0.856, 0.804$ and 0.808, respectively.

The QSPR study of Geometric-arithmetic energy reveals that the predicting power of $G-A$- energy for the physical properties Boiling points, Heats of vaporization and Critical temperatures of alkanes with correlation coefficient values $r = 0.870, 0.89$ and 0.833 respectively.

In addition the results for degree sum energy revealed that the recent advocated idea of using degree sum energy doesn't pass the test.

The so called Laplacian energy shows remarkably good correlation with the Boiling points, Molar volumes, Molar refractions, Heats of vaporization, Surface tensions and Critical temperatures of alkanes with correlation coefficient values $r = 0.951, 0.964, 0.972, 0.924, 0.83$ and $r = 0.935$ respectively. Further, the correlation coefficient values lies between 0.014 to 0.972. In fact the predicting power of Laplacian energy to the critical pressures of alkanes is almost nil.

The sum connectivity energy shows similar correlation properties [ ]. The QSPR study in Table 10 reveals

that the predicting power of sum connectivity energy is remarkably good. Infarct the sum connectivity energy can be use as a tool to predict the Heats of vaporization of alkanes. The correlation coefficient value of sum connectivity energy with the Heats of vaporization of alkanes is 0.931. Further the range of correlation coefficient value is 0.025 to 0.931. In fact, the predicting power of sum connectivity energy with Critical pressures of alkanes is almost nil.

The QSPR study of Vertex randic energy does not pass the test.

From practical point of view, topological indices for which the absolute values of correlation coefficient are less than 0.8 can be characterized as useless. Thus the QSPR study of 9 topological indices with physical properties of 68 alkanes helps us to characterize useful topological indices with absolute value of correlation coefficient lies between 0.8 to 0.972.

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