QSPR Study on Benzene Derivatives to some Physico–Chemical Properties by using Topological Indices

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ABSTRACT QSPR study on benzene derivatives have been made using recently introduced topological methodology. In this study the relationship between the Randic' (^1x), Balaban (J), Szeged (Sz),Harary (H), Wiener (W), HyperWiener(WW) and Wiener Polarity (W_P) to the thermal energy (E_{th}), heat capacity (C_V) and entropy (S) of benzene derivatives is represented. Physicochemical properties are taken from the quantum mechanics methodology with HF level using the ab initio 6-31G basis sets. The multiple linear regressions (MLR) and back ward methods (with significant at the 0.05 level) were employed to give the QSPR models. The satisfactory obtained results show that combining the two descriptors (Sz, WW) are useful topological descriptors for predicted (C_V) and (S) of the 45 benzene derivatives. The training set models established by MLR method have not good correlation of (E_{th}), which means QSPR models could not predict the thermal energy of compounds.

KEYWORDS QSPR • Topological index • benzene derivatives • graph theory • multiple linear regressions (MLR).

1. INTRODUCTION

Benzene derivatives compounds are widely used industrial chemicals and thus have a high potential for environmental pollution. The eventual release and accumulation of these compounds into the environment in both terrestrial and aquatic systems requires an assessment of their environmental risk. Science experimental measurements of physicochemical properties are extremely time- consuming and expensive.

Quantitative structure – property relationships (QSPRs) have provided a valuable approach in research into physicochemical properties of organic chemicals [1]. Many investigators have used quantum – chemical parameters [2–5].Among the different approaches employing computational chemistry, those based on chemical graph theory have been useful in establishing QSPR [6].

The basic strategy of QSPR is to find the optimum quantitative relationship which can then be used for the prediction of the properties of molecular structures including those unmeasured or even unknown [7–9].

The premise of QSPR is that physicochemical properties can be correlated with molecular structure characteristics (geometric and electronic) expressed in terms of appropriate molecular descriptors [10].

QSPR have been traditionally developed by selecting, a priori, an analytical model (typically) linear, polynomial or lag–linear to quantity the correlation between selected molecular indices and desired physicochemical properties, followed by regression analysis to determine model parameters [11–13].

In the present study, the multiple linear regression (MLR) techniques and back ward methods are used for modeling the thermal energy (E_{th}), heat capacity (C_V) and entropy (S) of 45 benzene derivatives.

The proposed QSPR models were based on molecular descriptors (topological indices) that can be calculated for any compound utilizing only the knowledge of its molecular structure (molecular graph).

The topological indices used for the QSPR analysis were Wiener [14], Szeged [15], first order molecular connectivity [16], Balaban [17], HyperWiener [18], Wiener Polarity [19] and Harary [20] indices.

2. MATERIALS AND METHODS

2.1. QUANTUM CHEMISTRY CALCULATIONS

The thermal energy (E_{th}), heat capacity (C_V) and entropy (S) of 45 benzene derivatives are taken from the quantum mechanics methodology with Hartree–Fock (HF) level using the ab initio 6–31G basis sets. The quantum chemistry data of the 45 congeners are listed in Table 1.

2.2. TOPOLOGICAL INDICES

All the used topological indices were calculated using all hydrogen suppressed graph by deleting all the carbon hydrogen as well as heteroatomic hydrogen bonds from the

structure of the benzene derivatives. The descriptors were calculated with chemicalize software [21]. Six topological indices tested in the present study are recorded in Table 2.

2.3. STATISTICAL ANALYSIS

Structure- Property models (MLR models) are generated using the multilinear regression procedure of SPSS version 16. The thermal energy ($E_{th}\frac{kcal}{mol}$), heat capacity ($Cv\frac{cal}{molK}$) and entropy ($S\frac{cal}{molK}$) are used as the dependent variable and ^{1}x, J, Sz, H, W_P and WW indices as the independent variables. The models are assessed with R value (correlation coefficient), the R^2(coefficient of determination), the R^2- adjusted, the SD value (root of the mean square of errors), the F value (Fischer statistic) and the sig (significant).

3. RESULTS

Several linear QSPR models involving one, two, three, four and five descriptors are established and strongest multivariable correlations are identified by the back ward method are significant at the 0.05 level and regression analysis of the SPSS program.

In the first of this study we drown scattering plots of C_V, S and E_{th} versus the six topological indices, ^{1}x, J, W, Sz, WW and W_P. Some of these plots are given in Fig. (1–8), respectively. Distribution of the dependent variable against the independent variable for 45 chemicals employed in developing quantitative structure–properties relationship.

3.1. QSPR MODELS FOR HEAT CAPACITY (CV)

Model 1

$C_V = 18.000 – 0.573\,^1x - 4.038\,J – 0.051\,H – 0.103\,WW – 0.006\,WP + 0.257\,Sz$

N= 45 R= 0.966 R^2 =0.933 R^2_{adj} = 0.922 SD=2.342

F= 88.125 sig = 0.000 (1)

Model 2

$C_V = 18.045 – 0.574\,^1x - 4.048\,J – 0.051\,H – 0.103\,WW - 0.256Sz$

N= 45 R= 0.966 R^2 =0.933 R^2_{adj} = 0.924 SD=2.312

F= 108.531 sig = 0.000 (2)

Model 3

$C_V = 18.351 - 0.556^1x - 4.180\ J - 0.106\ WW - 0.266\ Sz$

N= 45 R= 0.966 R^2 =0.933 R^2_{adj} = 0.926 SD=2.284

F= 138.960 sig = 0.000 (3)

Model 4

$C_V = 16.779 - 3.975\ J - 0.102\ WW - 0.252\ Sz$

N= 45 R= 0.966 R^2 =0.933 R^2_{adj} = 0.928 SD=2.261

F= 188.938 sig = 0.000 (4)

Model 5

$C_V = 10.629 - 0.085\ WW + 0.216\ Sz$

N= 45 R= 0.964 R^2 =0.929 R^2_{adj} = 0.926 SD=2.292

F= 274.854 sig = 0.000 (5)

It turns out that the heat capacity (C_V) has a good correlation with all six topological indices as well as with WW and Sz (Eq. (5)).

3.2. QSPR MODELS FOR THERMAL ENERGY (ETH)

Model 6

$E_{th} = 112.146 - 1.952^1x - 16.645\ J + 1.496\ H - 0.167\ WW - 0.702\ W_P - 0.356\ Sz$

N= 45 R= 0.425 R^2 =0.181 R^2_{adj} = 0.052 SD=18.837

F= 1.400 sig = 0.240 (6)

Model 7

$E_{th} = 106.705 - 15.971\ J + 1.473\ H + 0.180\ WW + 0.689\ W_P - 0.396\ Sz$

N= 45 R= 0.425 R^2 =0.180 R^2_{adj} = 0.075 SD=18.603

F= 1.715 sig = 0.154 (7)

Model 8

E_{th} = 102.046- 14.980 J + 1.454 H + 0.130 WW - 0.271 Sz

N= 45 R= 0.422 R^2 =0.178 R^2_{adj} = 0.096 SD=18.396

F= 2.162 sig = 0.091 (8)

Model 9

E_{th} = 112.147- 22.272 J + 0.666 H + 0.021 WW

N= 45 R= 0.414 R^2 =0.171 R^2_{adj} = 0.111 SD=18.240

F= 2.828 sig = 0.050 (9)

Model 10

E_{th} = 108.116- 23.268 J + 1.190 H

N= 45 R= 0.408 R^2 =0.167 R^2_{adj} = 0.127 SD=18.074

F= 4.199 sig = 0.022 (10)

Model 11

E_{th} = 66.730+0.699 H

N= 45 R= 0.365 R^2 =0.134 R^2_{adj} = 0.113 SD=18.214

F= 6.629 sig = 0.014 (11)

It turns out that the correlation coefficient values of all models for E_{th}, is less than 0.2, which means that there is no strong linear relation between E_{th} and descriptors.

3.3. QSPR MODELS FOR ENTROPY (S)

Model 12

$S = 72.845 - 0.598^{1}X - 4.788\ J + 0.259\ H - 0.116\ WW + 0.334\ W_P + 0.272\ Sz$

N= 45 R= 0.948 R^2 =0.898 R^2_{adj} = 0.882 SD=4.008

F= 55.810 sig = 0.000 (12)

Model 13

$S = 71.179 - 4.581\ J + 0.252\ H - 0.112\ WW - 0.33\ W_P - 0.259\ Sz$

N= 45 R= 0.948 R^2 =0.898 R^2_{adj} = 0.885 SD= 3.960

F= 68.590 sig = 0.000 (13)

Model 14

$S = 72.903 - 5.259\ J - 0.130\ WW - 0.322\ W_P + 0.312Sz$

N= 45 R= 0.947 R^2 =0.897 R^2_{adj} = 0.887 SD= 3.930

F= 86.936 sig = 0.000 (14)

Model 15

$S = 70.664 - 4.772\ J - 0.153\ WW + 0.369\ Sz$

N= 45 R= 0.946 R^2 =0.895 R^2_{adj} = 0.888 SD= 3.910

F= 116.931 sig = 0.000 (15)

Model 16

$S = 63.280 - 0.133\ WW + 0.324\ Sz$

N= 45 R= 0.945 R^2 =0.893 R^2_{adj} = 0.888 SD= 3.911

F= 174.741 sig = 0.000 (16)

It turns out that the entropy(S) has a good correlation with all six topological indices as well as with WW and Sz (Eq. (16)).

4. DISCUSSION

We studied the relationship between topological indices and the thermal energy (E_{th}), heat capacity (C_V) and entropy (S).

The elaborated QSPR models (Eqs 1 – 5) reveal that the heat capacity of the benzene derivatives could be explained by two, three, four, five and six parameter. All of models can explain about 93% of the experimental variance of the dependent variable C_V. The combination of the two parameters (WW, Sz) increases remarkably the predictive power of the QSPR model given by Eq. (5) ($R^2 = 0.929$, $R^2_{adj} = 0.926$, SD = 2.29, F = 274.854).

As can be seen from the statistical parameters of the above equation, a high F of Fischer (F = 274.854) which confirms that the model (5) predicts the heat capacity (dependent variable) in a statistically satisfactory significant manner.

The back ward values of the entropy shows that all of models (Eqs 12 – 16) can explain about 0.90% of the variance of the entropy. The combination of two parameters (WW, Sz) recorded in Eq (16) has highest F of Fischer (F = 174.741) which explain that the model (16) for predict entropy is better than another models. The QSPR models (Eqs 6 – 11) explains only 18% of the variance of the thermal energy besides a low F and a low standard deviation (SD) which confirms that all of models (Eqs 6 – 11) could not use to predicts the thermal energy.

The comparison between the observed data and predicted values using Eq (16) of entropy (S) is presented in Table 3. The linear relations between the observed and predicted values of the entropy of 45 benzene derivatives show in Figure (9).

The comparison between the observed data and predicted values using Eq (5) of C_V is presented in Table 3. The linear relations between the observed and predicted values of the heat capacity of 45 benzene derivatives show in Figure (10).

5. CONCLUSION

The aforementioned results and discussion lead us to conclude that combining the two descriptors (Sz, WW) can be used successfully for modeling and predicting the heat capacity (C_V) and entropy (S) of 45benzene derivatives. The training set models established by MLR method have not good correlation of the thermal energy (E_{th}), which means QSPR models could not predict the thermal energy of compounds.

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Table 1. Benzene derivatives and their thermal energy (E_{th}), heat capacity (C_V) and entropy (S)

compounds	No.	E_{th} $kcal/mol$	Cv $cal/molK$	S $cal/molK$
Bromobenzene	1	65.29	18.974	77.412
Phenol	2	74.241	19.556	73.301
1,2-Dichlorobenzene	3	59.638	22.459	81.422
3-Chlorotoluene	4	84.812	24.561	86.151
1,3-Dihydroxybenzene	5	77.539	24.356	78.827
3-Hydroxyanisole	6	97.706	28.52	85.825
4-Methyl-3-nitroaniline	7	103.88	36.498	97.218
2,4-Dimethylphenol	8	113.333	31.213	95.395
2,6-Dimethylphenol	9	113.476	30.971	88.024
3-Nitrotoluene	10	93.604	28.973	92.842
2,6-Dinitrotoluene	11	93.307	39.695	104.851
4-Methyl-2,6-dinitroaniline	12	105.713	44.947	114.965
5-Methyl-2,6-dinitroaniline	13	105.837	44.81	107.737
5-Methyl-2,4-dinitroaniline	14	105.62	45.252	109.238
2,4-Dinitrotoluene	15	93.169	39.727	105.107
4-Nitrophenol	16	77.413	27.692	86.473
4-Chlorotoluene	17	77.206	31.85	96.426
2,4,6-Trichlorophenol	18	57.376	30.862	93.417
Toluene	19	82.941	27.892	89.047
3-Methyl-6-nitroaniline	20	104.149	35.841	96.864
4-Methyl-2-nitroaniline	21	106.04	33.951	94.282
1,2,4-Trichlorobenzene	22	53.93	26.321	88.346
3,4-Dichlorotoluene	23	79.161	28.303	93.362
2,4-Dichlorotoluene	24	79.266	28.227	88.762
Chlorobenzene	25	65.308	18.726	74.858
1,3,5-Trinitrobenzene	26	74.783	43.544	111.19
1,2,3,4-Tetrachlorobenzene	27	48.143	29.99	94.375

Table 1. (Continued).

2,3,4,5,6-Pentachlorophenol	28	45.776	38.209	105.427
1,3-Dichlorobenzene	29	59.625	22.593	81.815
2-Chlorophenol	30	68.741	23.201	79.752
3-Methylphenol	31	93.75	25.379	83.997
2,3-Dinitrotoluene	32	93.312	39.473	103.012
1,4-Dimethylbenzene	33	109.926	26.47	90.836
2,3,4,5-Tetrachlorophenol	34	51.504	34.552	99.256
2,3,6-Trinitrotoluene	35	96.277	47.777	115.335
4-Methylphenol	36	93.737	25.413	83.681
4-Methyl-3,5-dinitroaniline	37	105.556	45.32	110.557
1,3,5-Trichlorobenzene	38	53.896	26.473	88.731
Benzene	39	70.931	14.87	67.85
2-Nitrotoluene	40	93.788	28.598	87.958
1,4-Dinitrobenzene	41	75.38	32.677	96.457
2-Methyl-3,6-dinitroaniline	42	107.521	43.693	107.087
2-Methyl-4,6-dinitrophenol	43	96.803	43.786	108.582
2,5-Dinitrotolueno	44	93.252	39.676	105.278
1,2-Dinitrobenzene	45	75.477	32.524	95.425

Table 2. Benzene derivatives and their topological indices used in present study

Comp. No.	$^1\chi$	J	H	HW	WP	Sz
1	3.39	1.82	12.92	71	5	78
2	3.39	1.82	12.92	71	5	78
3	3.8	2.28	16.17	106	8	106
4	3.79	2.23	16.08	110	7	108
5	3.79	2.23	16.08	110	7	108
6	4.33	1.98	19.15	176	9	146
7	5.11	2.25	26.67	315	14	232
8	4.2	2.09	19.53	160	10	144
9	4.22	2.15	19.67	151	11	140
10	4.7	2.32	22.72	245	11	186
11	6.04	2.4	34.6	545	19	348
12	6.43	2.7	39.2	669	31	420
13	6.45	2.72	39.13	667	22	418
14	6.43	2.65	38.83	698	21	430
15	6.02	2.33	34.3	576	18	360
16	4.7	2.26	22.6	262	11	192
17	3.79	2.19	16.03	115	7	110
18	4.61	2.49	23.28	215	13	184
19	3.39	1.82	12.92	71	5	78
20	5.11	2.22	26.6	327	14	236
21	5.11	2.27	26.67	315	14	232
22	4.2	2.09	19.53	160	10	144
23	4.2	2.09	19.53	160	10	144
24	4.2	2.09	19.53	160	10	144
25	3.39	1.82	12.92	71	5	78
26	6.91	2.46	42.6	906	21	516
27	4.63	2.52	23.37	211	14	182
28	5.46	2.76	31.6	357	21	282
29	3.79	2.23	16.08	110	7	108
30	3.8	2.28	6.17	106	8	106
31	3.79	2.23	16.08	110	7	108
32	6.04	2.47	34.83	511	19	336
33	3.79	2.19	16.03	115	7	110
34	5.04	2.39	27.32	281	17	230
35	7.36	2.83	47.97	1036	26	588
36	2.18	2.19	16.3	115	7	110
37	6.43	2.7	39.02	669	21	420
38	4.18	2.08	19.5	159	9	144
39	3	2	10	42	3	54
40	4.72	2.4	22.9	231	12	180
41	5.61	2.3	29.74	521	15	314
42	6.45	2.64	38.87	717	22	434
43	6.43	2.66	38.85	691	21	428
44	6.02	2.28	34.14	616	18	372
45	5.63	2.54	30.43	416	16	278

Table 3. Comparison between predicted and observed values of entropy and heat capacity of respect benzene derivatives.

Comp. No.	Observed (S)	Predicted (S)	Residual	Observed (C_V)	Predicted (C_V)	Residual
1	77.41	79.11	1.70	18.97	21.44	2.47
2	73.30	79.11	5.81	19.57	21.44	1.87
3	81.42	83.53	2.11	22.46	24.52	2.06
4	86.15	83.64	-2.51	24.56	24.61	0.05
5	78.83	83.64	4.81	24.36	24.61	0.25
6	85.82	87.18	1.36	28.52	27.20	-1.32
7	97.22	96.55	-0.67	36.50	33.97	-2.53
8	95.40	88.66	6.74	31.21	28.13	-3.08
9	88.02	88.56	0.54	30.97	28.03	-2.94
10	92.84	90.96	-1.88	28.97	29.98	1.01
11	104.85	103.55	-1.30	39.70	39.47	-0.23
12	114.96	110.38	-4.58	44.95	44.48	-0.47
13	107.74	110.00	2.26	44.81	44.22	-0.59
14	109.24	109.77	0.53	45.25	44.18	-1.07
15	105.11	103.31	-1.80	39.73	39.43	-0.30
16	86.47	90.64	4.17	27.69	29.83	2.14
17	96.43	83.62	12.81	31.85	24.61	-7.24
18	93.42	94.30	0.88	30.86	32.09	1.23
19	89.05	79.11	-9.94	27.89	21.44	-6.45
20	96.86	96.25	-0.61	35.84	33.81	-2.03
21	94.28	96.55	2.27	33.95	33.97	0.02
22	88.35	88.66	0.31	26.32	28.13	1.81
23	93.36	88.66	-4.70	28.30	28.13	-0.17
24	88.76	88.66	-0.10	28.23	28.13	-0.10
25	74.86	79.11	4.25	18.73	21.44	2.71
26	111.19	109.97	-1.22	43.54	45.08	1.54
27	94.38	94.18	-0.20	29.99	32.01	2.02
28	105.43	107.17	1.74	38.21	41.20	2.99
29	81.82	83.64	1.82	22.59	24.61	2.02
30	79.75	83.53	3.78	23.20	24.52	1.32
31	84.00	83.64	-0.36	25.38	24.61	-0.77
32	103.01	104.18	1.17	39.47	39.77	0.30
33	90.84	83.49	-7.35	26.47	24.53	-1.94
34	99.26	100.29	1.03	34.55	36.34	1.79
35	115.34	116.00	0.66	47.78	49.58	1.80
36	83.68	83.62	-0.06	25.41	24.61	-0.80
37	110.58	110.38	-0.20	45.32	44.48	-0.84
38	88.73	88.79	0.06	26.47	28.22	1.75
39	67.85	75.19	7.34	14.87	18.72	3.85
40	87.96	90.88	2.92	28.60	29.87	1.27
41	96.46	95.72	-0.74	32.68	34.17	1.49
42	107.09	108.54	1.45	43.69	43.43	-0.26
43	108.58	110.05	1.47	43.79	44.34	0.55
44	105.28	101.88	-3.40	39.68	38.62	-1.06
45	95.42	98.02	2.60	32.52	35.32	2.8

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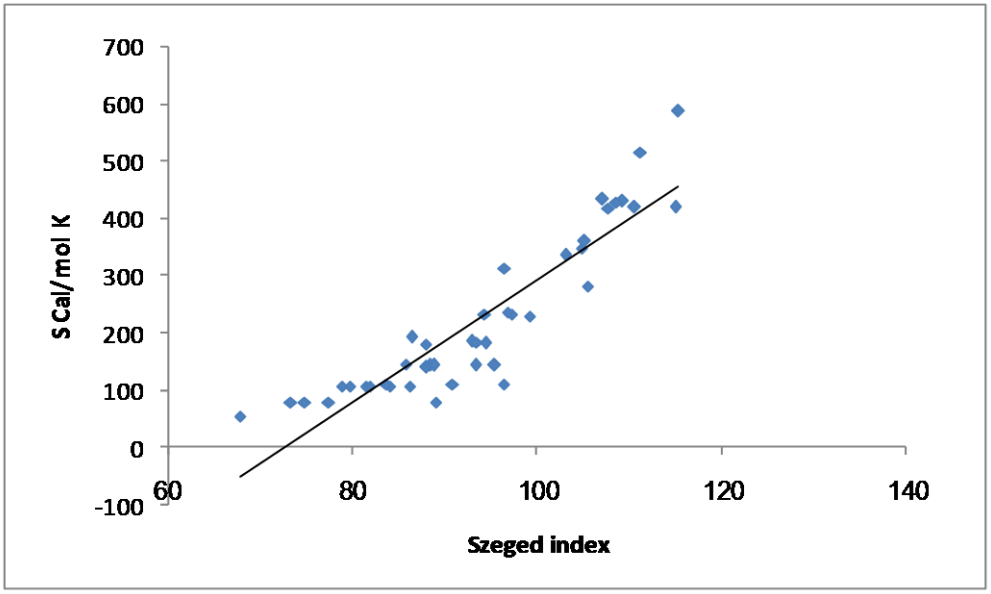

Figure 1. Plots of the Szeged index (Sz) versus entropy of 45 benzene derivatives.

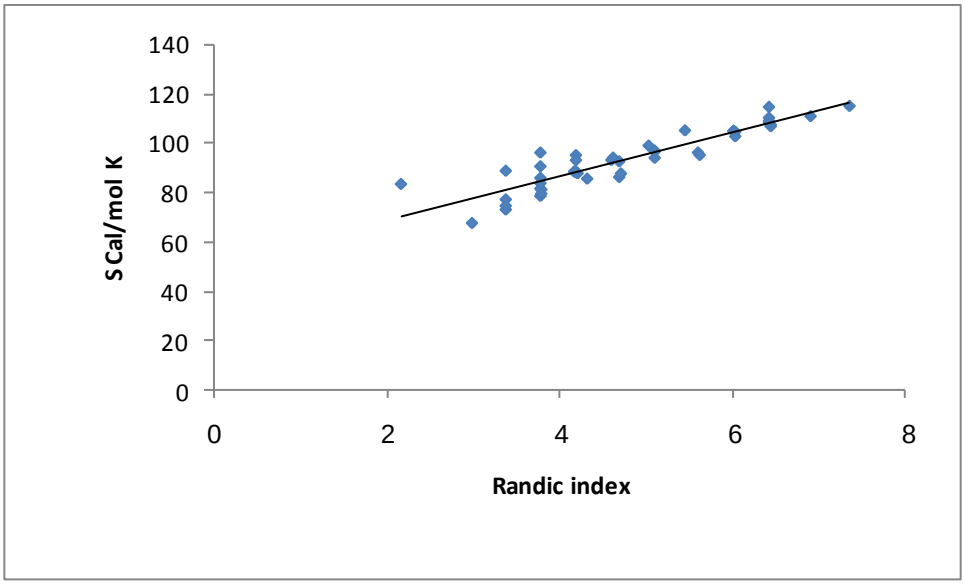

Figure 2. Plots of the Randić index (^{1}x) versus entropy of 45 benzene derivatives.

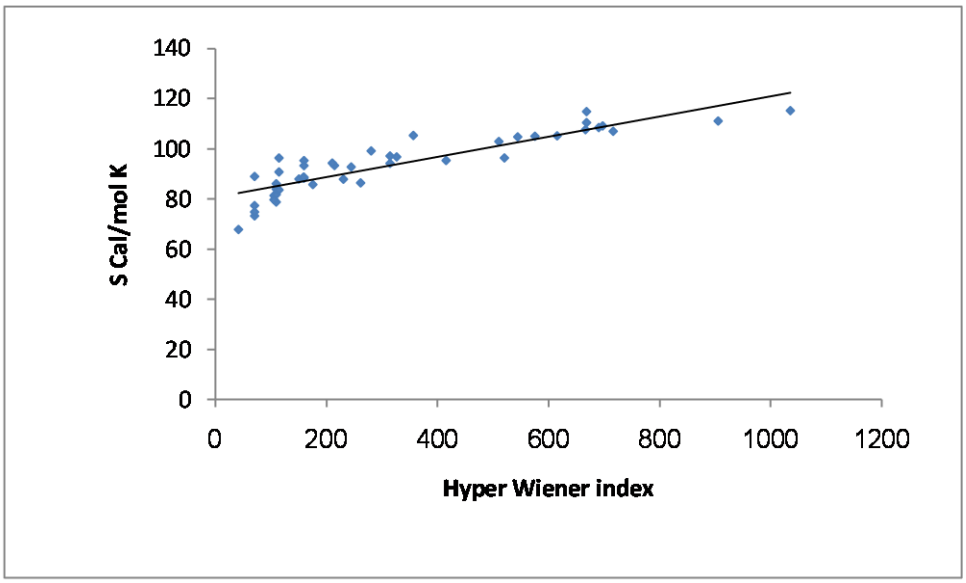

Figure 3. Plots of the Hyper–Wiener (WW) index versus entropy of 45 benzene derivatives.

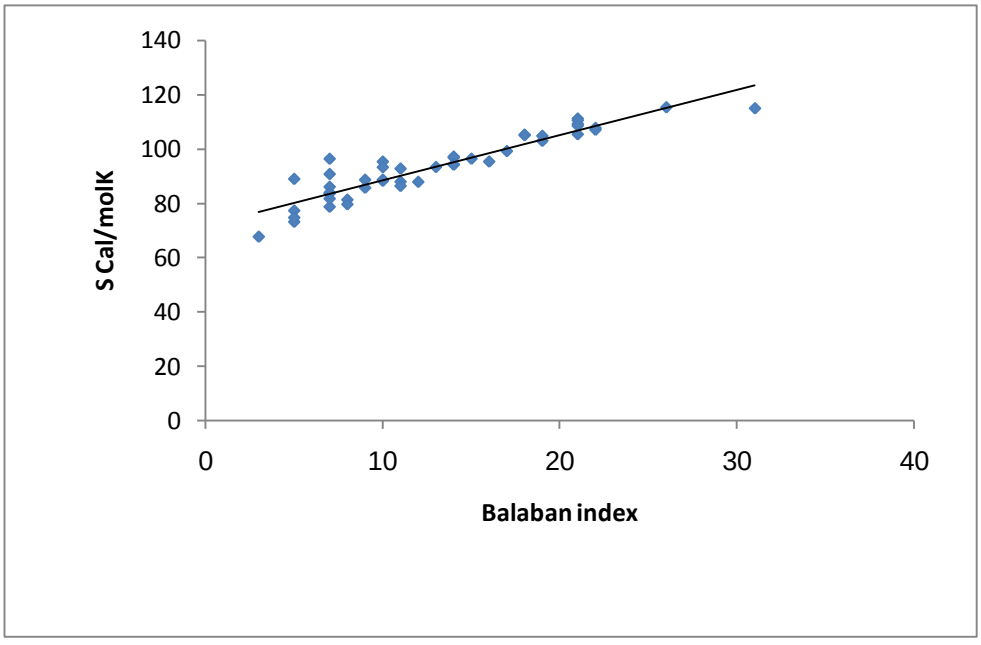

Figure 4. Plots of the Balaban index (J) versus entropy of 45 benzene derivatives.

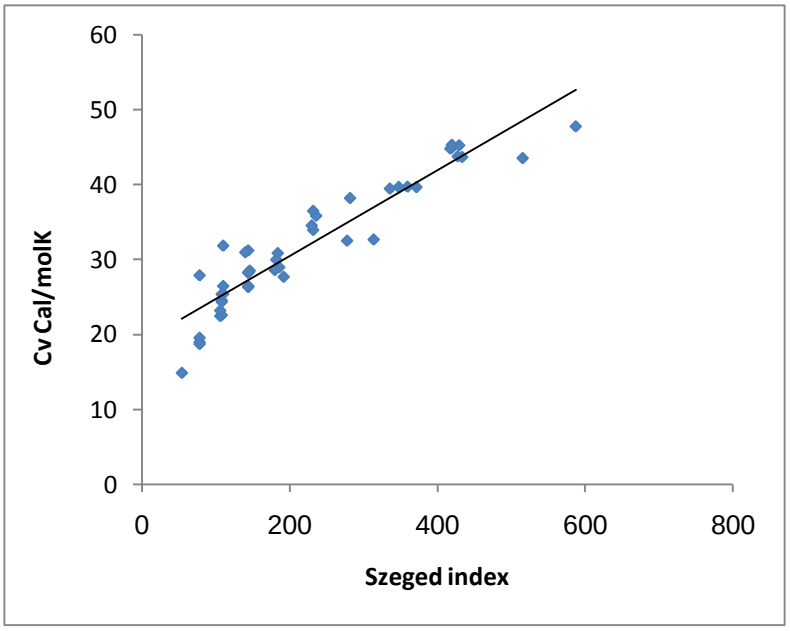

Figure 5. Plots of the Szeged index (Sz) indexversus heat capacity (Cv) of 45 benzene derivatives.

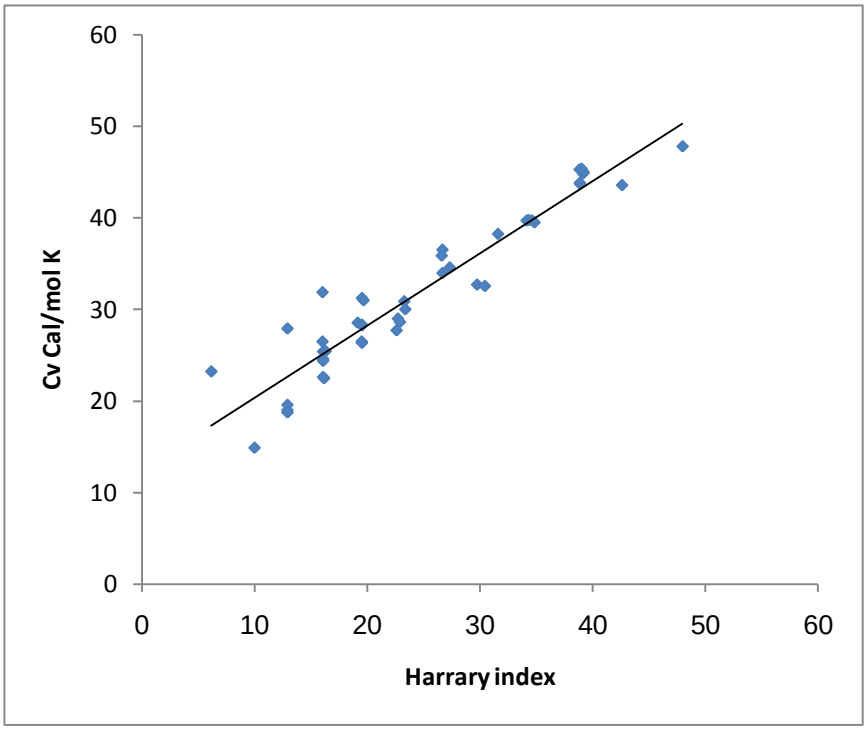

Figure 6. Plots of the Harrary index(H) versus heat capacity (Cv) of 45 benzene derivatives.

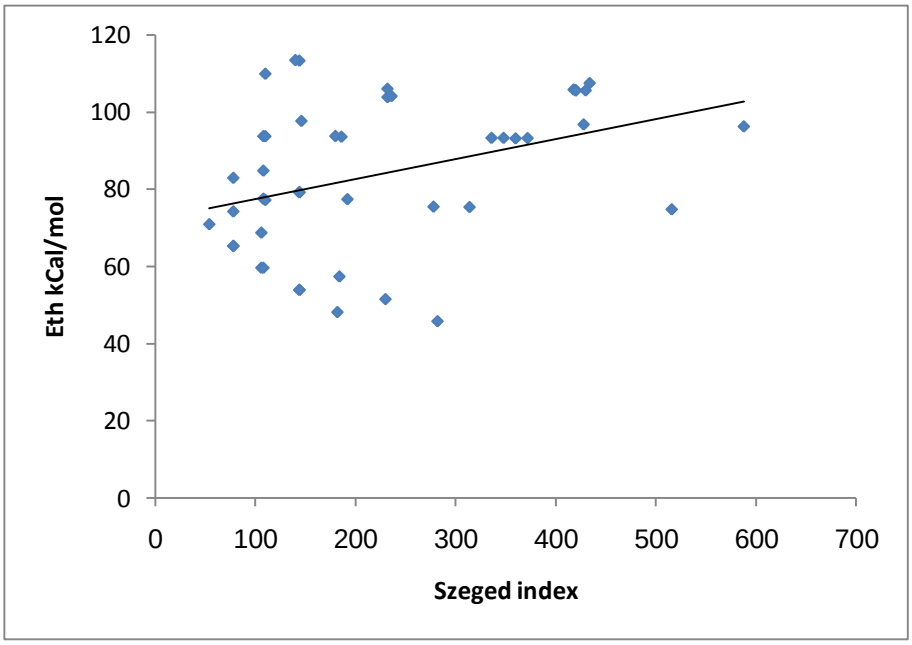

Figure 7. Plots of the Szeged index (Sz) index versus thermal energy (E_{th}) of 45 benzene derivatives .

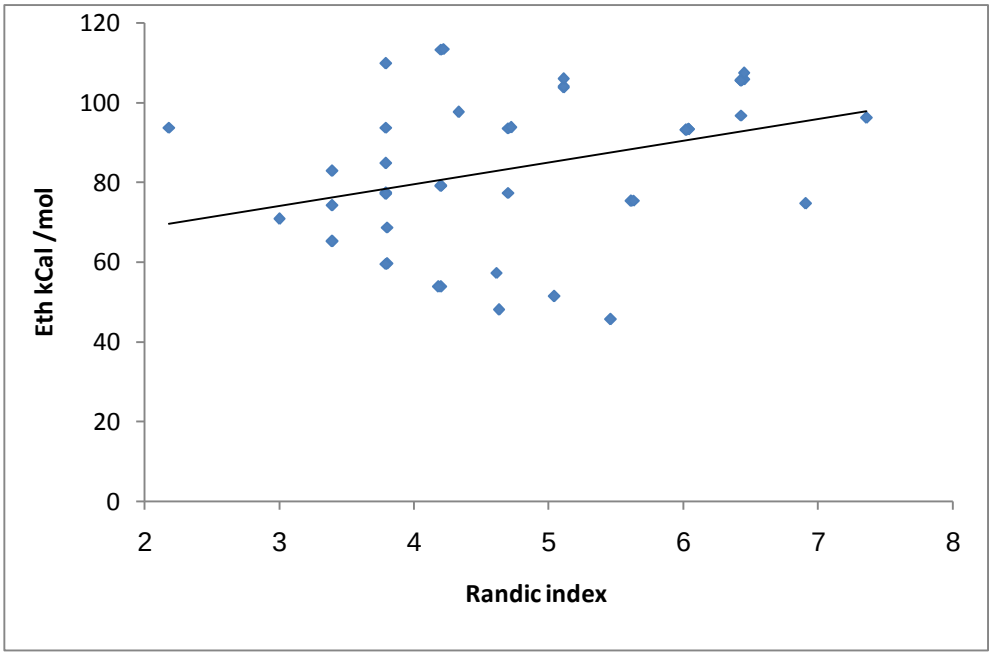

Figure 8. Plots of the Randić index (^1x) index versus thermal energy (E_{th}) of 45 benzene derivatives**.**

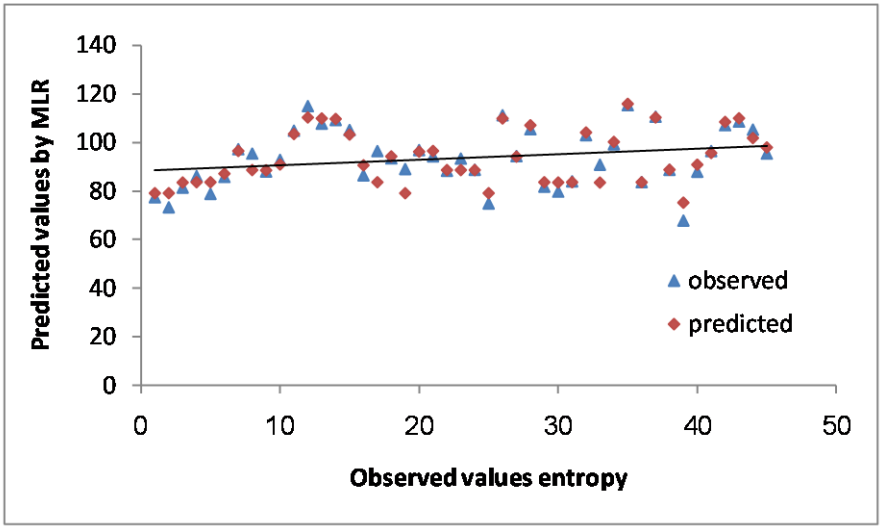

Figure 9. Comparison between the predicted and observed values of entropy by MLR.

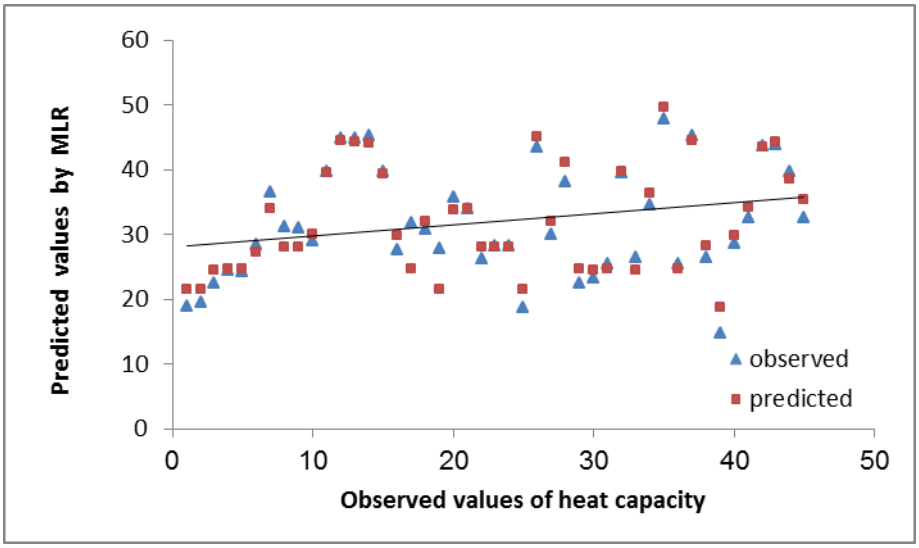

Figure 10. Comparison between the predicted and observed values of thermal energy by MLR