



## ESTIMATION OF THE STANDARD ENTHALPY OF FORMATION OF ALKANES IN GAS STATE BY CALCULATING SIZE, STRUCTURAL AND ELECTRONIC PARAMETERS OF THE MOLECULES

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A quantitative analysis is made on the correlation of thermodynamic properties, *i.e.*, standard enthalpy of formation ( $\Delta H_f^0$ ) with Kier's molecular connectivity index ( $^1X^v$ ), van der Waals volume ( $vW$ ), electrotopological state index ( $E$ ) and refractotopological state index ( $R$ ) in gas state of alkanes. The regression analysis reveals significant linear correlations of the standard enthalpy of formation ( $\Delta H_f^0$ ) with  $^1X^v$ ,  $vW$ ,  $E$  and  $R$ . The equations obtained by regression analysis may be used to estimate the standard enthalpy of formation ( $\Delta H_f^0$ ) of alkanes in gas state.

### INTRODUCTION

The standard enthalpy of formation is a basic thermodynamic property. It is used in chemical engineering calculations. Experimental measurements of the standard enthalpy of formation ( $\Delta H_f^0$ ) imply experimental difficulties and they are not always feasible. The corresponding methods have real drawbacks. Consequently, it is necessary to resort to a theoretical calculation of these parameters. This option is now accessible due to an important, fruitful and current field of research.

The additive approach applied to the estimation of thermo-physical properties was systematically developed by S.W. Benson and coworkers.<sup>1-3</sup> Many topological distances based indices as molecular descriptors for QSAR<sup>4,5</sup> and additive schemes<sup>6</sup> have been developed for the estimation of the enthalpy of formation of organic compounds.

One of the most important points in such research is the selection of adequate descriptors containing the information stored in the molecular structure. The quite satisfactory results of applying

regression analysis used to calculate heats of formation seem to indicate that this way is a suitable one to compute the enthalpy of formation of molecules. Since results are good enough and errors are nearly the same as experimental uncertainties, the equations seem to be a suitable method to systematize data and to derive certain rules regarding the structural elements and group contribution to the molecular enthalpy of formation.

There are a wide variety of molecular descriptors to be used as independent variables and this large number of possibilities allows one to make quite different choices to perform the calculation and to interpret the results in a meaningful way. In view of the above, it is thought that enthalpies of formation which depend upon the size, structure, electronic environment and complexity of the molecules, may be quantitatively correlated with size, structure and electronic parameters, *i.e.* first order valence connectivity ( $^1X^v$ ), van der Waals volume ( $vW$ ), electrotopological state index ( $E$ ) and refractotopological state index ( $R$ ) in alkanes. Previously we have established a significant

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quantitative correlation of these parameters with diamagnetic susceptibility of many organic compounds.<sup>7,8</sup> The aim of this paper is to obtain the correlation equations of  $(\Delta H_f^0)$  with  ${}^1X^v$ ,  $vW$ ,  $E$  and  $R$  parameters.

### 1. Calculation of Kier<sup>9</sup> molecular connectivity ( ${}^1X^v$ ):

The chi is calculated by a hydrogen suppressed graph of the molecule.<sup>10</sup> The first order valence connectivity ( ${}^1X^v$ ) is given by eq. 1:

$${}^1X^v = \sum (\delta i^v \cdot \delta j^v)^{-1/2} \quad (1)$$

Here, the sum is composed of the overall connections or edges in such a graph;  $\delta i^v$  and  $\delta j^v$

are numbers assigned to each atom reflecting the numbers of atoms adjacent or connected to atom ( $i$ ) and ( $j$ ) which are formally bound. The atom connectivity term ( $\delta i^v$ ) is defined as:

$$\delta i^v = \frac{Zi^v - hi}{Z - Zi^v - 1} \quad (2)$$

Where  $Zi^v$  = number of valence electron of atom ( $i$ ),  
 $Z$  = atomic number of atom ( $i$ ) and  
 $hi$  = number of hydrogen atoms attached to atom ( $i$ ).

Table (1) shows the atom connectivity ( $\delta i^v$ ) values in different groups as calculated by eq. (2).

Table 1

Atom connectivity ( $\delta i^v$ ) values in different groups

Groups	$\delta i^v$	Groups	$\delta i^v$
-CH <sub>3</sub>	01	=CH <sub>2</sub>	02
≡CH	03	-OH	05
-NH <sub>2</sub>	03	O	06
-NH-	04	C=O	06
-C≡N	05	Furan O	06
-C=NH	04	O=N O	06
N or Pyridine N	05	H <sub>2</sub> O	04
NH <sub>3</sub>	02	F	07
NH <sub>4</sub>	01	Cl	0.778
>N< <sup>+</sup>	06	Br	0.259
=N H <sub>2</sub> <sup>+</sup>	03	I	0.156

### 2. Calculation of van der Waals Volume (vW):

Another atomic parameter accounting for the size of a molecule, the van der Waals volume ( $vW$ )

may be calculated as suggested by Bond.<sup>11</sup> The atoms are assumed to be spherical and necessary corrections for the overlap in the hydrogen chain are also incorporated.<sup>12</sup>

$$vW = \sum n_i a_i + [ \sum \text{corrections for bonds} + \sum \text{corrections for no. of branching} ] \quad (3)$$

Where,  $vW$  = van der Waals volume of the molecules,

$n_i$  = no. of atoms,

$a_i$  = van der Waals volume of atom  $i$ .

Table 2 shows the van der Waals volume of different atoms and table 3 shows correction

values of van der Waals volume for sphere overlapping due to covalent bonding and for branching. The value of the van der Waals volume may be calculated with eq. 3.

Table 2

van der Waals volume of different atoms

Atom	Sphere volume $10^2 \text{ \AA}^3$	Atom	Sphere volume $10^2 \text{ \AA}^3$	Atom	Sphere volume $10^2 \text{ \AA}^3$
C	0.206	H	0.056	N	0.141
O	0.115	S	0.244	F	0.115
Aliphatic Cl	0.206	Aromatic Cl	0.244	Aliphatic Br	0.244
Aromatic Br	0.287	Aliphatic I	0.335	Aromatic I	0.388

Table 3

Correction values of van der Waals volume for sphere overlapping due to covalent bonding and for branching

Bond	Correction value $10^2 \text{ \AA}^3$	Bond	Correction value $10^2 \text{ \AA}^3$	Bond	Correction value $10^2 \text{ \AA}^3$
C-C	-0.078	C-H	-0.043	C-N	-0.065
C-O	-0.056	C-S	-0.066	C-F	-0.056
Aliph. C-Cl	--0.058	Arom C-Cl	-0.066	Aliph. C-Br	-0.060
Arom. C-Br	-0.068	Aliph. C-I	-0.063	Arom. C-I	-0.072
C-B	-0.113	H-H	-0.030	N-H	-0.038
N-N	-0.050	N-O	-0.042	N-S	-0.061
O-H	-0.034	O-B	-0.079	S-H	-0.040
S-S	-0.062	S-F	-0.052	C=C	-0.094
C=N	-0.072	C=O	-0.068	C=S	-0.081
N=N	-0.061	N=O	-0.053	S=O	-0.057
C≡C	-0.0101	C≡N	-0.079	Arom. C=C	-0.086
Branching for Saturated bond Except bonding with H	-0.050				

### 3. Calculation of electrotopological state index (E-State):

This index is developed from chemical graph theory and uses the chemical graph (hydrogen - suppressed skeleton) for generation of atom-level structure indices. This index recognizes that every atom in a molecule is unique, and this uniqueness arises from differences in the electronic and topological environment of each atom. This descriptor is formulated as an intrinsic value  $I_i$  plus a perturbation given by the electronic influence of the topological environment of the molecule.<sup>13-15</sup> Intrinsic state valence  $I_i$  of each atom is calculated as follow:

$$I_i = [(2/N)^2 \delta v + 1] / \delta \quad (4)$$

where  $N$  is the principal quantum number of the atom  $i$ ,  $\delta v$  the number of valence electrons in the skeleton ( $Z_v - h_i$ ),  $\delta$  the number of  $\sigma$  electrons in the skeleton ( $\sigma - h$ ). For a skeleton,  $Z_v$  is the total number of electrons on the atom,  $\sigma$  is the number of electrons in the  $\sigma$  orbitals,  $h$  the number of bonded hydrogen atom. The E-state for an atom  $i$  in molecule ( $S_i$ ) is given by

$$S_i = I_i + \sum \Delta I_i \quad (5)$$

$\Delta I_i$  = quantifies the perturbation effect on the intrinsic atom value. This perturbation is assumed to be a function of the difference in the intrinsic values  $I_i$  and  $I_j$ :

$$\Delta I_i = \sum (I_i - I_j) / r_{ij}^2 \quad (6)$$

where,  $r_{ij}$  is the number of atoms in the shortest path between atoms  $i$  and  $j$  including both  $i$  and  $j$ . The difference in intrinsic values  $\Delta I_i$ , for a pair of skeletal atoms encode both electronic and topological attributes that arise from electronegativity differences and skeletal

connectivity. Therefore, the total of sum of the differences in intrinsic values,  $\sum \Delta I_i$ , due to perturbation for a whole molecule is zero, i.e.,  $\sum \Delta I_i = 0$  so,

$$S_i = I_i \quad (7)$$

$$\text{Therefore, the E- state for a molecule} = \sum n_i S_i \quad \text{or} \quad \sum n_i I_i \quad (8)$$

where  $n_i$  = no. of atoms.

Table 4 shows the intrinsic state valence  $I_i$  of atoms in some groups.

$E$  values of the molecules can be calculated with eq. 8.

Table 4

Intrinsic state valence  $I_i$  of atoms in some groups

Group	$I_i$	Group	$I_i$	Group	$I_i$
> C <	1.250	>CH-	1.333	-CH <sub>2</sub> -	1.5
> C =	1.667	-S-	1.833	-CH <sub>3</sub> , =CH-, > N	2.00
-I	2.12	≡C -, -NH-	2.5	-Br	2.75
= CH <sub>2</sub> , =N-	3.00	-SH	3.222	-O-	3.500
=CH, -NH <sub>2</sub>	4.00	-Cl	4.111	≡N, -OH	6.00
=O	7.00	-F	8.000		

#### 4. Calculation of refractotopological state index (R- state):

The R state index is also developed from the chemical graph theory. This index is based on the influence of dispersive forces of each atom on the other atoms in the molecule, modified by molecular topology. Crippen *et al*<sup>16</sup> reported the atomic refractivity values of the topological environment of each skeleton atom in the molecule.

The evaluation of the individual atomic refractivity value (Calculated by Ghose and Crippen<sup>16</sup> and given in table 5) is based on the idea that the sum of the atomic values ( $\alpha_i$ ) is related to the molecular value of the molar refractivity:

$$R(\text{molecule})_{\text{calc.}} = \sum n_i \alpha_i \quad (9)$$

where,  $n_i$  = no. of atoms;

$\alpha_i$  = atomic refractivity value.

The R-values of molecules are calculated with eq. 9.

Table 5

Atomic refractivity values as calculated by Ghose and Crippen used in the analysis

Atom Type	Atomic Refractivity	Atom Type	Atomic Refractivity	Atom Type	Atomic Refractivity
C(sp <sup>3</sup> )	2.816	C(sp <sup>2</sup> )	3.828	C(sp)	3.897
C(Ar)	3.509	C=X	3.089	H	0.916
-O-	1.635	=O	1.796	O=N	2.141
N(sp <sup>3</sup> )	3.010	N(sp <sup>2</sup> ), N(sp)	3.201	N(Ar)	2.766
NO <sub>2</sub>	3.505	Ar-N=X	3.810	F	1.063
Cl	5.611	Br	8.678	I	13.874
S(sp <sup>3</sup> )	7.319	S(sp <sup>2</sup> )	9.168	R-SO-R	6.076

## RESULTS AND DISCUSSION

The values of the standard enthalpy of formation ( $\Delta H_f^0$ ) of gases are taken from literature.<sup>17-21</sup> Standard heat enthalpies ( $\Delta H_f^0$ ) are taken in kilo calories per mole at one atmospheric pressure at 298.15K in gas phase. The values of  ${}^1\chi^v$ ,  $vW$ ,  $E$  and  $R$  are calculated as discussed above and are correlated with standard enthalpies ( $\Delta H_f^0$ ) of alkanes.

$$\Delta H_f^0 = -9.829 (\pm 0.175) {}^1\chi^v - 4.871 (\pm 0.670) I - 11.288 \quad (10)$$

$$N = 44, r = 0.994, s = 1.889, F(2, 41) = 1776.123$$

$$\Delta H_f^0 = -31.724 (\pm 0.477) vW - 4.979 (\pm 0.574) I - 7.628 \quad (11)$$

$$N = 45, r = 0.996, s = 1.711, F(2,42) = 2362.53$$

In regression analysis, the statistical parameters are as:

$N$  = number of data points,

$r$  = correlation coefficient,

$s$  = standard deviation and

$F$  = the ratio between the variance of calculated and observed data.

Both equations show almost 100 % correlation, because both equations show correlation coefficients nearly equal to one ( $r = 0.994, 0.996$ ), low values of standard deviations ( $s$ ) and confidence intervals. Inclusion of indicator variable shows that branching in chains plays an important role in the correlations of the molecular connectivity ( ${}^1\chi^v$ ) & van der Waals volume ( $vW$ ) with the standard enthalpies ( $\Delta H_f^0$ ) of the alkanes. In equations (10) & (11), the  $F$  values are significant at 99% level [ $F_{42}^2(0.01) = 5.18$ ] and are accounting for 98.8% & 99.2% variance ( $r^2 = 0.988$  &  $0.992$ ) respectively.

The correlations of the standard enthalpies ( $\Delta H_f^0$ ) with the electrotopological state index ( $E$ ) and refractotopological state index ( $R$ ) are given by equations (12) & (13).

The regression analysis reveals that the correlations of the standard enthalpies ( $\Delta H_f^0$ ) with the molecular connectivity ( ${}^1\chi^v$ ) & van der Waals volume ( $vW$ ) show very low level of significance, but with the inclusion of the indicator variable ( $I$ ), i.e.,  $I = 0$  for straight chain and  $I = 1$  for branched alkanes, shows high level of significance and are shown by equations (10) & (11).

$$\Delta H_f^0 = -3.259 (\pm 0.023) E - 7.573 \quad (12)$$

$$N = 45, r = 0.999, s = 0.810, F(1, 43) = 19512.99$$

$$\Delta H_f^0 = -1.033 (\pm 0.013) R - 11.114 \quad (13)$$

$$N = 46, r = 0.997, s = 1.452, F(1,44) = 6581.835$$

These equations show again a high level of significance, because the correlation coefficients and the  $F$  value are again at 99% [ $F_{44}^1(0.01) = 7.31$ ] and are accounting for 99.8% & 99.4% variance ( $r^2 = 0.998$  &  $0.994$ ). Standard deviations have low value. Therefore, these equations show perfect correlations.

The experimental values of the standard enthalpies of formation ( $\Delta H_f^0$ ) of some alkanes and the theoretical calculated values with equations (10),(11), (12) and (13) show good agreement and are listed in tables 6. & 7.

Table 6

Experimental and theoretical calculated values of  $\Delta H_f^0$  by 1Xv

&vW parameters in alkanes						
Name of compound	${}^1X^v$	$vW$	I	$\Delta H_f^0$		
				Exp.value	Cald.Eq.10	Cald.Eq.11
Methane	0.000	0.258	0	-17.890	*	-15.813
Ethane	1.000	0.412	0	-20.240	-21.117	-20.699
Propane	1.414	0.566	0	-24.820	-25.186	-25.584
n-Butane	1.914	0.720	0	-30.150	-30.100	-30.470
2-Methyl propane	1.731	0.670	1	-32.150	-33.173	-33.862

Table 6 (continued)

n-Pentane	2.414	0.874	0	-35.000	-35.015	-35.355
2-Methyl butane	2.269	0.824	1	-36.920	-38.461	-38.748
2,2-Dimethyl propane	2.000	0.774	1	-39.170	-35.817	-37.162
n-Hexane	2.914	1.028	0	-39.960	-39.930	-40.241
2-Methyl pentane	2.769	0.978	1	-41.660	-43.375	-43.633
3-Methyl pentane	2.807	0.978	1	-41.020	-43.749	-43.633
2,2-Dimethyl butane	2.560	0.928	1	-44.350	-41.321	-42.047
2,3-Dimethyl butane	2.641	0.928	1	-42.490	-42.107	-42.047
Heptane	3.414	1.182	0	-44.880	-44.844	-45.126
2-Methyl hexane	3.269	1.132	1	-46.590	-48.290	-48.519
3-Methyl hexane	3.307	1.132	1	-45.960	-48.663	-48.519
2,2-Dimethyl pentane	3.061	1.082	1	-49.270	-46.235	-46.933
2,3-Dimethyl pentane	3.179	1.082	1	-47.620	-47.405	-46.933
2,4-Dimethyl pentane	3.124	1.082	1	-48.280	-46.865	-46.933
2,2,3-Trimethyl butane	2.942	1.032	1	-48.950	-45.076	-45.346
Octane	3.914	1.336	0	-49.820	-49.759	-50.011
2-Methyl heptane	3.769	1.286	1	-51.500	-53.204	-53.404
3-Methyl heptane	3.807	1.286	1	-50.820	-53.578	-53.404
4-Methyl heptane	3.807	1.286	1	-50.690	-53.578	-53.404
2,2-Dimethyl hexane	3.560	1.236	1	-53.710	-51.150	-51.818
2,3-Dimethyl hexane	3.679	1.236	1	-51.130	-52.320	-51.818
2,4-Dimethylhexane	3.662	1.236	1	-52.440	-52.153	-51.818
2,5-Dimethylhexane	3.624	1.236	1	-53.210	-51.779	-51.818
3,3-Dimethylhexane	3.620	1.236	1	-52.610	-51.740	-51.818
3,4-Dimethylhexane	3.717	1.236	1	-50.910	-52.693	-51.818
Nonane	4.414	1.490	0	-54.740	-54.673	-54.897
2,2,3-Trimethylpentane	3.480	1.186	1	-52.610	-50.364	-50.232
2,2,4-Trimethylpentane	3.415	1.186	1	-53.570	-49.725	-50.232
2,3,3-Trimethylpentane	3.502	1.186	1	-51.730	-50.580	-50.232
2,3,4-Trimethylpentane	3.551	1.186	1	-51.970	-51.062	-50.232
3-Ethyl pentane	3.345	1.132	1	-45.330	-49.037	-48.519
3-Methyl-3-ethyl pentane	3.680	1.236	1	-51.380	-52.329	-51.818
2-Methyl-3-ethyl pentane	3.717	1.236	1	-50.480	-52.693	-51.818
Undecane	5.414	1.798	0	-64.600	-64.502	-64.668
Hexadecane	7.914	2.568	0	-89.230	-89.075	-89.095
Nonadecane	9.414	3.030	0	-104.000	-103.818	-103.752
Octadecane	8.914	2.876	0	-99.080	-98.904	-98.866
Pentadecane	7.414	2.414	0	-84.310	-84.16	-84.210
Tetradecane	6.914	2.260	0	-79.380	-79.246	-79.324
Tridecane	6.414	2.106	0	-74.450	-74.331	-74.439
I = 0 for Straight Chain	I = 1 for Branched Chain					

Table 7  
Experimental and theoretical calculated values of  $\Delta H_f^0$  by E

Name of compound	E	R	$\Delta H_f^0$		
			Exp.value	Cald.Eq.12	Cald.Eq.13
Methane	*	6.478	-17.890	*	-17.806
Ethane	4.000	11.125	-20.240	-20.611	-22.606
Propane	5.500	15.771	-24.820	-25.500	-27.405
n-Butane	7.000	20.418	-30.150	-30.389	-32.205
2-Methyl propane	7.333	20.418	-32.150	-31.475	-32.205
n-Pentane	8.500	25.065	-35.000	-35.279	-37.006
2-Methyl butane	8.833	25.065	-36.920	-36.364	-37.006
2,2-Dimethyl propane	9.250	25.065	-39.170	-37.723	-37.006
n-Hexane	10.000	29.712	-39.960	40.168	-41.806
2-Methyl pentane	10.333	29.712	-41.660	-41.253	-41.806
3-Methyl pentane	10.333	29.712	-41.020	-41.253	-41.806
2,2-Dimethyl butane	10.750	29.712	-44.350	-42.612	-41.806
2,3-Dimethyl butane	10.666	29.712	-42.490	-42.338	-41.806
Heptane	11.500	34.359	-44.880	-45.057	-46.606
2-Methyl hexane	11.833	34.359	-46.590	-46.142	-46.606
3-Methyl hexane	11.833	34.359	-45.960	-46.142	-46.606
2,2-Dimethyl pentane	12.250	34.359	-49.270	-47.501	-46.606
2,3-Dimethyl pentane	12.166	34.359	-47.620	-47.228	-46.606
2,4-Dimethyl pentane	12.166	34.359	-48.280	-47.228	-46.606
2,2,3-Trimethyl butane	12.583	34.359	-48.950	-48.587	-46.606
Octane	13.000	39.005	-49.820	-49.946	-51.405
2-Methyl heptane	13.333	39.005	-51.500	-51.031	-51.405
3-Methyl heptane	13.333	39.005	-50.820	-51.031	-51.405
4-Methyl heptane	13.333	39.005	-50.690	-51.031	-51.405
2,2-Dimethyl hexane	13.750	39.005	-53.710	-52.391	-51.405
2,3-Dimethyl hexane	13.666	39.005	-51.130	-52.117	-51.405
2,4-Dimethylhexane	13.666	39.005	-52.440	-52.117	-51.405
2,5-Dimethylhexane	13.666	39.005	-53.210	-52.117	-51.405
3,3-Dimethylhexane	13.750	39.005	-52.610	-52.391	-51.405
3,4-Dimethylhexane	13.666	39.005	-50.910	-52.117	-51.405
Nonane	14.500	43.652	-54.740	-54.835	-56.206
2,2,3-Trimethylpentane	14.083	39.005	-52.610	-53.476	-51.405
2,2,4-Trimethylpentane	14.083	39.005	-53.570	-53.476	-51.405
2,3,3-Trimethylpentane	14.083	39.005	-51.730	-53.476	-51.405
2,3,4-Trimethylpentane	13.999	39.005	-51.970	-53.202	-51.405
3-Ethyl pentane	11.833	34.359	-45.330	-46.142	-46.606
3-Methyl-3-ethyl pentane	13.750	39.005	-51.380	-52.391	-51.405
2-Methyl-3-ethyl pentane	13.666	39.005	-50.480	-52.117	-51.405
2,2,3,3-Tetramethylbutane	14.500	39.005	-53.990	-54.835	-51.405
Undecane	17.500	52.946	-64.600	-64.613	-65.806

Table 7 (continued)

Hexadecane	25.000	76.180	-89.230	-89.059	-89.806
Nonadecane	29.500	90.120	-104.000	-103.727	-104.206
Octadecane	28.000	85.473	-99.080	-98.838	-99.406
Pentadecane	23.500	71.533	-84.310	-84.170	-85.006
Tetradecane	22.000	66.886	-79.380	-79.281	-80.206
Tridecane	20.500	62.239	-74.450	-74.392	-75.406

## CONCLUSION

Therefore, the standard enthalpies of formation ( $\Delta H_f^0$ ) of alkanes can be estimated with equations (10), (11), (12) and (13) simply by calculating the molecular connectivity ( ${}^1\chi^v$ ), van der Waals volume ( $vW$ ), electrotopological state index ( $E$ ) and refractotopological state index ( $R$ ) parameters.

## REFERENCES

1. S.W. Benson and J.H. Buss, *J. Chem. Phys.*, **1958**, *29*, 546-72.
2. S.W. Benson, F.R. Cruickshank, D.M. Golden, G.R. Haugen, H.E. O'Neal, A.S. Rodgers, R.J. Shaw and R. Walsh, *Chem. Rev.*, **1969**, *69*, 279-321.
3. M. Luria and S.W. Benson, *J. Chem. Eng. Data*, **1977**, *22*, 90-100.
4. A. Mercader, E.A. Castro and A.A. Toropov, *Int. J. Mol. Sci.* **2001**, *2*, 121-132.
5. P. Duchowicz and E.A. Castro, *Journal of the Korean Chemical Society*, **2000**, *44*, 501.
6. N. Cohen, *J. Phys. Chem. Ref. Data*, **1996**, *25*, 1411.
7. B.L. Gorski, G.S. Kalwania and M. Sharma, *Indian J. Chem., Sec. A*, **1993**, *32A*, 889-890.
8. B.L. Gorski, G.S. Kalwania and M. Sharma, *J. Indian Chem. Soc.*, **1998**, *75*, 373-374.
9. L.B. Kier and L.H. Hall, "Molecular Connectivity in Chemistry and Drug Research", Academic Press, New York, 1976.
10. M. Randic, *J. Am. Chem. Soc.*, **1975**, *97*, 6609-6615.
11. A. Bondi, *J. Phys. Chem.*, **1964**, *68*, 441.
12. A. Moriguchi, *Chem. Pharm. Bull. (Jpn.)*, **1975**, *23*, 247.
13. L.H. Hall, B. Mohnney and L.B. Kier, *J. Chem. Inf. Compt. Sci.*, **1991**, *1*, 31.
14. L.H. Hall, B. Mohnney and L.B. Kier, *Quant. Struct- Net., Relat*, **1991**, *10*, 43-51.
15. L.B. Kier and L.H., Hall, *Pharmae Res.*, **1990**, *7*, 801-807.
16. A.K. Ghose and G.M. Crippen, *J. Chem. Inf. Comput. Sci.* **1987**, *27.1*, 21-35.
17. F.D. Rossini, K.S. Pitzer, R.L. Arnett, R.M. Braum and G.C. Pimentel, "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds", Carnegie Press Pittsburgh, Pa., 1953.
18. J.G. Aston, *Chem. Rev.*, **1940**, *27*, 59-73.
19. K.S. Pitzer, *Chem. Rev.*, **1940**, *27*, 39-57.
20. M. Sounders, Jr., C.S. Mathewa and C.O. Hurd, *Ind. Eng. Chem.*, **1949**, *41*, 1048-1056.
21. F.D. Rossini, *Chem. Rev.*, **1940**, *27*, 1-16.