

# Topological Indices Based on Vertex, Edge, Ring, and Distance: Application to Various Physicochemical Properties of Diverse Hydrocarbons

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This paper developed the Edge degree-Distance Index (EDI) and Sum of edges ( $S_e$ ) based on the edge and distance of molecular graph. This set of topological indices, EDI,  $S_e$  combined with VDI, OEI, and RDI proposed in our previous paper can characterize the molecular structures of diverse hydrocarbons well. The regression analyses against nine physicochemical properties, such as boiling points (Bp), critical properties (Tc, Pc, Vc), heat capacities (Cp), and so on, of 1038 diverse hydrocarbons were investigated, and good correlations were obtained.

## 1. INTRODUCTION

Over the years people have been endeavoring to improve the prediction of physical and biological properties of organic compounds. There were two major threads of research. On one hand, some studied on the various properties such as normal boiling points,<sup>1–3</sup> critical properties,<sup>4–6</sup> thermodynamic properties,<sup>5–9</sup> and so on<sup>10–13</sup> for a specific kind of compounds. On the other hand, a lot of papers focused on a certain property for a diverse set of compounds, for example, Stanton<sup>14</sup> studied the normal boiling points of small multifunctional organic molecules; Cao investigated the water solubility,<sup>15</sup> boiling points,<sup>16</sup> respectively, for alkanes and alcohols; another paper<sup>17</sup> reported the prediction of ionization potential for haloalkanes, amines, alcohols, and ethers. But there were only a few papers that studied the various properties for a structurally diverse swatch. The difficulty, in general, is that most of the developed descriptors or descriptor sets render the molecular structural features only in term of some aspect, which is deficient to illuminate the exact relationship between structure and various properties. However, it is expected and pursued by computer chemists that the prospective molecular descriptors will be of rich structural information and good structural interpretation, furthermore, they will have good correlations with multifarious properties of compounds which encompass as much structural diversity as possible.

Our previous paper<sup>18</sup> introduced a set of topological indices, named as Odd–Even Index (OEI), Vertex degree-Distance Index (VDI), and Ring degree-Distance Index (RDI) based on the vertex, ring, and distance of molecular graph. It was found that these topological indices can characterize the molecular structures of paraffins and cycloalkanes (including polycyclic and spirocycloalkanes) and correlate with their boiling points satisfactorily. But they are deficient in telling the single bond from the double or triple bond of the unsaturated and benzenoid hydrocarbons. In response to this challenge, this paper developed another topological index, the Edge degree-Distance Index (EDI) to distinguish

saturated and unsaturated structures. Furthermore, the sum of edges ( $S_e$ ) in molecular graph is also calculated. These two new indices, EDI and  $S_e$ , combined with OEI, VDI, and RDI are expected to characterize the molecular structures of hydrocarbons. As mentioned in the above benchmark, the newly developed descriptors should have good correlations with multifarious properties of compounds. The paper regressed this set of topological indices against nine physicochemical properties such as boiling points, critical properties, and vapor pressures for 1038 hydrocarbons with 1–20 carbon atoms (consisting of 424 alkanes, 399 alkenes and alkynes, 215 benzenoid hydrocarbons). The results show good correlations with all these properties, which confirm the availability of this set of topological indices.

## 2. CALCULATION OF DESCRIPTORS

Vertex, distance, and ring (in cyclic hydrocarbons) are the fundamental structural elements of molecular graph, based on which three topological indices, Odd–Even Index (OEI), Vertex degree-Distance Index (VDI), and Ring degree-Distance Index (RDI), have been defined in the previous paper.<sup>18</sup> They are restated briefly as follows:

### 1. Odd–Even Index (OEI)

$$OEI = \sum_{i=1}^N \sum_{j \neq i}^N [(-1)^{D_{ij}-1} S] \quad (1)$$

where  $N$  is the number of vertices in molecular graph and  $S$  is the derivative matrix from distance matrix  $D$ . The elements of  $S$  are the squares of the reciprocal distances  $(D_{ij})^{-2}$ , i.e.,  $S_{ij} = 1/D_{ij}^2$  (when  $i = j$ , let  $1/D_{ij}^2 = 0$ ).

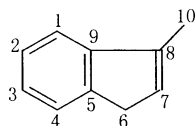
### 2. Vertex degree-Distance Index (VDI)

$$VDI = \left( \prod_{i=1}^N f_i \right)^{1/N} \quad (2)$$

where  $f_i$  is the element of vector  $VS$  obtained by  $V$ -multiply- $S$  (here  $V$  is the vertex degree matrix<sup>18</sup>):

$$VS = [f_1, f_2, \dots, f_N] \quad (3)$$

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**Figure 1.** The hydrogen-suppressed molecular graph of 3-methyl-1H-indene.

### 3. Ring degree-Distance Index (RDI)

$$\text{RDI} = \left( \prod_{i=1}^N g_i \right)^{1/N} \quad (4)$$

where  $g_i$  is the element of vector  $RS$  obtained by  $R$ -multiply- $S$  (here  $R$  is the ring degree matrix<sup>18</sup>):

$$RS = [g_1, g_2, \dots, g_N] \quad (5)$$

In alkanes, each pair of adjacent vertices is linked by a single bond. While in unsaturated hydrocarbons, there are double and/or triple bonds that are responsible for the differences of properties between the saturated and unsaturated hydrocarbons with the same molecular skeleton. However, vertex degree matrix ( $V$ ) or distance matrix ( $D$ ) is unable to tell the unsaturated molecular graph from the saturated one (in the case of the same skeleton), which results in the same values of VDI and OEI, respectively. To resolve this problem, we represent the molecular graph of hydrocarbons as follows: vertex stands for carbon atom, one edge typifies the single bond (C–C), while double and triple bonds are shown with two and three edges, respectively. Thus the molecular graphs of saturated and unsaturated hydrocarbons, such as normal butane, 2-butene, and 1,3-butadiene, are distinguishable.

This paper defines the number of edges linked to vertex  $i$  as edge degree,  $E_i$ . Vector  $E$  ( $1 \times N$ ) is employed to represent the edge degrees of molecular graph. According to the algorithm of Vertex degree-Distance Index (VDI), a new topological index, Edge degree-Distance Index (EDI) was developed based on the edge degree vector  $E$  and the derivative distance matrix  $S$ :

### 4. Edge degree-Distance Index (EDI)

$$\text{EDI} = \left( \prod_{i=1}^N h_i \right)^{1/N} \quad (6)$$

where  $h_i$  is the elements of vector  $ES$  obtained by  $E$ -multiply- $S$ :

$$ES = [h_1, h_2, \dots, h_N] \quad (7)$$

### 5. The sum of edges ( $S_e$ )

$S_e$  equals to the half sum of the edge degrees ( $E_i$ ) of each vertex in molecular graph:

$$S_e = \frac{1}{2} \sum_{i=1}^N E_i \quad (8)$$

We take 3-methyl-1H-indene for example to compute the indices OEI, VDI, RDI, EDI, and  $S_e$ . Figure 1 is the hydrogen-suppressed molecular graph of 3-methyl-1H-indene (where the digits are the random numberings of each vertex).

The calculation steps are as follows:

(a) The distance matrix  $D$  and its derivative matrix  $S$

$$D = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 3 & 3 & 2 & 1 & 3 \\ 1 & 0 & 1 & 2 & 3 & 4 & 4 & 3 & 2 & 4 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 4 & 3 & 5 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 3 & 2 & 4 \\ 2 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 1 & 3 \\ 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 3 \\ 3 & 4 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 2 \\ 2 & 3 & 4 & 3 & 2 & 2 & 1 & 0 & 1 & 1 \\ 1 & 2 & 3 & 2 & 1 & 2 & 2 & 1 & 0 & 2 \\ 3 & 4 & 5 & 4 & 3 & 3 & 2 & 1 & 2 & 0 \end{bmatrix}$$

$S =$

$$\begin{bmatrix} 0 & 1 & 1/4 & 1/9 & 1/4 & 1/9 & 1/9 & 1/4 & 1 & 1/9 \\ 1 & 0 & 1 & 1/4 & 1/9 & 1/16 & 1/16 & 1/9 & 1/4 & 1/16 \\ 1/4 & 1 & 0 & 1 & 1/4 & 1/9 & 1/16 & 1/16 & 1/9 & 1/25 \\ 1/9 & 1/4 & 1 & 0 & 1 & 1/4 & 1/9 & 1/9 & 1/4 & 1/16 \\ 1/4 & 1/9 & 1/4 & 1 & 0 & 1 & 1/4 & 1/4 & 1 & 1/9 \\ 1/9 & 1/16 & 1/9 & 1/4 & 1 & 0 & 1 & 1/4 & 1/4 & 1/9 \\ 1/9 & 1/16 & 1/16 & 1/9 & 1/4 & 1 & 0 & 1 & 1/4 & 1/4 \\ 1/4 & 1/9 & 1/16 & 1/9 & 1/4 & 1/4 & 1 & 0 & 1 & 1 \\ 1 & 1/4 & 1/9 & 1/4 & 1 & 1/4 & 1/4 & 1 & 0 & 1/4 \\ 1/9 & 1/16 & 1/25 & 1/16 & 1/9 & 1/9 & 1/4 & 1 & 1/4 & 0 \end{bmatrix}$$

(b) The vectors of  $V$ ,  $R$ , and  $E$

$$V = [2 \ 2 \ 2 \ 2 \ 3 \ 2 \ 2 \ 3 \ 3 \ 1]$$

$$R = [1 \ 1 \ 1 \ 1 \ 2 \ 1 \ 1 \ 1 \ 2 \ 0]$$

$$E = [3 \ 3 \ 3 \ 3 \ 4 \ 2 \ 3 \ 4 \ 4 \ 1]$$

(c) The  $V$ -multiply- $S$  vector  $VS$

$$VS = [7.7778 \ 6.2292 \ 6.1581 \ 7.5903 \ 9.5833 \ 7.6806 \\ 7.4444 \ 8.3194 \ 10.4722 \ 5.3578]$$

(d) The  $R$ -multiply- $S$  vector  $RS$

$$RS = [4.3333 \ 3.2083 \ 3.2083 \ 4.3333 \ 5.1111 \ 4.2847 \\ 3.3472 \ 4.2847 \ 5.1111 \ 2.3594]$$

(e) The  $E$ -multiply- $S$  vector  $ES$

$$ES = [10.7500 \ 9.0139 \ 8.8942 \ 10.4236 \ 12.6944 \ 10.7153 \\ 9.2917 \ 11.1042 \ 14.3333 \ 7.2450]$$

(f) The values of OEI, VDI, RDI, EDI, and  $S_e$

$$\text{OEI} = 1 \times 22 + (-1/4) \times 30 + (1/9) \times 24 + \\ (-1/16) \times 12 + (1/25) \times 2 = 16.4967$$

$$\text{VDI} = (7.7778 \times 6.2292 \times 6.1581 \times 7.5903 \times \\ 9.5833 \times 7.6806 \times 7.4444 \times 8.3194 \times 10.4722 \times \\ 5.3578)^{1/10} = 7.5212$$

$$\text{RDI} = (4.3333 \times 3.2083 \times 3.2083 \times 4.3333 \times \\ 5.1111 \times 4.2847 \times 3.3472 \times 4.2847 \times 5.1111 \times \\ 2.3594)^{1/10} = 3.8588$$

$$\text{EDI} = (10.7500 \times 9.0139 \times 8.8942 \times 10.4236 \times \\ 12.6944 \times 10.7153 \times 9.2917 \times 11.1042 \times 14.3333 \times \\ 7.2450)^{1/10} = 10.2731$$

$$S_e = 1/2 \times (3 + 3 + 3 + 3 + 4 + 2 + 3 + 4 + 4 + 1) =$$

**Table 1.** Indices  $N$ , VDI, OEI, EDI, RDI, and  $S_e$  of Some Hydrocarbons

no. <sup>a</sup>	$N$	VDI	OEI	EDI	RDI	$S_e$	no. <sup>a</sup>	$N$	VDI	OEI	EDI	RDI	$S_e$
1	1	0.0000	0.0000	0.0000	0	0	435	5	3.8514	6.4444	4.6363	0	5
2	2	1.0000	2.0000	1.0000	0	1	436	5	3.8514	6.4444	5.0190	0	5
3	3	2.1634	3.5000	2.1634	0	2	437	6	3.7591	8.4967	4.3763	0	6
4	4	2.9131	5.2222	2.9131	0	3	438	6	3.7591	8.4967	4.5606	0	6
5	4	3.3677	4.5000	3.3677	0	3	439	6	3.7591	8.4967	4.5606	0	6
6	5	3.4010	6.8194	3.4010	0	4	440	6	3.7591	8.4967	4.5766	0	6
7	5	3.8514	6.4444	3.8514	0	4	441	6	3.7591	8.4967	4.5766	0	6
8	5	4.5895	5.0000	4.5895	0	4	442	6	4.1451	7.9167	4.9200	0	6
9	6	3.7591	8.4967	3.7591	0	5	443	6	4.1925	8.2639	4.8510	0	6
10	6	4.1451	7.9167	4.1451	0	5	444	6	4.1451	7.9167	4.7935	0	6
11	6	4.1925	8.2639	4.1925	0	5	824	6	5.2222	9.6667	7.8333	2.6111	9
12	6	4.8758	7.1667	4.8758	0	5	825	7	5.7200	10.9861	8.1986	2.4730	10
13	6	4.6112	7.8889	4.6112	0	5	826	8	6.1701	12.5278	8.5530	2.3742	11
14	7	4.0367	10.1183	4.0367	0	6	827	8	6.1234	12.1806	8.5016	2.3742	11
15	7	4.3801	9.6739	4.3801	0	6	828	8	6.1117	12.3856	8.4866	2.3742	11
16	7	4.4146	9.8161	4.4146	0	6	829	8	5.7813	12.7606	7.9296	2.0874	11
17	7	5.0050	8.5139	5.0050	0	6	830	8	5.7813	12.7606	8.5347	2.0874	12
18	7	4.8234	9.5833	4.8234	0	6	831	8	5.7813	12.7606	7.9296	2.0874	13
19	7	4.7465	8.8889	4.7465	0	6	832	9	6.5491	13.9444	8.8566	2.3001	12
20	7	5.0972	9.2083	5.0972	0	6	833	9	6.4935	13.8022	8.7961	2.3001	12
425	2	1.0000	2.0000	2.0000	0	2	834	9	6.4600	13.2500	8.7626	2.3001	12
426	3	2.1634	3.5000	3.2436	0	3	835	9	6.1929	14.1772	8.2959	2.0514	12
427	4	2.9131	5.2222	3.7851	0	4	836	9	6.1449	14.0350	8.2393	2.0514	12
428	4	2.9131	5.2222	4.0509	0	4	837	9	6.1284	14.1044	8.2182	2.0514	12
429	4	2.9131	5.2222	4.0509	0	4	838	9	5.8046	14.3372	7.6686	1.7084	12
430	4	3.3677	4.5000	4.4892	0	4	839	9	6.1888	14.0350	8.1562	1.8296	12
431	5	3.4010	6.8194	4.1145	0	5	840	9	6.1929	14.1772	8.8473	2.0514	13
432	5	3.4010	6.8194	4.3540	0	5	841	9	6.1449	14.0350	8.7906	2.0514	13
433	5	3.4010	6.8194	4.3540	0	5	842	9	6.1284	14.1044	8.7679	2.0514	13
434	5	3.8514	6.4444	4.7818	0	5	843	9	6.1888	14.0350	8.8356	1.8296	13

<sup>a</sup> The molecular structures shown in Figure 3.**Table 2.** Regression Expressions of Nine Physicochemical Properties

no.	equations	$r$	$s$	$F$	$n$
1	$\ln(721\text{-Bp}) = 6.8619 - 0.1048N^{2/3} + 0.0284VDI - 0.0085OEI - 0.0143EDI - 0.0122RDI$	0.9926	8.26 °C	1379.21	1038
2	$\ln(1160\text{-Tc}) = 6.8274 + 0.0350N - 0.0416VDI - 0.0310OEI + 0.0173RDI - 0.0223S_e$	0.9881	16.13 °C	1095.94	139
3	$\ln(\text{Pc}-0.4405) = 2.3041 - 0.7123N^{2/3} + 0.0338VDI + 0.0625OEI + 0.0920EDI$	0.9855	0.188 MPa	1045.33	129
4	$Vc = -1.4162 + 104.92N - 44.2576VDI - 37.1381S_e + 24.6269EDI$	0.9975	14.84 cm <sup>3</sup> ·mol <sup>-1</sup>	4259.39	90
5	$\ln(5.8653 - D) = 1.6847 - 0.0121N^{2/3} + 0.0080VDI + 0.0006OEI - 0.0081EDI - 0.0076RDI$	0.9799	0.0185 g·cm <sup>-3</sup>	2347.04	493
6	$n_D = 1.2703 + 0.0254N^{2/3} - 0.0304VDI + 0.0345EDI + 0.0125RDI$	0.9675	0.0136	2735.84	752
7	$\log P_v = 8.0183 - 0.6040N^{2/3} + 0.2013VDI - 0.2377OEI - 0.1992EDI + 0.0763S_e$	0.9956	0.118	3867.66	179
8	$Cp = 14.1128 + 49.7541N - 19.4661VDI + 11.4664EDI - 3.5173RDI - 17.7836S_e$	0.9983	4.38 J·mol <sup>-1</sup> ·K <sup>-1</sup>	4465.54	84
9	$H_v = 0.0663 + 3.5612N - 4.1046VDI + 2.3656OEI + 4.2610EDI - 2.3779S_e$	0.9955	1.34 kJ·mol <sup>-1</sup>	3339.93	159

**Table 3.** Experimental and Estimated Boiling Points ( $Bp_{exp}$ ,  $Bp_{calc}$ ) of Some Hydrocarbons

no.	$Bp_{exp}^a$	$Bp_{calc}^b$	no.	$Bp_{exp}^a$	$Bp_{calc}^b$	no.	$Bp_{exp}^a$	$Bp_{calc}^b$	no.	$Bp_{exp}^a$	$Bp_{calc}^b$	no.	$Bp_{exp}^a$	$Bp_{calc}^b$
1	-161.5	-139.1	13	57.9	46.7	429	0.8	1.8	441	67.1	65.8	832	176.1	164.8
2	-88.6	-85.4	14	98.5	88.7	430	-6.9	-7.4	442	62.1	58.6	833	169.3	164.5
3	-42.1	-47.6	15	90.0	83.3	431	29.9	32.1	443	54.2	59.0	834	164.7	162.2
4	-0.5	-10.0	16	92.0	83.7	432	36.9	34.4	444	53.9	57.4	835	165.2	165.3
5	-11.7	-19.2	17	79.2	71.3	433	36.3	34.4	824	80.0	95.8	836	161.3	165.0
6	36.0	25.0	18	89.7	78.8	434	31.2	27.7	825	110.6	119.2	837	162.0	165.4
7	27.8	18.3	19	80.4	75.7	435	20.1	26.2	826	144.5	142.7	838	159.2	164.9
8	9.4	2.3	20	86.0	74.3	436	38.5	30.0	827	139.1	141.3	839	152.4	162.1
9	68.7	58.1	425	-103.7	-73.9	437	63.4	64.0	828	138.3	142.4	840	169.8	169.7
10	60.2	51.2	426	-47.6	-35.8	438	68.8	65.7	829	136.1	143.0	841	164.0	169.4
11	63.2	52.8	427	-6.2	-0.9	439	67.9	65.7	830	145.0	148.0	842	172.8	169.8
12	49.7	40.0	428	3.7	1.8	440	66.4	65.8	831	143.0	143.0	843	165.4	167.5

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 1 of Table 2.

The above calculations were all finished quickly by computer. With the same method, this paper calculated the five indices OEI, VDI, RDI, EDI, and  $S_e$  for 1038 hydrocarbons. Some of them (the first 20 examples of each kind of hydrocarbons) are listed in Table 1, and the rest can be seen in the Supporting Information.

Known from Table 1, EDI is the most structurally distinguishable index among the descriptors VDI, OEI, EDI, RDI, and  $S_e$ . For the given 1038 hydrocarbons, the EDIs are all different from each other (except for the *cis/trans* isomers). The more unsaturated the molecule is, the larger is the EDI. VDI and OEI just distinguish molecules with

**Table 4.** Experimental and Estimated Critical Temperatures ( $T_{c,exp}$ ,  $T_{c,calc}$ ) of Some Hydrocarbons

no.	$T_{c,exp}^a$	$T_{c,calc}^b$	no.	$T_{c,exp}^a$	$T_{c,calc}^b$	no.	$T_{c,exp}^a$	$T_{c,calc}^b$	no.	$T_{c,exp}^a$	$T_{c,calc}^b$	no.	$T_{c,exp}^a$	$T_{c,calc}^b$
1	190.56	204.31	29	553.50	552.52	162	708.00	711.51	426	364.90	373.93	825	591.75	607.95
2	305.32	287.35	30	550.00	552.95	163	723.00	729.66	427	419.50	428.45	826	630.30	637.76
3	369.83	356.22	31	562.00	554.88	164	736.00	746.87	428	435.50	428.45	827	617.00	631.08
4	425.12	411.96	32	568.80	563.38	165	747.00	763.38	429	428.60	428.45	828	616.20	634.18
5	407.80	409.36	33	565.50	558.72	166	768.00	794.14	430	417.90	425.90	829	617.15	635.67
6	469.70	453.48	34	563.50	560.35	167	398.00	462.41	431	464.80	469.05	832	664.50	662.37
7	460.40	458.49	35	543.80	538.01	168	460.00	486.26	432	475.00	469.05	833	649.10	659.01
8	433.80	448.55	36	573.50	567.80	171	511.70	499.12	433	471.00	469.05	834	637.30	649.65
9	507.60	490.75	37	566.40	561.27	181	553.80	538.72	434	470.00	473.95	835	651.00	660.71
10	497.70	489.46	38	567.10	559.78	195	532.70	536.66	435	452.70	473.95	836	637.00	657.51

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 2 of Table 2.**Table 5.** Experimental and Estimated Critical Pressures ( $P_{c,exp}$ ,  $P_{c,calc}$ ) of Some Hydrocarbons

no.	$P_{c,exp}^a$	$P_{c,calc}^b$	no.	$P_{c,exp}^a$	$P_{c,calc}^b$	no.	$P_{c,exp}^a$	$P_{c,calc}^b$	no.	$P_{c,exp}^a$	$P_{c,calc}^b$	no.	$P_{c,exp}^a$	$P_{c,calc}^b$
1	4.599	5.353	27	2.530	2.551	157	1.820	1.829	287	3.040	3.106	825	4.108	4.231
2	4.872	4.596	28	2.630	2.623	159	1.680	1.710	316	3.340	2.752	826	3.732	3.875
3	4.248	4.160	29	2.560	2.568	161	1.570	1.606	425	5.041	4.996	827	3.541	3.780
4	3.796	3.769	30	2.490	2.569	162	1.480	1.514	426	4.600	4.549	828	3.511	3.818
5	3.640	3.809	31	2.650	2.609	163	1.400	1.433	427	4.020	4.046	829	3.609	3.689
6	3.370	3.373	32	2.690	2.653	164	1.340	1.361	428	4.210	4.136	832	3.454	3.538
7	3.380	3.472	33	2.610	2.586	165	1.290	1.296	429	4.100	4.136	833	3.232	3.488
8	3.196	3.479	34	2.730	2.686	166	1.070	1.186	430	4.000	4.175	834	3.127	3.372
9	3.025	3.043	35	2.570	2.517	167	5.540	5.920	431	3.560	3.572	835	3.380	3.390
10	3.040	3.075	36	2.820	2.747	168	4.980	4.982	432	3.690	3.641	836	3.250	3.344

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 3 of Table 2.**Table 6.** Experimental and Estimated Critical Volumes ( $V_{c,exp}$ ,  $V_{c,calc}$ ) of Some Hydrocarbons

no.	$V_{c,exp}^a$	$V_{c,calc}^b$	no.	$V_{c,exp}^a$	$V_{c,calc}^b$	no.	$V_{c,exp}^a$	$V_{c,calc}^b$	no.	$V_{c,exp}^a$	$V_{c,calc}^b$	no.	$V_{c,exp}^a$	$V_{c,calc}^b$
1	98.6	103.5	19	418.0	417.0	37	460.0	473.0	195	318.0	295.9	578	221.0	218.8
2	145.5	151.7	20	414.0	410.1	38	442.0	479.7	203	353.0	366.2	640	112.2	126.6
3	200.0	196.6	21	416.0	422.6	39	455.0	474.2	223	375.0	362.3	641	163.5	175.5
4	255.0	249.7	22	398.0	402.3	40	461.0	455.0	224	369.0	360.8	642	208.0	217.9
5	259.0	240.7	23	492.0	494.4	41	555.0	558.5	247	410.0	431.5	715	245.0	226.7
6	311.0	307.9	24	488.0	488.2	76	624.0	623.3	425	131.1	139.1	824	256.0	255.6
7	306.0	299.0	25	464.0	487.7	151	689.0	688.5	426	184.6	186.1	825	316.0	310.4
8	307.0	284.5	26	476.0	487.8	157	754.0	754.0	427	240.8	234.0	826	370.0	367.0
9	368.0	368.6	27	478.0	477.4	159	823.0	819.8	428	233.8	240.5	827	375.0	367.8
10	368.0	361.0	28	468.0	480.6	161	894.0	885.9	429	237.7	240.5	828	378.0	367.9

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 4 of Table 2.**Table 7.** Experimental and Estimated Densities ( $D_{exp}$ ,  $D_{calc}$ ) of Some Hydrocarbons

no.	$D_{exp}^a$	$D_{calc}^b$	no.	$D_{exp}^a$	$D_{calc}^b$	no.	$D_{exp}^a$	$D_{calc}^b$	no.	$D_{exp}^a$	$D_{calc}^b$	no.	$D_{exp}^a$	$D_{calc}^b$
6	0.6262	0.6411	359	0.7936	0.7727	560	0.7340	0.7464	744	0.8354	0.8340	923	0.8734	0.8861
7	0.6201	0.6426	360	0.8023	0.7785	561	0.7396	0.7441	746	0.9064	0.9034	924	0.8880	0.8720
13	0.6616	0.6621	373	0.7912	0.7602	564	0.7503	0.7527	747	0.8472	0.8250	925	0.8590	0.8714
14	0.6837	0.6771	374	0.7976	0.8124	565	0.7576	0.7569	748	0.8483	0.8250	926	0.8585	0.8710
15	0.6787	0.6787	375	0.7813	0.8147	566	0.7528	0.7569	750	0.7824	0.8146	927	0.8744	0.8641
16	0.6860	0.6783	377	0.8101	0.7897	567	0.7537	0.7553	755	0.8005	0.8177	928	0.8594	0.8634
17	0.6739	0.6827	380	0.7970	0.7881	568	0.7497	0.7553	757	0.8150	0.8185	929	0.8710	0.8571
18	0.6951	0.6792	382	0.7963	0.7936	569	0.7584	0.7647	758	0.8040	0.8164	930	0.8590	0.8574
19	0.6727	0.6814	384	0.7902	0.7745	570	0.7658	0.7764	761	0.7996	0.8146	931	0.8586	0.8569
20	0.6936	0.6806	385	0.8131	0.7814	572	0.7764	0.7986	763	0.8140	0.7997	932	0.8649	0.8634

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 5 of Table 2.

different molecular skeleton, so the combination of EDI can improve the characterization of molecular graphs. RDI indicates the rigidity of ring. The molecules with larger rigidity will get the larger RDI. For all the noncyclic compounds, their RDIs are equal to 0.

### 3. RESULTS AND DISCUSSION

**3.1. Data Sets.** In this paper, 1038 boiling points (Bp),<sup>18,19</sup> 139 critical temperatures ( $T_c$ ),<sup>19</sup> 129 critical pressures ( $P_c$ ),<sup>19</sup>

90 critical volumes ( $V_c$ ),<sup>19</sup> 493 densities ( $D$ ) at 20 °C,<sup>19</sup> 752 refractive indexes ( $n_D$ ) at 20 °C,<sup>19</sup> 179 vapor pressures ( $\log P_v$ ),<sup>10</sup> 84 heat capacities ( $C_p$ ) in liquid,<sup>19</sup> and 159 heats of vaporization ( $H_v$ )<sup>19</sup> were taken as the data sets to examine the QSPR capability of these topological indices.

**3.2. Regression Analyses.** It has been proved that the addition of  $N$  (the number of carbon atoms) to other molecular descriptors can improve the correlations with the physicochemical properties of hydrocarbons.<sup>16,18</sup> Therefore,

**Table 8.** Experimental and Estimated Refractive Indexes ( $n_{D\text{exp}}$ ,  $n_{D\text{calc}}$ ) of Some Hydrocarbons

no.	$n_D^a\text{exp}$	$n_D^b\text{calc}$	no.	$n_D^a\text{exp}$	$n_D^b\text{calc}$	no.	$n_D^a\text{exp}$	$n_D^b\text{calc}$	no.	$n_D^a\text{exp}$	$n_D^b\text{calc}$	no.	$n_D^a\text{exp}$	$n_D^b\text{calc}$
4	1.3326	1.3465	165	1.4390	1.4671	447	1.4045	1.4063	630	1.4498	1.4556	856	1.5043	1.5118
6	1.3575	1.3589	166	1.4425	1.4802	448	1.3800	1.4018	631	1.4481	1.4552	857	1.5107	1.5123
7	1.3537	1.3607	171	1.4065	1.3968	449	1.3889	1.4018	632	1.4445	1.4561	858	1.4981	1.5115
9	1.3749	1.3700	172	1.3668	1.3915	450	1.3995	1.4026	634	1.4577	1.4427	859	1.5035	1.5025
10	1.3715	1.3716	173	1.3829	1.3897	451	1.3763	1.3999	635	1.5135	1.4427	860	1.4955	1.5018
11	1.3765	1.3718	174	1.3713	1.3897	452	1.4122	1.4144	636	1.5079	1.4497	861	1.4967	1.5015
12	1.3688	1.3746	175	1.3786	1.3832	453	1.3969	1.3996	638	1.5122	1.4544	862	1.4996	1.4994
13	1.3750	1.3735	176	1.3866	1.3926	454	1.3998	1.3991	639	1.4722	1.4667	863	1.4935	1.4989
14	1.3878	1.3802	177	1.4120	1.4196	455	1.4060	1.4045	642	1.3962	1.4062	864	1.4922	1.4987
15	1.3848	1.3816	181	1.4266	1.4088	456	1.4045	1.4045	643	1.3921	1.4248	865	1.5006	1.5055

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 6 of Table 2.**Table 9.** Experimental and Estimated Vapor Pressures ( $\log P_{V\text{exp}}$ ,  $\log P_{V\text{calc}}$ ) of Some Hydrocarbons

no.	$\log P_{V\text{exp}}$	$\log P_{V\text{calc}}$	no.	$\log P_{V\text{exp}}$	$\log P_{V\text{calc}}$	no.	$\log P_{V\text{exp}}$	$\log P_{V\text{calc}}$	no.	$\log P_{V\text{exp}}$	$\log P_{V\text{calc}}$	no.	$\log P_{V\text{exp}}$	$\log P_{V\text{calc}}$
2	6.622	6.663	39	3.486	3.503	222	3.934	3.915	451	4.760	4.643	828	3.068	3.038
3	5.979	6.087	41	2.764	2.837	223	3.727	3.825	452	4.222	4.381	829	3.107	2.993
4	5.387	5.490	42	2.927	2.949	224	3.788	3.743	453	4.369	4.366	830	2.912	2.949
5	5.546	5.663	43	2.921	2.906	247	2.876	3.069	454	3.876	3.837	832	2.335	2.561
6	4.835	4.944	44	2.959	2.922	278	3.217	3.308	455	3.810	3.806	833	2.458	2.595
7	4.962	5.034	49	3.094	3.101	279	3.332	3.413	457	3.850	3.807	834	2.527	2.726
9	4.307	4.394	58	3.347	3.249	280	3.480	3.420	481	3.882	3.881	835	2.530	2.545
10	4.449	4.533	68	3.103	3.226	281	3.286	3.248	484	4.172	4.096	836	2.628	2.581
11	4.402	4.450	70	3.427	3.721	282	3.412	3.248	486	3.367	3.323	837	2.600	2.565
12	4.631	4.712	75	2.988	2.957	283	3.457	3.331	487	3.331	3.296	838	2.666	2.554

<sup>a</sup> From ref 10. <sup>b</sup> Calculated by eq 7 of Table 2.**Table 10.** Experimental and Estimated Heat Capacities ( $C_{p\text{exp}}$ ,  $C_{p\text{calc}}$ ) of Some Hydrocarbons

no.	$C_p^a\text{exp}$	$C_p^b\text{calc}$	no.	$C_p^a\text{exp}$	$C_p^b\text{calc}$	no.	$C_p^a\text{exp}$	$C_p^b\text{calc}$	no.	$C_p^a\text{exp}$	$C_p^b\text{calc}$	no.	$C_p^a\text{exp}$	$C_p^b\text{calc}$
4	140.9	136.5	26	251.1	250.9	171	128.8	125.2	432	151.7	157.7	825	157.3	158.5
6	167.2	164.5	30	249.2	248.5	181	154.9	155.0	433	157.0	157.7	826	186.1	186.1
7	164.8	160.9	31	246.6	246.1	224	184.8	183.4	434	157.2	153.8	827	183.0	186.5
9	195.6	193.6	35	239.1	243.8	278	216.3	219.1	435	156.1	152.2	828	181.5	186.5
10	193.7	190.6	36	245.6	242.6	280	209.2	210.2	436	152.8	156.5	829	183.2	187.6
11	190.7	190.2	37	247.3	244.9	281	210.2	212.2	437	183.3	182.9	830	182.0	176.7
12	191.9	184.7	41	284.4	284.1	282	209.4	212.2	454	211.8	211.9	832	216.4	214.5
13	189.7	186.8	68	271.5	269.1	283	209.4	212.5	486	241.0	241.5	833	215.0	214.9
14	224.7	223.4	70	266.3	270.6	284	212.8	212.5	487	239.0	243.0	834	209.3	215.1
15	222.9	220.7	75	278.2	275.9	285	212.1	212.6	488	239.0	243.0	838	214.7	217.4

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 8 of Table 2.**Table 11.** Experimental and Estimated Heat of Vaporization ( $H_{V\text{exp}}$ ,  $H_{V\text{calc}}$ ) of Some Hydrocarbons

no.	$H_V^a\text{exp}$	$H_V^b\text{calc}$	no.	$H_V^a\text{exp}$	$H_V^b\text{calc}$	no.	$H_V^a\text{exp}$	$H_V^b\text{calc}$	no.	$H_V^a\text{exp}$	$H_V^b\text{calc}$	no.	$H_V^a\text{exp}$	$H_V^b\text{calc}$
2	5.16	9.70	35	35.14	34.91	177	27.49	28.39	435	23.77	25.17	522	36.86	37.90
3	14.79	14.61	36	37.27	38.22	181	33.01	30.85	436	27.06	26.81	523	37.03	37.90
4	21.02	19.99	37	37.75	38.24	195	31.64	29.20	437	30.61	30.48	534	37.23	36.22
5	19.23	18.35	38	38.52	39.08	221	34.20	33.57	438	32.19	31.27	537	37.27	39.41
6	26.43	25.02	39	37.99	39.05	223	36.40	34.40	439	31.60	31.27	555	50.43	50.04
7	24.85	24.21	40	42.90	36.55	224	35.36	35.23	440	31.23	31.34	569	60.78	59.98
8	21.84	20.91	41	46.55	45.52	233	34.77	35.59	441	31.55	31.34	573	80.25	80.00
9	31.56	30.23	58	40.16	41.61	273	38.85	38.46	442	30.48	29.84	577	23.21	23.84
10	29.89	28.92	61	41.41	43.15	278	41.08	39.45	443	28.62	30.18	578	20.86	22.73
11	30.28	29.75	70	38.49	37.02	279	39.44	38.48	444	28.71	29.31	642	23.35	22.59

<sup>a</sup> From ref 19. <sup>b</sup> Calculated by eq 9 of Table 2.

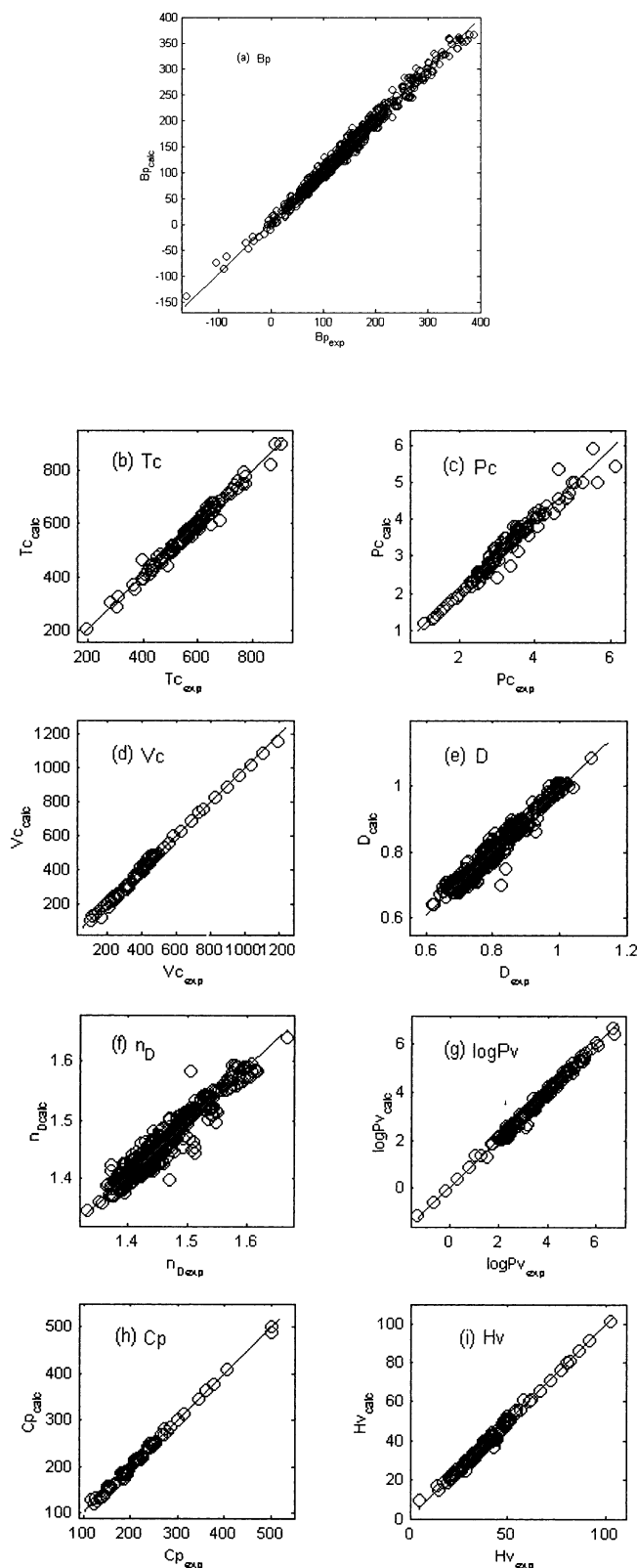
this paper also took  $N$  as a parameter (combined with the five topological indices defined above) to correlate with the properties of the title compounds. We have tried many regression analyses for each property with the various combinations among the six parameters  $N$ ,  $VDI$ ,  $OEI$ ,  $EDI$ ,  $RDI$ , and  $S_e$ . The best correlation results are listed in Table 2.

The regression equations in Table 2 all employ only 4–5 indices and obtain good correlations, especially for  $Bp$ ,  $Vc$ ,  $Pv$ ,  $Cp$ , and  $Hv$ . For the boiling points ( $Bp$ ), critical

temperatures ( $T_c$ ), critical pressures ( $P_c$ ), densities ( $D$ ), and vapor pressures ( $P_v$ ), the nonlinear regressions are better than the linear ones. This paper only lists some experimental and estimated values for each property in Tables 3–11, respectively, and the tables about the whole datas are shown in the Supporting Information. The numberings of compounds in tables are consistent with those in Figure 3.

Known from Table 3, the prediction of boiling points is satisfactory for such a comprehensive sample. Most of the estimated boiling points ( $Bp_{\text{calc}}$ ) are very close to the





**Figure 2.** The plots of the estimated vs experimental properties for hydrocarbons.

experimental ones ( $Bp_{exp}$ ). The largest deviation is  $-29.8$  °C for ethene. We also noted that Wessel<sup>20</sup> ever studied the boiling points of 296 hydrocarbons with six molecular descriptors and obtained  $r = 0.997$ ,  $rms = 6.3$  K. Plavšić and his collaborators<sup>3</sup> compared the Bp-Structure relationships with different descriptors for 22 condensed benzenoids. In

the eight regression equations, the worst is  $s = 38.5$  °C and the best is  $s = 7.8$  °C. The previous results achieved important progress, but they all only reached a relatively narrow range of compounds. This paper correlated the Bps of 1038 hydrocarbons with five indices, the good agreement between  $Bp_{calc}$  and  $Bp_{exp}$  was still obtained ( $r = 0.9926$ ,  $s = 8.26$  °C). In Figure 2(a), the plot of  $Bp_{calc}$  vs  $Bp_{exp}$  was shown.

In Table 4, the deviations of critical temperature ( $Tc_{exp} - Tc_{calc}$ ) for paraffins are smaller, while larger for cyclic and unsaturated hydrocarbons. It is amazing that the estimated Tcs ( $Tc_{calc}$ ) largely deviate from the experimental ones ( $Tc_{exp}$ ) for normal cycloalkanes, such as cyclopropane (no. 167), cyclooctane (no. 247), and so on. The correlation of Tc is worse than that of Bp, one reason of which may be that Tc is more difficult to measure accurately than Bp. The plot of  $Tc_{calc}$  vs  $Tc_{exp}$  was shown in Figure 2(b).

The four-index regression equation for critical pressures (Pc) obtains  $r = 0.9855$ ,  $s = 0.188$  MPa for 129 diverse hydrocarbons. In Table 5, some of the estimated results were listed. We plotted the estimated versus the experimental Pc in Figure 2(c).

The prediction of critical volumes with four indices gets the high correlation coefficient ( $r = 0.9975$ ) and low standard deviation ( $s = 14.84$  cm<sup>3</sup>·mol<sup>-1</sup>). Most of the  $Vc_{calc}$  have good agreement with  $Vc_{exp}$ , but some have large deviations, such as nos. 38 and 167, the deviations of which are  $-37.7$  and  $38.6$ , respectively (seen in Table 6). Figure 2(d) shows the correlation of  $Vc_{calc}$  and  $Vc_{exp}$ .

493 densities of hydrocarbons at 20 °C were reproduced with eq 5 of Table 2. Known from Table 7 (or the Supporting Information), the majority of deviations are less than 0.0100, but for 2,2,3,3-tetramethylbutane (no. 40), the  $D_{calc}$  deviates from  $D_{exp}$  by 0.1243, which is an outlier seen from Figure 2(e).

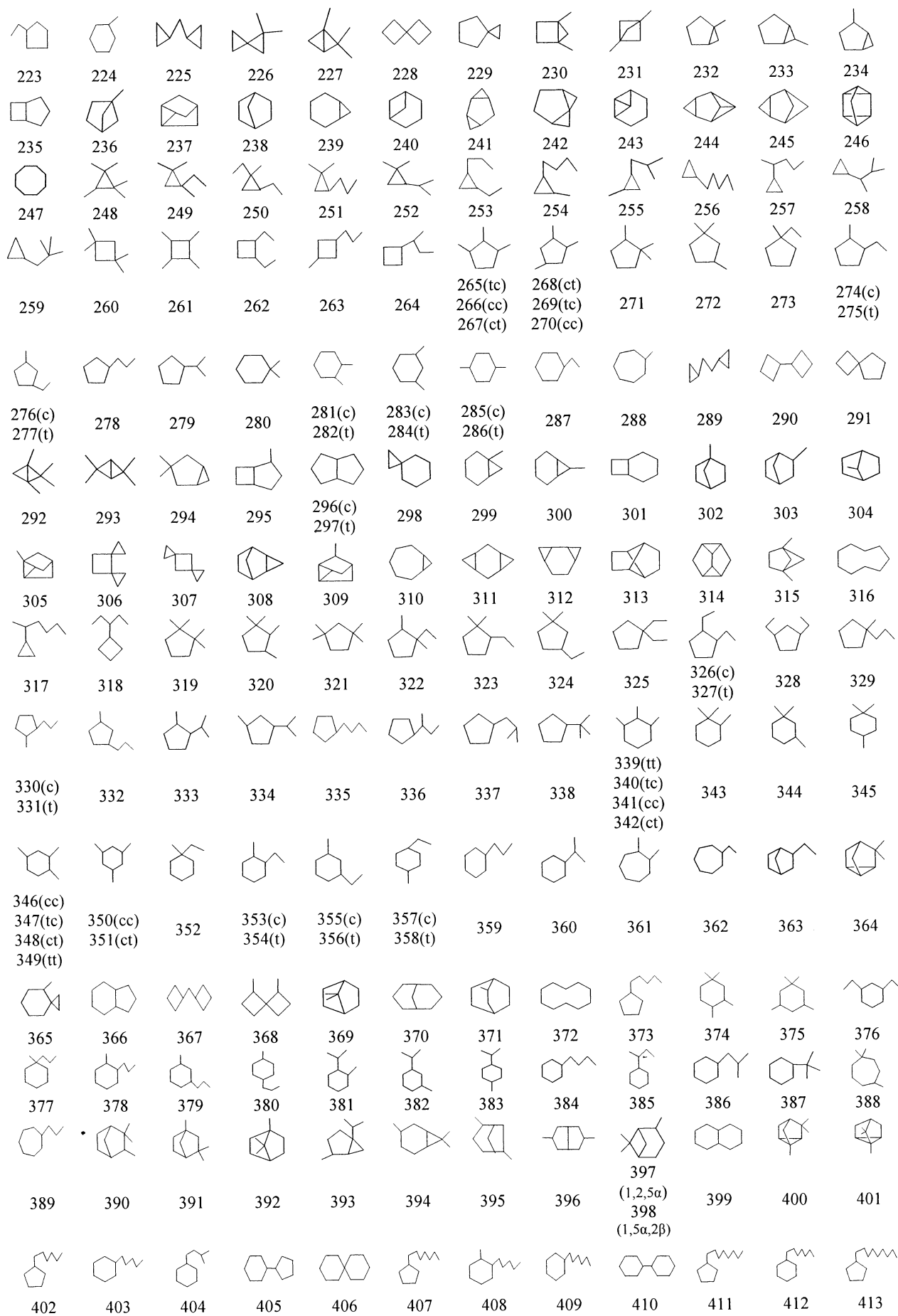
It is shown in Table 8 that the  $n_{Dcalc}$  of alkanes (except for no. 40, 2,2,3,3-tetramethylbutane), alkenes, and alkynes are estimated with little difference to  $n_{Dexp}$ , while for the condensed benzenoids, some  $n_{Dcalc}$  are far from the  $n_{Dexp}$ , the largest deviation is  $-0.0779$  for no. 982 (2,3-dimethylnaphthalene). The relatively low correlation coefficient ( $r = 0.9675$ ) reminds us that some information about the condensed structure perhaps is still not counted by the four indices in eq 6 of Table 2 and the improvement will be continued. We plotted  $n_{Dcalc}$  against  $n_{Dexp}$  in Figure 2(f).

The five-descriptor equation attained a satisfactory correlation ( $r = 0.9956$ ) and low standard deviation ( $s = 0.118$ ) for the logarithm of vapor pressures of 179 diverse hydrocarbons. The  $\log Pv_{calc}$  are very close to the  $\log Pv_{exp}$ , which can be seen in Table 9 and Figure 2(g). A previous paper<sup>10</sup> predicted the  $\log Pv$  of 290 diverse compounds and obtained  $rms = 0.26$  with eight descriptors by neural network approach.

The heat capacities (Cp) of 84 hydrocarbons are perfectly correlated with five indices  $N$ , VDI, EDI, RDI, and  $S_e$  ( $r = 0.9983$ ,  $s = 4.38$  J·mol<sup>-1</sup>·K<sup>-1</sup>). Known from Table 10 (or the Supporting Information), in the studied 84 compounds, only four deviations are larger than 10 J·mol<sup>-1</sup>·K<sup>-1</sup>. Figure 2(h) is the plot of  $Cp_{calc}$  vs  $Cp_{exp}$ .

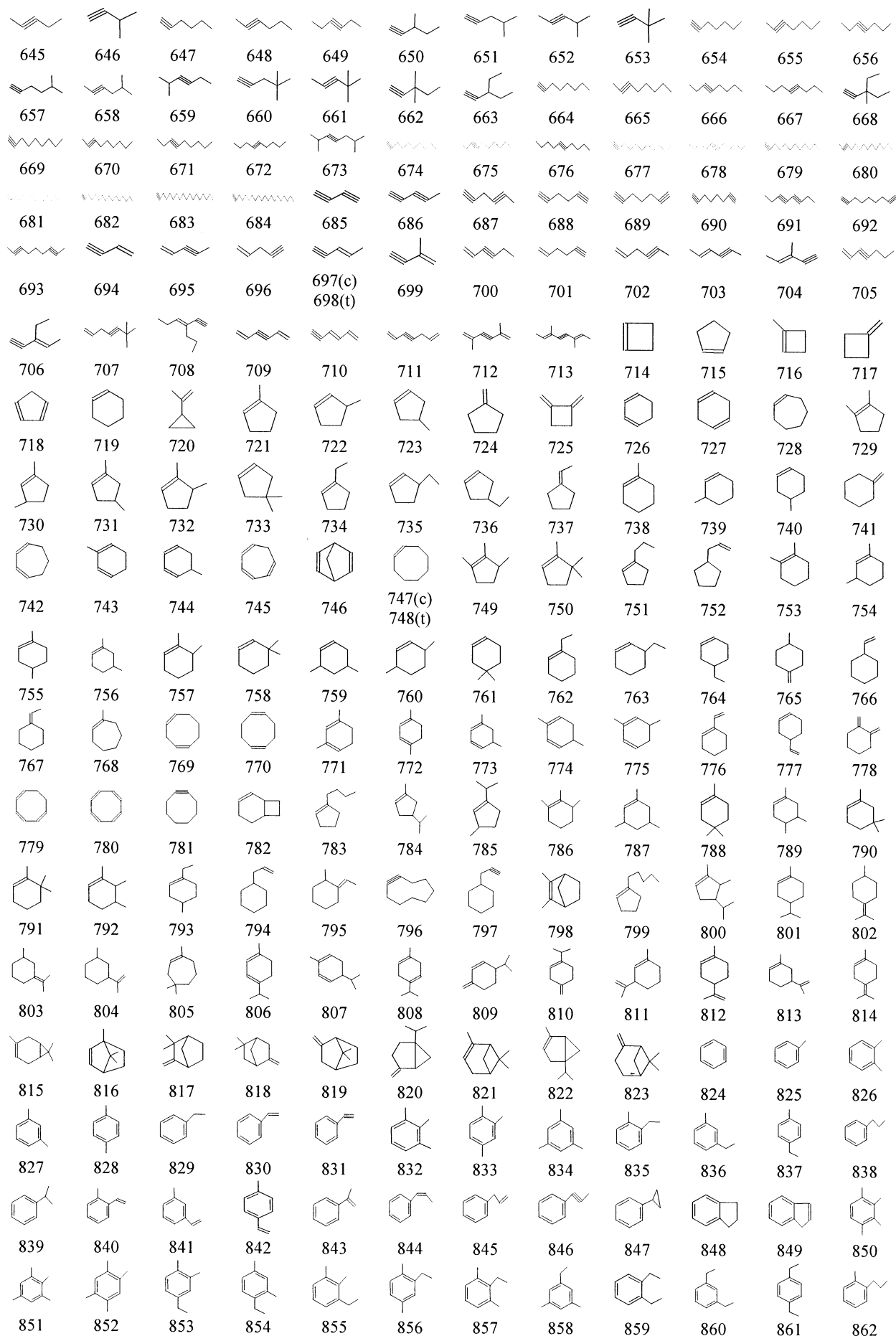
The high correlation coefficient ( $r = 0.9955$ ) and low standard deviation ( $s = 1.34$  kJ·mol<sup>-1</sup>) of eq 9 in Table 2

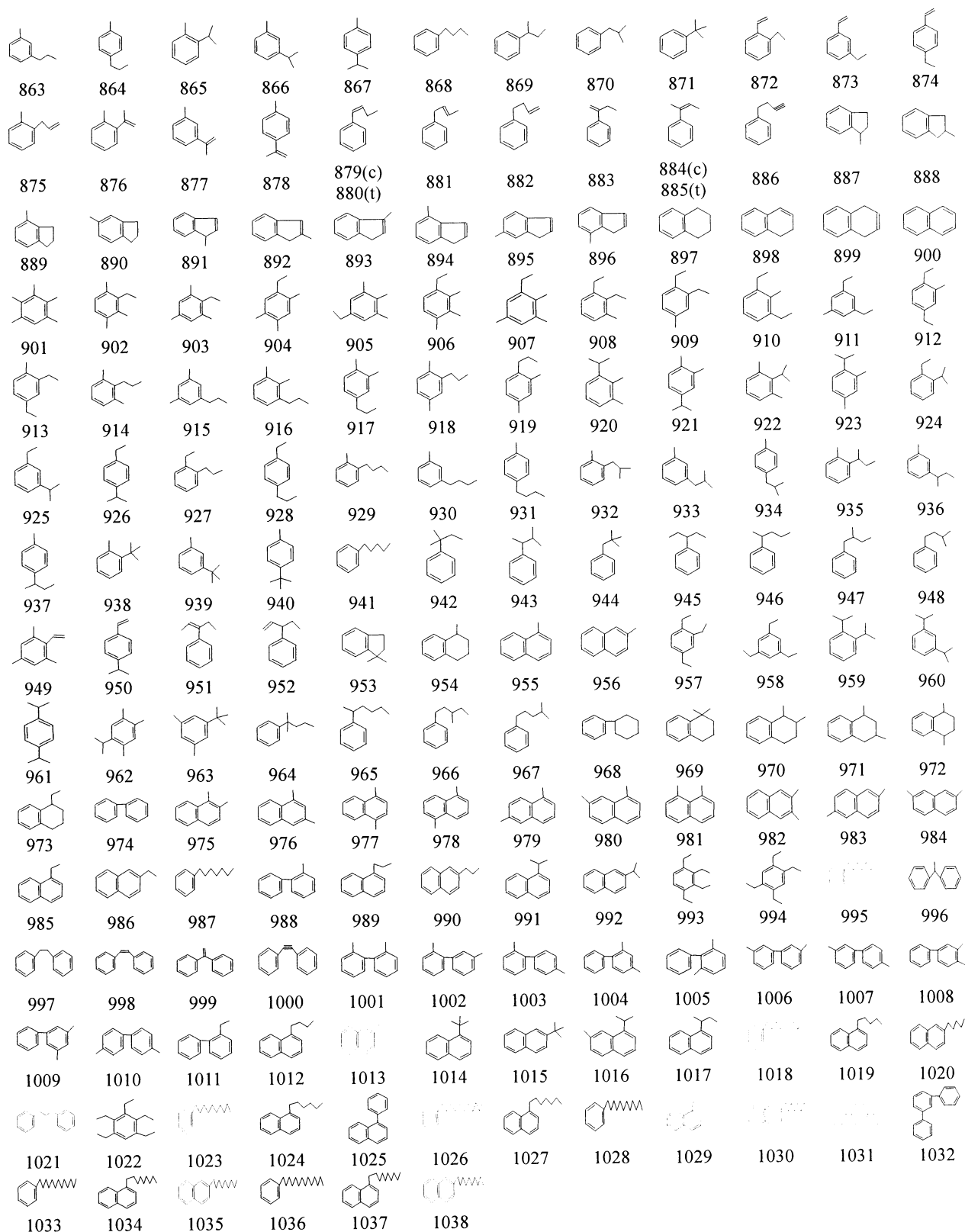






414	415	416	417	418	419	420	421	422	423	424	425
426	427	428(c) 429(t)	430	431	432(c) 433(t)	434	435	436	437	438(c) 439(t)	440(c) 441(t)
442	443	444	445	446(c) 447(t)	448(c) 449(t)	450	451	452	453	454	455(c) 456(t)
457(c) 458(t)	459	460	461	462	463	464	465(c) 466(t)	467(c) 468(t)	469(c) 470(t)	471	472
473	474	475	476	477	478	479(c) 480(t)	481	482	483	484	485
486	487(c) 488(t)	489(c) 490(t)	491(c) 492(t)	493	494	495	496	497	498	499	500
501	502	503	504	505	506	507	508	509	510	511	512
513	514	515	516	517	518	519	520(c) 521(t)	522(c) 523(t)	524(c) 525(t)	526	527
528	529	530	531	532	533	534	535	536	537	538	539
540	541	542	543(c) 544(t)	545	546	547	548	549	550	551	552
553	554	555	556	557(c) 558(t)	559	560	561	562	563	564	565(c) 566(t)
567(c) 568(t)	569	570	571	572	573	574	575	576	577	578	579
580(c) 581(t)	582	583	584	585	586	587(c) 588(t)	589	590	591	592(tt) 593(tc) 594(cc)	595
596	597	598	599	600	601	602	603	604	605	606	607
608	609	610	611	612	613	614	615	616	617	618	619
620	621	622	623	624	625	626	627	628	629	630	631
632	633	634(c) 635(t)	636	637	638	639	640	641	642	643	644





**Figure 3.** The molecular structures of 1038 hydrocarbons.

indicate the good relationship between the heat of vaporization ( $H_v$ ) and the topological indices of this paper. Some of the estimated  $H_v$  (i.e.  $H_{v,calc}$ ) are listed in Table 11. Most of the  $H_{v,calc}$  are in good agreement with the  $H_{v,exp}$ , but no. 2 (ethane) has the largest deviation by  $-4.54$ , which was shown in Figure 2(i).

#### 4. CONCLUSION

Nine physicochemical properties of a comprehensive data set consisting of 1038 diverse hydrocarbons were estimated with the four- or five-parameter regression models. The good correlation results indicate that the set of topological indices,

VDI, OEI, RDI, EDI, and  $S_e$  derived from the fundamental structural elements, vertex, edge, ring, and distance of molecular graph, express most of the molecular structural information. VDI and OEI can characterize the molecular skeleton, RDI is responsible for the rigidity resulting from the cyclic structure, while EDI and  $S_e$  count for the molecular unsaturated state. Thus the combination of these indices together forms an integrated series which can represent the molecular structures not only of alkanes but also of alkenes, alkynes, and benzenoid hydrocarbons.

#### ACKNOWLEDGMENT

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**Supporting Information Available:** Complete Tables 1–11. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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