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TOPOLOGICAL INDICES : INTER-RELATIONS AND COMPOSITION

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Abstract. The linear relationships between pairs of topological indices were investigated in three series of hydrocarbons with wide structural variation, i.e., 37 alkanes, 36 polyalkylbenzenes and 48 monocyclic structures with side chains. One evidenced strong intercorrelations between $\varepsilon - \chi - Z - w - \bar{I}_D^w - M_1 - N_2 - x_1$ and DRCI - DRGI. Results provided by the topologycal branching equation here formulated for alkanes indicate that M_1, $\bar{I}_D^w$, χ, ε, w and Z have as dominant feature the van der Waals volume, B,C and Q express predominantly the chain branching, and x_1, $\bar{I}_C$ and RCI have comparable weights for these two factors. The dependence of boiling points at normal pressure in the three series of hydrocarbons was also investigated, the best results being obtained for χ and ε.

SYMBOLS and DEFINITIONS

N_2	the number of distinct ways the acyclic C-C-C fragment can be superimposed on the molecular graph M. Gordon, G.R. Scantlebury, Trans. Faraday Soc., 60, 605 (1964)
x_1	the largest eigenvalue of the characteristic polynomial of the graph L. Lovasz, J. Pelikan, Period. Math. Hung., 3, 175 (1973)
w	half-sum of the off-diagonal elements of the distance matrix H. Wiener, J. Amer. Chem. Soc., 69, 2636 (1947)
$Z = \sum_k p(G,k)$	where p(G,k) is the number of ways in which k edges are chosen from the graph G so that no two of them are adjacent H. Hosoya, Bull. Chem. Soc. Japan, 44, 2332 (1971)
$M_1 = \sum_{\text{all vert.}} v_i^2$	where v_i is the degree of vertex i in the hydrogen suppressed graph; and
$M_2 = \sum_{\text{all edges}} (v_i v_j)$	where v_i and v_j are the degree of the two ends of the edge (ij) I. Gutman et al., J. Chem. Phys., 62, 3339 (1975)
$B = \sum_i \delta_i^2$	where δ_i is the number of vertices deleted at step i on running a tree-graph towards ist centre

$C = \frac{1}{2}\ (B-2N + U)$

$C' = (B-2N+U)/[(N-2)^2-2+U]$ where $U = [1-(-1)^N]$ and N stands for the number of the graph vertices

$Q = \frac{1}{2}\sum_i iV_i - 2N+3$, and

$Q' = {}^2(3V_4+V_3)/[2(N-2)(N-3)]$ where V_i stands for the number of vertices of degree $i \leq 4$
A.T. Balaban, Theor. Chim. Acta, 53, 355 (1979)

$X = \sum_{\text{all edges}} (v_i v_j)^{-1/2}$ with v_i and v_j being the degree of the two ends of the edge (ij)
M. Randić, J. Amer. Chem. Soc., 97, 6609 (1975)

$\bar{I}_{ORB}$ information content on the graph orbits
N. Rashevsky, Bull. Math. Biophys., 30, 229 (1955);
E. Trucco, ibid, 18, 129, 237 (1956)

$\bar{I}_{CHR}$ chromatic information content of the graph
A. Mowshowitz, Bull. Math. Biophys., 30, 175, 225, 387, 533 (1968)

$\bar{I}_D^E$ information index for the equality of distance in graph; and

$\bar{I}_D^W$ information index for the magnitude of distance
D. Bonchev, N. Trinajstić, J. Chem. Phys., 67, 4517 (1977)

$\bar{I}_Z$ and $\bar{I}_X$ information analogues of the Hosoya and Randić indices
D.Bonchev, N. Trinajstić, J. Chem. Phys., 67, 4517 (1977)

ε	Electropy index W.T. Yee, K. Sakamoto, Y.J. I'Haya, Rep. Univ. Electro-Comm., 27, 53 (1976)
RCI, DRCI, RGI, DRGI	topological indices based on the generalized concept for the graph centre D. Bonchev, A.T. Balaban, Ov. Mekenyan, J. Chem. Inf. Comp. Sci., 20, 106 (1980)
r,s and F	stand for correlation coefficient, standard deviation and Fisher statistic, respectively

1. Introduction

The large number of existing topological indices[1] raises the question to what extent they are orthogonal. In other words, it is possible that some topological indices existing in the literature express predominantly the same type of structural information ; the differences then reside in the scaling factors.

Another problem is the meaning of the topological indices. We are interested to identify which topological indices, and to what extent, espress steric effects.

Finally, we investigate the correlation ability of topological indices, calculating the dependence of boiling points for three series of hydrocarbons on topological indices.

2. Inter-relations Among Topological Indices

In the following treatment, the existence of linear relationships (1) between pairs of topological indices T_i and T_j was investigated :

$$T_i = a + b\, T_j \qquad , \qquad i \neq j \tag{1}$$

For avoiding chancy correlations, three series of hydrocarbons with wide structural variation were considered : 37 alkanes (Table 1), 36 polyalkylbenzenes (Table 2) and 48 monocyclic structures with side - chains depicted in Figure 1 (Table 3). The three tables list the structures, their topological indices and the boiling points at normal pressure of the corresponding hydrocarbons.

The pairwise linear correlations between topological indices T_i and T_j are displayed in matrix form in Tables 4 - 6. These matrices are symmetrical and indicate the correlation coefficients $r(T_i,T_j)$, $i \leqslant j$.

The strong intercorrelations T_i vs. T_j evidenced by all three series of structures are presented in more detail in Table 7 A.

Figure 2 presents as a graph the most strongly intercorrelated topological indices together with their correlation

coefficient r averaged for the three series. One can note two disjoint graphs.

The present data supplement those indicated in previous papers.[2,3] On comparing the data from Tables 4 - 6 with those from ref. 3, two conclusions emerge : i) Some inter-relations T_i *vs.* T_j for one of the three series are statistically significant, yet they are due only to structural similarities in that series. Tables 7 B and 7 C illustrate this parallelism between topological indices generated by structural similarity; ii) Equation (1) translated into Figure 2 evidences the following two classes of strongly intercorrelated topological indices : *class 1* : Z, w, I_D^W, χ , ξ , M_1, N_2, x_1, and *class 2* : DRCI and DRGI. The other topological indices are practically not intercorrelated with the above indices or among themselves (the centric and quadratic indices are also intercorrelated as seen in the alkane series, Table 4, but since no data are available for the other two series, they have not been included in Tables 7 A - C or in Figure 2).

3. Which Topological Indices, and to What Extent, Express Steric Effects

For 29 chemical structures, in ref. 4 a numerical integration[4,5] (Monte Carlo) of van der Waals envelopes was effected resulting in van der Waals volumes (WV). On correlating these volumes with molar refractions (MR), equation (2) was obtained:

$$MR = -1.966 + 0.323\ WV \qquad (2)$$

$$(r=0.95,\ s=2.01,\ F=128.53,\ EV=0.91)$$

This indicates that the MR values depend with about 90% on the van der Waals volume, and only about 10% on other factors such as electronic components.

It has been argued[6] that topological indices reflect the molecular branching. In the previous paper[3], we observed correlations between MR and topological indices, therefore it is plausible that some topological indices contain steric com-

ponents reflecting molecular volumes.

We therefore proceeded to identify the topological indices which reflect substantially the molecular volume by studying correlations MR vs. T_i. For 17 topological indices calculated for a restricted alkane series, ref.3 demonstrated that Z, I_D^W, χ and M_1 are proportional van der Waals volumes. Since MR's are calculated incrementally (either from atomic refractions or from bond refractions) , evidently the number of carbon atoms in a alkane is proportional to MR.

Since steric effects depend both on the molecular volume and on its shape, we tested the validity of the following topological branching equation (3) for acyclic structures :

$$T_i = a + b\ NCA + c\ NBP + d\ NSC \qquad (3)$$

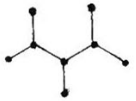
where NCA indicates the number of carbon atoms (i.e., the number of vertices in the molecular hydrogen - depleted graph of the hydrocarbon) ;

NBP is the number of branching points (i.e., the number of vertices with degree $\geqslant 3$ in the above graph) ; and

NSC is the number of side- chains (i.e., after the longest path has been defined on an acyclic graph, from the branching points one enumerates the side - chains).

For example, structures 18 and 35 from Table 1 have the following characteristics :

(no. 18)



(no. 35)

NCA = 7 ; NBP = 1 ; NSC = 2. NCA = 8; NBP = 3 ; NSC=3.

One can imagine that for acyclic structures grouped in Table 1, NCA measures the volume, while NBP and NSC express together the branching of the alkane. If we adopt the notation[6] V_i for the number of vertices of degree i, then for carbon trees (i.e., acyclic graphs corresponding to alkanes) we have :

$$NCA = V_1 + V_2 + V_3 + V_4$$

$$NBP = V_3 + V_4 \quad ; \quad NSC = V_3 + 2V_4 = V_1 - 2$$

whence we obtain the number of vertices with degree two :

$$V_2 = NCA - (NBP + NSC) - 2$$

Thus, separately and lumped together as a sum, the two parameters NBP and NSC reflect the branching since V_2 (whose maximal value is NCA-2 for n-alkanes and whose minimal value is zero) also reflects the degree of branching.

It should be mentioned that several topological indices are linearly dependent[6] on V_3 and V_4 like NBP and NSC :

$$M_1 = 2\,(3V_4 + V_3) + 4NCA - 6$$
$$N_2 = 3V_4 + V_3 + NCA - 2$$
$$Q = 3V_4 + V_3$$

The correlation (3) proved to be valid for the following topological indices : B, C, Q, M_1, $\bar{I}^{w}_{D}$, χ , x_1, $\bar{I}_C$, ε and RGI. The results are presented in Table 8.

Results provided by eqn.(3) indicate that some indices from Table 8 (M_1, $\bar{I}^{w}_{D}$, χ , ε , w and Z) express steric effects, having as dominant feature the van der Waals volume or the number of carbon atoms, while other indices (B, C, Q) express predominantly the chain branching, and still other indices (x_1, $\bar{I}_C$, RCI) have comparable weights for these two factors.

The number of endpoints V_1 in the molecular graph is reflected with a considerable weight in the centric indices B,C, and (by extension) Q because the outer shell of endpoints is squared and summed into these indices. Since NSC = V_1 - 2, it is not surprising to find that B,C and Q correlate well with NSC, little with NBP and not at all with NCA (cf. Table 8).

The topological indices which do not appear in Table 8). cannot be represented according to eqn. (3) : the correlation coefficients r range from 0.337 ($\bar{I}^{\varepsilon}_{p}$) to 0.829 ($\bar{I}_Z$), therefore it is improbable that these other indices could represent steric effects.

The above results from the two preceding sections suggest how to explore the systematic construction of topological superindices[7] SI :

$$SI = \sum_{j=1}^{m} T_j \qquad (4)$$

$$SI = \{ T_1, \cdots, T_m \} \qquad (5)$$

One should sum T_is belonging to the same class in Figure 2. The number m of topological indices constituting the superindex should be selected according to the requested discriminating ability of the superindex among isomeric graphs. For instance:

$$SI = \bar{I}_D^w + \chi \quad , \text{ or } \quad SI = M_1 + \varepsilon + \bar{I}_D^w + \chi$$

reflect the volume parameter, while

$$SI = B + C \ , \text{ or } SI = {}^{x}_{1} + RCI$$

reflect the molecular shape.

The SI defined by relation (5) will contain as entries only orthogonal T_is.

The results from Table 8 indicate that χ, ε, $\bar{I}_D^w$ and w may be used with equivalent results in QSAR.

4. Comparative Study of the Correlation Ability of Topological Indices

As an illustration, the dependence of boiling points at normal pressure[8] (B.p.) on topological indices T_i (Tables 1-3) was investigated :

$$B.p. = a + bT_i \qquad (6)$$

Results are grouped in Tables 9 - 11.

The data from Tables 9 - 11, especially the higher values for χ and ε show the usefulness of topological indices for describing thermodynamic properties which depend on molecular weight, volume, and branching.

Table 1. Alkanes : boiling temperature and topological indices.

No.	Alkane	T_B	B	C	M_1	Q	C'	Q'	N_2	$\bar{I}_D^E$	W	Z
1.	n-C_4	-0.50	8	0	10	0	0.000	0.000	2	1.4592	10	5
2.	i-C_4	-11.72	10	1	12	1	1.000	1.000	3	1.0000	9	4
3.	n-C_5	36.07	9	0	14	0	0.000	0.000	3	1.8464	20	8
4.	2-Me-C_4	27.85	13	2	16	1	0.500	0.333	4	1.5219	18	7
5.	2,2-Me_2-C_3	9.50	17	4	20	3	1.000	1.000	6	0.9710	16	5
6.	n-C_6	68.74	12	0	18	0	0.000	0.000	4	2.1493	35	13
7.	2-Me-C_5	60.27	14	1	20	1	0.143	0.167	5	1.9086	32	11
8.	3-Me-C_5	63.28	14	1	20	1	0.143	0.167	5	1.8256	31	12
9.	2,2-Me_2-C_4	49.74	24	6	24	3	0.857	0.500	7	1.5058	28	9
10.	2,3-Me_2-C_4	57.99	20	4	22	2	0.571	0.333	6	1.5656	29	10
11.	n-C_7	98.43	13	0	22	0	0.000	0.000	5	2.3983	56	21
12.	2-Me-C_6	90.05	17	2	24	1	0.167	0.100	6	2.2126	52	18
13.	3-Me-C_6	91.85	17	2	24	1	0.167	0.100	6	2.1359	50	19
14.	3-Et-C_5	93.47	19	3	24	1	0.250	0.100	6	1.9502	48	20
15.	2,2-Me_2-C_5	79.20	21	4	28	3	0.333	0.300	8	1.9035	46	14
16.	2,3-Me_2-C_5	89.78	21	4	26	2	0.333	0.200	7	1.8842	46	17
17.	2,4-Me_2-C_5	80.50	21	4	26	2	0.333	0.200	7	1.9561	48	15
18.	3,3-Me_2-C_5	86.06	21	4	28	3	0.333	0.300	8	1.7723	44	16
19.	2,2,3-Me_3-C_4	80.88	29	8	30	4	0.667	0.400	99	1.5567	42	13

Table 1. (continued)

No.	Alkane	T_B	B	C	M_1	Q	C'	Q'	N_2	$\bar{I}_D^E$	W	Z
2o.	n-C_8	125.66	16	o	26	o	o.ooo	o.ooo	6	2.[illegible]oo	84	34
21.	2-Me-C_7	117.65	18	1	28	1	o.o59	o.o67	7	2.4621	79	29
22.	3-Me-C_7	118.93	18	1	28	1	o.o59	o.o67	7	2.3942	76	31
23.	4-Me-C_7	117.71	18	1	28	1	o.o59	o.o67	7	2.3637	75	3o
24.	3-Et-C_6	118.53	22	3	28	1	o.176	o.o67	7	2.2158	72	32
25.	2,2-Me_2-C_6	1o6.84	24	4	32	3	o.235	o.2oo	9	2.2165	71	23
26.	2,3-Me_2-C_6	115.61	24	4	3o	2	o.235	o.133	8	2.1894	7o	27
27.	2,4-Me_2-C_6	1o9.43	24	4	3o	2	o.235	o.133	8	2.2o84	71	26
28.	2,5-Me_2-C_6	1o9.1o	24	4	3o	2	o.235	o.133	8	2.2623	74	25
29.	3,3-Me_2-C_6	111.97	24	4	32	3	o.235	o.2oo	9	2.o991	67	25
3o.	3,4-Me_2-C_6	117.73	24	4	3o	2	o.235	o.133	8	2.1o55	68	29
31.	2-Me,3-Et-C_5	115.65	26	5	3o	2	o.294	o.133	8	1.9766	67	28
32.	3-Me,3-Et-C_5	118.26	26	5	32	3	o.294	o.2oo	9	1.8979	64	28
33.	2,2,4-Me_3-C_5	99.24	3o	7	34	4	o.412	o.267	1o	1.9506	66	19
34.	2,2,3-Me_3-C_5	1o9.84	3o	7	34	4	o.412	o.267	1o	1.8922	63	22
35.	2,3,4-Me_3-C_5	113.47	3o	7	32	3	o.412	o.2oo	9	1.9438	65	24
36.	2,2,3,3-Me_4-C_4	1o6.3o	4o	12	38	6	o.7o6	o.4oo	12	1.55o2	58	17
37.	2,3,3-Me_3-C_5	114.76	3o	7	34	4	o.412	o.267	1o	1.8288	62	23

Table 1. (continued)

No.	$\bar{I}_D^W$	$\bar{I}_z$	χ	x_1	$\bar{I}_C$	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$	$\bar{I}_\chi$	ξ	RCI	DRCI	MCI	RGI	DRGI
1.	2.4464	1.37o9	1.9142	1.618	1.oooo	1.oooo	1.oooo	o.9183	86.2	8	8	52	8	8
2.	2.5o33	o.8113	1.7321	1.732	o.8113	o.8113	o.8113	o.oooo	84.8	1o	1o	57	1o	1o
3.	3.1464	1.4o56	2.4142	1.732	1.5219	o.97o9	1.5219	1.oooo	116.9	9	9	95	9	9
4.	3.1972	1.3788	2.27o1	1.848	1.37o9	o.97o9	1.9219	1.5ooo	115.6	13	7	76	11	7
5.	3.25oo	o.7219	2.oooo	2.ooo	o.7219	o.7219	o.7219	o.oooo	111.6	17	17	116	17	17
6.	3.7o42	1.6143	2.9142	1.8o2	1.585o	1.oooo	1.585o	o.97o9	149.1	12	12	164	12	12
7.	3.7417	1.3486	2.77o2	1.9o2	1.4592	o.9183	2.2516	1.9219	147.8	14	8	123	14	8
8.	3.76oo	1.65oo	2.8o82	1.932	1.4592	1.oooo	1.9183	1.5219	147.8	14	1o	146	14	1o
9.	3.7979	1.3516	2.56o7	2.o74	1.2516	o.9183	1.7925	1.37o9	143.9	2o	12	15o	2o	12
1o.	3.7883	1.361o	2.6425	2.ooo	o.9183	1.oooo	o.9183	o.7219	146.5	2o	2o	196	2o	2o
11.	4.169o	1.69o9	3.4142	1.848	1.95o2	o.9852	1.95o2	o.9183	182.6	13	13	252	13	13
12.	4.1958	1.6122	3.27oo	1.932	1.8424	o.9852	2.5216	1.9183	181.3	17	9	185	15	9
13.	4.21o2	1.6798	3.3o81	1.97o	1.8424	o.9852	2.8o74	1.9183	181.3	17	7	14o	15	7
14.	4.24o6	1.72oo	3.3461	2.ooo	1.4488	o.9852	1.4488	1.oooo	181.3	19	19	29o	19	19
15.	4.24o5	1.2958	3.o6o7	2.1o1	1.3788	o.8631	2.1281	1.7925	177.4	21	13	225	21	13
16.	4.2512	1.6457	3.18o7	2.o53	1.4488	o.9852	2.5216	1.7925	18o.o	19	9	185	19	9
17.	4.23o4	1.2729	3.1251	2.ooo	1.3788	o.8631	1.3788	o.9183	18o.o	21	21	297	21	21
18.	4.2656	1.6774	3.1213	2.136	1.3788	o.9852	1.95o2	1.585o	177.4	21	13	252	21	13
19.	4.2845	1.3143	2.9434	2.175	1.3788	o.9852	1.8424	1.4592	176.1	29	15	261	21	15
2o.	4.8o16	1.8o88	3.9142	1.879	2.oooo	1.oooo	2.oooo	o.8631	217.2	16	16	376	16	16

Table 1. (continued)

No.	$\bar{I}_D^w$	$\bar{I}_z$	χ	x_1	$\bar{I}_C$	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$	$\bar{I}_\chi$	$\mathcal{E}$	RCI	DRCI	MCI	RGI	DRGI
21.	4.587o	1.6647	3.77o1	1.95o	1.9o56	o.9544	2.75oo	1.8424	215.9	18	1o	264	18	1o
22.	4.6o49	1.8266	3.8o81	1.989	1.9o56	1.oooo	3.oooo	1.95o2	215.9	18	1o	259	18	1o
23.	4.612o	1.6751	3.8o81	2.ooo	1.9o56	o.9544	2.25oo	1.95o2	215.9	18	14	35o	18	14
24.	4.6352	1.8286	3.851o	2.o28	1.8113	1.oooo	2.5ooo	1.4488	215.9	22	12	3o3	2o	12
25.	4.62o1	1.592o	3.56o6	2.112	1.75oo	o.9544	2.4o56	1.8424	212.o	24	14	319	22	2o
26.	4.6364	1.67o9	3.68o7	2.o74	1.8113	1.oooo	2.75oo	2.1281	214.6	22	12	264	2o	12
27.	4.6322	1.6479	3.6739	2.o42	1.75oo	o.9544	2.75oo	1.4488	214.6	22	12	264	22	12
28.	4.612o	1.6136	3.6259	2.ooo	1.5ooo	1.oooo	1.5ooo	1.3788	214.6	24	24	436	24	12
29.	4.6498	1.6726	3.6213	2.157	1.75oo	o.9544	2.75oo	1.95o2	212.o	24	14	252	22	1o
3o.	4.6516	1.8439	3.7188	2.o95	1.5ooo	1.oooo	2.oooo	1.95o2	214.7	24	16	376	24	16
31.	4.6625	1.6856	3.7188	2.1o1	1.4o56	o.9544	2.25oo	1.95o2	214.7	26	14	316	26	14
32.	4.6751	1.8673	3.6819	2.189	1.4o56	1.oooo	1.8113	1.4488	212.o	26	2o	394	26	2o
33.	4.6539	1.21o8	3.4165	2.149	1.2988	o.8113	2.1556	1.8424	21o.7	3o	16	351	3o	16
34.	4.6751	1.62o3	3.4814	2.2o6	1.4o56	o.9544	2.4o56	2.1281	21o.7	26	14	319	26	14
35.	4.6679	1.64o3	3.5534	2.136	1.4o56	o.9544	1.75oo	o.8631	213.3	26	22	41o	26	22
36.	4.7o64	1.2533	3.25oo	2.3o3	o.8113	1.oooo	o.8113	o.5917	2o6.8	4o	4o	484	4o	4o
37.	4.6833	1.6668	3.5o4o	2.222	1.4o56	1.oooo	2.5ooo	2.2359	21o.7	26	12	312	26	12

Table 2. Alkylbenzenes : boiling temperature and topological indices.

No.	Structure	M_1	N_2	w	$\bar{I}_D^E$	$\bar{I}_D^W$	Z	$\bar{I}_Z$	χ	$\bar{I}_\chi$	x_1
1.	Benzene(B)	24	6	27	1.5219	3.7821	18	1.6122	3.0000	0.0000	2.0000
2.	Toluene	30	3	42	1.7608	4.2548	26	1.6479	3.3940	1.3788	2.1010
3.	Et-B	34	9	64	2.0597	4.6423	44	1.8228	3.9320	1.4056	2.1358
4.	o-Xylene	36	10	60	1.8352	4.6729	39	1.7697	3.8047	1.9056	2.1935
5.	m-Xylene	36	10	61	1.8922	4.6638	37	1.6344	3.7880	1.5000	2.1753
6.	p-Xylene	36	10	62	1.9905	4.6494	38	1.7669	3.7880	1.5000	2.1701
7.	n-Pr-B	38	10	94	2.3334	4.9761	70	1.8611	4.4320	1.3516	2.1490
8.	i-Pr-B	40	11	88	2.1499	5.0047	62	1.8144	4.3047	1.8366	2.1940
9.	1-Me,2-Et-B	40	11	86	2.0751	5.0174	65	1.8758	4.3427	2.1133	2.2216
10.	1-Me,3-Et-B	40	11	88	2.1499	5.0047	63	1.8459	4.3260	1.6577	2.2001
11.	1-Me,4-Et-B	40	11	90	2.2501	4.9860	64	1.8722	4.3260	1.6577	2.1940
12.	1,2,3-Me_3-B	42	12	82	1.9032	5.0368	58	1.8406	4.2154	1.9749	2.2638
13.	1,2,4-Me_3-B	42	12	84	2.0375	5.0214	56	1.8067	4.1987	1.7527	2.2458
14.	1,3,5-Me_3-B	42	12	84	1.9591	5.0257	52	1.5922	4.1820	0.9183	2.2361
15.	n-Bu-B	42	11	133	2.5657	5.2731	144	1.9687	4.9320	1.2955	2.1543
16.	i-Bu-B	44	12	126	2.4245	5.2958	96	1.8393	4.7880	1.5219	2.1753
17.	s-Bu-B	44	12	121	2.3375	5.3135	106	1.9806	4.8427	2.0464	2.2143
18.	t-Bu-B	48	14	114	2.1811	5.3317	80	1.7931	4.6053	1.8464	2.2882
19.	1,2-Et_2-B	44	12	117	2.2027	5.3329	109	1.9842	4.8807	1.8464	2.2470
20.	1,3-Et_2-B	44	12	121	2.3375	5.3135	109	1.9798	4.8640	1.3710	2.2216

Table 2. (continued)

No.	Structure	M_1	N_2	w	$\bar{I}_D^E$	$\bar{I}_D^W$	Z	$\bar{I}_Z$	χ	$\bar{I}_\chi$	x_1
21.	1,4-Et_2-B	44	12	125	2.4572	5.2874	108	1.9901	4.8640	1.3710	2.2143
22.	1-Me,2-n-Pr-B	44	12	121	2.3375	5.2135	103	1.9406	4.8427	2.0464	2.2310
23.	1-Me,3-n-Pr-B	44	12	124	2.4005	5.3009	100	1.8644	4.8260	1.6855	2.2089
24.	1-Me,4-n-Pr-B	44	12	127	2.4926	5.2827	101	1.9260	4.8260	1.6855	2.2026
25.	1-Me,2-i-Pr-B	46	13	114	2.1509	5.3392	91	1.8482	4.7154	1.9710	2.2672
26.	1-Me,3-i-Pr-B	46	13	117	2.2245	5.3256	89	1.8402	4.6987	1.8464	2.2428
27.	1-Me,4-i-Pr-B	46	13	120	2.3442	5.3056	88	1.8246	4.6986	1.8464	2.2361
28.	1,2-Me_2,3-Et-B	46	13	113	2.1345	5.3420	97	1.9479	4.7534	2.2464	2.2844
29.	1,2-Me_2,4-Et-B	46	13	117	2.2783	5.3200	95	1.9459	4.7367	1.9610	2.2627
30.	1,3-Me_2,2-Et-B	46	13	112	2.0823	5.3482	95	1.8757	4.7534	2.2464	2.2883
31.	1,3-Me_2,4-Et-B	46	13	116	2.2475	5.3253	93	1.8717	4.7367	1.9610	2.2672
32.	1,3-Me_2,5-Et-B	46	13	116	2.2000	5.3310	89	1.8403	4.7200	1.1568	2.2552
33.	1,4-Me_2,2-Et-B	46	13	115	2.1863	5.3334	94	1.9368	4.7367	1.9610	2.2682
34.	1,2,3,4-Me_4-B	48	14	109	2.0400	5.3537	87	1.9450	4.6261	1.8464	2.3180
35.	1,2,3,5-Me_4-B	48	14	110	2.0634	5.3502	82	1.8356	4.6094	1.5219	2.3072
36.	1,2,4,5-Me_4-B	48	14	111	2.1110	5.3437	83	1.8530	4.0694	1.5219	2.3028

Table 2. (continued)

No.	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$	$\mathcal{E}$	RCI	DRCI	MCI	RGI	DRGI	$T_B(^oC)$
1.	1.0000	0.0000	119.58	36	36	216	36	36	80.10
2.	0.9852	2.2359	146.88	29	11	204	14	11	110.63
3.	1.0000	2.5000	179.52	22	16	335	20	12	136.19
4.	1.0000	2.0000	175.62	32	16	376	24	16	144.41
5.	0.9544	2.2500	175.62	32	18	350	22	14	139.10
6.	1.0000	1.5000	175.62	24	24	404	40	24	138.35
7.	0.9911	2.7255	213.40	23	17	427	23	17	159.22
8.	0.9911	2.5033	212.08	27	15	462	27	15	152.39
9.	0.9911	3.1699	209.49	29	9	285	27	9	165.15
10.	0.9911	3.1699	209.49	29	9	285	23	9	161.31
11.	0.9911	2.7255	209.49	21	13	358	29	13	161.99
12.	0.9911	1.8911	205.59	45	15	453	27	15	176.08
13.	0.9911	3.1699	205.59	29	9	285	23	9	169.35
14.	0.9183	1.5850	205.59	45	27	612	27	27	164.72
15.	1.0000	2.9219	248.36	26	14	520	24	14	183.27
16.	0.9710	2.7219	247.03	28	16	619	28	16	172.76
17.	1.0000	2.9219	247.03	30	18	595	30	18	173.30
18.	0.9710	2.4464	243.13	34	20	683	36	20	169.12
19.	1.0000	2.3219	244.45	36	20	720	36	20	183.42
20.	1.0000	2.5219	244.45	30	18	686	30	18	181.10
21.	1.0000	1.9219	244.45	28	28	757	44	28	183.75
22.	1.0000	3.3219	244.45	30	14	436	30	12	184.25
23.	0.9710	3.3219	244.45	28	12	436	28	12	181.75
24.	1.0000	2.9219	244.45	26	18	560	24	14	183.45
25.	0.9710	3.1219	243.13	34	12	484	36	12	178.35
26.	1.0000	3.1219	243.13	36	22	644	30	12	175.20
27.	0.9710	2.7219	243.13	26	16	564	34	16	177.25
28.	1.0000	3.3219	240.54	38	14	479	36	12	193.91
29.	1.0000	3.3219	240.54	30	14	485	30	12	189.75
30.	0.9710	2.7219	240.54	38	20	587	36	16	190.01
31.	1.0000	3.3219	240.54	28	10	385	28	10	188.41
32.	0.9710	2.7219	240.54	42	24	581	28	16	183.75
33.	1.0000	3.3219	240.54	36	12	385	30	10	186.91

Table 2. (continued)

No.	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$	ε	RCI	DRCI	MCI	RGI	DRGI	T_B(°C)
34.	1.0000	1.5219	236.65	44	20	720	36	20	205.04
35.	0.9710	2.1710	236.65	44	20	559	46	16	198.15
36.	1.0000	1.5219	236.65	36	36	880	52	36	196.85

Table 3. Cyclic structures : boiling temperature and topological indices.

No.	T_B	M_1	N_2	w	$\bar{I}_D^E$	$\bar{I}_D^W$	Z	$\bar{I}_Z$	χ	$\bar{I}_\chi$
1.	-32.8	12	3	3	0.0000	1.5850	4	0.8113	1.5000	1.5850
2.	0.7	18	5	8	0.9183	2.5000	6	1.2516	1.8940	1.5000
3.	12.5	16	4	8	0.9183	2.5000	7	1.3788	2.0000	0.0000
4.	20.5	26	8	15	1.0000	3.2402	8	1.2988	2.2072	1.5219
5.	32.6	28	7	16	1.3710	3.2028	9	1.3516	2.3047	1.5219
6.	35.9	22	6	17	1.4855	3.1751	10	1.3610	2.4320	1.3709
7.	36.3	22	6	16	1.3610	3.2028	10	1.3610	2.3940	1.5219
8.	49.3	20	5	15	1.0000	3.2402	11	1.3486	2.5000	0.0000
9.	52.5	32	10	26	1.4295	3.7962	12	1.3250	2.6280	2.2516
10.	56.0	30	9	26	1.4295	3.7962	13	1.3143	2.7072	1.5850
11.	56.8	30	9	27	1.5219	3.7821	14	1.5917	2.7679	1.7925
12.	62.9	30	9	27	1.5219	3.7821	14	1.5917	2.7321	1.0000
13.	58.3	28	8	28	1.5656	3.7710	14	1.2958	2.8047	1.9183
14.	59.0	28	8	28	1.7056	3.7534	14	1.2958	2.7880	0.9183
15.	62.8	28	8	29	1.5219	3.7454	15	1.5628	2.8427	1.7925
16.	64.0	28	8	27	1.5219	3.7821	15	1.5628	2.8047	1.9183
17.	69.2	26	7	31	1.8892	3.7198	16	1.5306	2.9320	1.4592
18.	71.8	26	7	26	1.4295	3.7962	16	1.5306	2.8940	1.4592
19.	70.6	26	7	29	1.7819	3.7454	17	1.6457	2.9320	1.4592
20.	80.7	24	6	27	1.5219	4.0043	18	1.6122	3.0000	0.0000
21.	75.9	40	13	39	1.4937	4.2849	16	1.2718	2.9572	1.3788
22.	82.1	36	11	41	1.5751	4.2715	20	1.5784	3.1507	2.2350
23.	88.7	34	10	43	1.7822	4.2512	24	1.6968	3.3286	1.3788

Table 3. (continued).

No.	T_B	M_1	N_2	w	$\bar{I}_D^E$	$\bar{I}_D^W$	Z	$\bar{I}_Z$	χ	$\bar{I}_\chi$
24.	107.8	34	10	42	1.7608	4.2548	23	1.6668	3.2679	1.8424
25.	87.9	34	10	39	1.4937	4.2849	21	1.5492	3.2072	1.5566
26.	98.0	34	10	44	1.8727	4.2373	23	1.6668	3.2701	1.8424
27.	92.8	32	9	48	2.1106	4.1968	24	1.6403	3.3427	2.1281
28.	92.7	32	9	44	1.8727	4.2373	24	1.6403	3.3047	1.9502
29.	99.7	32	9	41	1.7170	4.2595	23	1.5920	3.2880	1.3788
30.	113.0	30	8	48	2.1106	4.1968	27	1.6709	3.4320	1.4488
31.	103.7	30	8	43	1.8375	4.2398	27	1.6709	3.4320	1.4488
32.	101.1	30	8	42	1.7608	4.2548	26	1.6479	3.3940	1.3788
33.	118.9	28	7	42	1.5850	4.2675	29	1.6647	3.5000	0.0000
34.	104.0	44	14	59	1.8179	4.6744	28	1.6319	3.5179	1.8113
35.	113.7	40	12	56	1.5567	4.6995	32	1.6359	3.6280	2.5000
36.	121.5	38	11	59	1.8179	4.6744	37	1.7850	3.7679	1.8113
37.	119.8	38	11	59	1.8179	4.6744	34	1.6320	3.7072	1.5000
38.	116.4	38	11	58	1.7340	4.6849	36	1.7806	3.7154	1.9056
39.	119.3	36	10	69	2.1924	4.9524	37	1.6344	3.7880	1.5000
40.	126.4	36	10	62	1.9242	4.6553	38	1.6397	3.8047	1.9056
41.	128.1	36	10	61	1.8922	4.6638	40	1.7700	3.8427	2.1556
42.	126.5	36	10	60	1.8352	4.6729	39	1.7697	3.8427	1.9056
43.	122.3	36	10	61	1.8922	4.6638	37	1.6344	3.7880	1.5000
44.	121.8	36	10	62	1.9906	4.6494	38	1.7669	3.7880	1.5000
45.	130.9	34	9	67	2.1595	4.6184	43	1.7515	3.9320	1.4056
46.	131.8	34	9	64	2.0597	4.6423	44	1.8228	3.9320	1.4056
47.	134.0	34	9	61	1.8410	4.6718	42	1.7538	3.8490	1.2988
48.	151.1	32	8	64	1.9502	4.6556	47	1.8006	4.0000	0.0000

Table 3. (continued)

No.	x_1	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$	ε	RCI	DRCI	MCI	RGI	DRGI
1.	2.0000	1.5850	0.0000	52.8	9	9	27	9	9
2.	2.1701	1.5000	1.5000	78.7	10	6	42	10	6
3.	2.0000	1.0000	0.0000	80.8	16	16	64	16	16
4.	2.3429	1.3729	1.5219	104.2	17	9	95	17	9
5.	2.3028	1.5219	1.5219	106.8	13	9	88	9	9
6.	2.2143	1.5219	1.9219	108.1	13	7	76	11	7
7.	2.1358	0.9709	1.9219	108.1	13	7	71	11	7
8.	2.0000	1.5219	0.0000	109.8	25	25	125	25	25
9.	2.4458	1.2516	2.2516	134.1	18	8	123	18	8
10.	2.2882	0.9183	1.9183	135.4	18	14	143	18	10
11.	2.3788	1.4592	2.2516	135.4	20	8	118	18	8
12.	2.4142	1.4592	1.0000	136.6	18	18	189	18	18
13.	2.2784	1.4592	1.9583	138.0	20	12	164	20	12
14.	2.2361	0.9183	1.5850	138.0	12	12	164	20	12
15.	2.3342	1.4592	2.5850	138.0	14	8	118	14	8
16.	2.2470	1.0000	1.5850	138.0	20	12	164	20	12
17.	2.2283	1.4592	2.2516	139.3	14	8	123	14	8
18.	2.1149	1.4592	1.9183	139.3	18	10	143	14	10
19.	2.1753	1.0000	2.2516	139.3	14	12	138	14	12
20.	2.0000	1.0000	0.0000	140.6	36	36	216	36	36
21.	2.5616	1.1488	1.3788	162.8	25	21	286	21	21
22.	2.4309	1.3788	2.5216	166.7	29	11	221	21	11
23.	2.4142	1.4488	1.9502	168.0	21	13	252	21	13
24.	2.3244	0.9852	2.5216	168.0	21	13	197	21	13
25.	2.2562	1.3788	1.9502	168.0	25	13	252	21	13
26.	2.4383	1.3788	2.2359	169.2	19	11	209	19	11
27.	2.3429	1.3788	2.8074	170.6	17	7	140	15	7
28.	2.2361	0.9852	2.2359	170.6	19	15	218	19	11
29.	2.1987	1.4488	1.9502	170.6	21	13	252	21	13
30.	2.1889	0.9852	2.5216	171.9	17	9	173	15	9
31.	2.1515	1.4488	2.2359	171.9	19	11	209	19	11
32.	2.1010	0.9852	2.2359	171.9	29	11	204	15	11
33.	2.0000	1.4488	0.0000	173.2	49	49	343	49	49

Table 3. (continued)

No.	x_1	I_{CHR}	I_{ORB}	ε	RCI	DRCI	MCI	RGI	DRGI
34.	2.5831	1.2988	2.7500	196.6	26	10	264	26	10
35.	2.3371	1.2988	2.7500	200.5	40	10	264	26	10
36.	2.2922	1.4056	2.5000	201.8	26	12	292	26	12
37.	2.2361	0.9544	2.2500	201.8	34	18	340	22	14
38.	2.2904	1.4056	2.2500	203.1	30	14	343	26	14
39.	2.2143	0.9544	2.5000	204.4	22	18	312	22	12
40.	2.2105	1.4056	2.2500	204.4	26	14	361	26	14
41.	2.2427	1.4056	3.0000	204.4	26	8	204	26	8
42.	2.1935	1.0000	2.0000	204.4	32	16	376	24	16
43.	2.1753	0.9544	2.2500	204.4	32	18	350	22	14
44.	2.1701	1.0000	1.5000	204.4	24	24	404	40	24
45.	2.1648	1.4056	2.5000	205.7	22	12	303	20	12
46.	2.1358	1.0000	2.5000	205.7	22	16	335	20	12
47.	2.0912	1.4056	2.2500	205.7	34	14	340	18	14
48.	2.0000	1.0000	0.0000	207.1	64	64	512	64	64

Table 4. Alkanes : intercorrelation matrix

	B	C	M_1	Q	C'	Q'	M_2	$\bar{I}_D^E$	W	Z
B	1.00									
C	0.94	1.00								
M_1	0.91	0.73	1.00							
Q	0.89	0.95	0.73	1.00						
C'	0.34	0.57	0.04	0.59	1.00					
Q'	0.11	0.33	0.13	0.43	0.93	1.00				
M_2	0.96	0.84	0.98	0.86	0.22	0.04	1.00			
$\bar{I}_D^E$	0.03	0.29	0.39	0.32	0.81	0.82	0.18	1.00		
W	0.53	0.21	0.80	0.19	0.41	0.49	0.65	0.81	1.00	
Z	0.34	0.07	0.68	0.02	0.48	0.53	0.51	0.81	0.96	1.00
$\bar{I}_D^W$	0.72	0.45	0.92	0.42	0.26	0.40	0.82	0.68	0.93	0.86
$\bar{I}_Z$	0.12	0.15	0.39	0.23	0.72	0.80	0.21	0.80	0.68	0.78
χ	0.51	0.19	0.78	0.14	0.49	0.58	0.63	0.84	0.98	0.96
x_1	0.94	0.86	0.93	0.88	0.32	0.13	0.96	0.06	0.53	0.41
$\bar{I}_C$	0.13	0.42	0.23	0.43	0.76	0.73	0.43	0.92	0.76	0.70
$\bar{I}_{CHR}$	0.06	0.08	0.15	0.21	0.57	0.71	0.05	0.49	0.33	0.41
$\bar{I}_{ORB}$	0.14	0.10	0.42	0.06	0.49	0.50	0.29	0.69	0.62	0.63
$\bar{I}_\chi$	0.27	0.08	0.48	0.13	0.43	0.49	0.40	0.53	0.52	0.50
$\mathcal{E}$	0.67	0.37	0.89	0.34	0.33	0.45	0.77	0.73	0.97	0.92
RCI	0.98	0.92	0.91	0.88	0.31	0.09	0.96	0.05	0.54	0.41
DRCI	0.65	0.66	0.52	0.59	0.32	0.16	0.58	0.09	0.26	0.15
MCI	0.76	0.56	0.86	0.49	0.10	0.26	0.79	0.47	0.82	0.75
RGI	0.96	0.89	0.90	0.85	0.29	0.08	0.94	0.06	0.55	0.42
DRGI	0.65	0.65	0.52	0.58	0.31	0.15	0.57	0.08	0.27	0.15

Table 4 (continued)

	$\bar{I}_D^W$	$\bar{I}_Z$	χ	x_1	$\bar{I}_C$	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$
B							
C							
M_1							
Q							
C'							
Q'							
N_2							
$\bar{I}_D^E$							
W							
Z							
$\bar{I}_D^W$	1.00						
$\bar{I}_Z$	0.63	1.00					
χ	0.95	0.78	1.00				
x_1	0.75	0.19	0.54	1.00			
$\bar{I}_C$	0.53	0.76	0.71	0.05	1.00		
$\bar{I}_{CHR}$	0.31	0.79	0.43	0.03	0.45	1.00	
$\bar{I}_{ORB}$	0.58	0.64	0.67	0.27	0.80	0.31	1.00
$\bar{I}_\chi$	0.55	0.59	0.58	0.39	0.58	0.35	0.86
ε	0.99	0.67	0.98	0.68	0.58	0.34	0.62
RCI	0.72	0.11	0.52	0.92	0.13	0.06	0.11
DRCI	0.38	0.11	0.22	0.52	0.37	0.01	0.48
MCI	0.86	0.44	0.79	0.69	0.21	0.25	0.14
RGI	0.72	0.12	0.52	0.90	0.17	0.02	0.06
DRGI	0.37	0.11	0.22	0.51	0.36	0.01	0.48

Table 4 (continued)

	$\bar{I}_\chi$	ξ	RCI	DRCI	MCI	RGI	DRGI
B							
C							
M_1							
Q							
C'							
Q'							
N_2							
$\bar{I}_D^E$							
W							
Z							
$\bar{I}_D^W$							
$\bar{I}_Z$							
χ							
x_1							
$\bar{I}_C$							
$\bar{I}_{CHR}$							
$\bar{I}_{ORB}$							
$\bar{I}_\chi$	1.00						
ξ	0.57	1.00					
RCI	0.25	0.67	1.00				
DRCI	0.37	0.33	0.70	1.00			
MCI	0.21	0.86	0.79	0.71	1.00		
RGI	0.21	0.68	0.97	0.75	0.82	1.00	
DRGI	0.36	0.33	0.70	0.98	0.54	0.74	1.00

Table 5. Alkylbenzenes : intercorrelation matrix

	M_1	N_2	w	$\bar{I}_D^E$	$\bar{I}_D^W$	z	I_Z	χ	$\bar{I}_\chi$	x_1
M_1	1.00									
N_2	0.98	1.00								
w	0.88	0.80	1.00							
$\bar{I}_D^E$	0.61	0.49	0.87	1.00						
$\bar{I}_D^W$	0.97	0.93	0.94	0.70	1.00					
z	0.76	0.65	0.95	0.85	0.85	1.00				
$\bar{I}_Z$	0.62	0.53	0.77	0.74	0.73	0.83	1.00			
χ	0.89	0.81	0.99	0.86	0.97	0.94	0.82	1.00		
$\bar{I}_\chi$	0.59	0.58	0.45	0.32	0.61	0.38	0.53	0.12	1.00	
x_1	0.91	0.95	0.62	0.28	0.83	0.49	0.46	0.67	0.67	1.00
$\bar{I}_{CHR}$	0.08	0.13	0.06	0.15	0.03	0.19	0.57	0.08	0.20	0.11
$\bar{I}_{ORB}$	0.48	0.41	0.57	0.63	0.59	0.52	0.51	0.61	0.67	0.36
ε	0.93	0.86	0.99	0.83	0.98	0.92	0.77	0.99	0.54	0.72
RCI	0.30	0.39	0.02	0.42	0.16	0.01	0.15	0.03	0.02	0.49
DRCI	0.10	0.06	0.12	0.25	0.18	0.12	0.24	0.18	0.59	0.11
MCI	0.70	0.68	0.67	0.45	0.67	0.61	0.44	0.64	0.12	0.57
RGI	0.45	0.48	0.32	0.05	0.34	0.28	0.25	0.30	0.02	0.46
DRGI	0.16	0.13	0.17	0.26	0.24	0.15	0.24	0.30	0.60	0.17

Table 5 (continued)

	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$	ε	RCI	DRCI	MCI	RGI	DRGI
M_1								
N_2								
w								
$\bar{I}_D^E$								
$\bar{I}_D^W$								
z								
$\bar{I}_z$								
χ								
$\bar{I}_\chi$								
x_1								
$\bar{I}_{CHR}$	1.00							
$\bar{I}_{ORB}$	0.08	1.00						
ε	0.02	0.59	1.00					
RCI	0.34	0.32	0.09	1.00				
DRCI	0.09	0.77	0.16	0.34	1.00			
MCI	0.07	0.11	0.68	0.32	0.51	1.00		
RGI	0.08	0.34	0.34	0.37	0.61	0.62	1.00	
DRGI	0.06	0.84	0.21	0.26	0.94	0.46	0.62	1.00

Table 6. Cyclic structures : intercorrelation matrix

	M_1	N_2	w	$\bar{I}_D^E$	$\bar{I}_D^W$	z	$\bar{I}_z$	χ	$\bar{I}_\chi$
M_1	1.00								
N_2	0.97	1.00							
w	0.84	0.71	1.00						
$\bar{I}_D^E$	0.72	0.60	0.81	1.00					
$\bar{I}_D^W$	0.91	0.80	0.93	0.87	1.00				
z	0.71	0.54	0.96	0.73	0.86	1.00			
$\bar{I}_z$	0.66	0.51	0.81	0.83	0.85	0.82	1.00		
χ	0.81	0.67	0.98	0.85	0.96	0.96	0.88	1.00	
$\bar{I}_\chi$	0.45	0.52	0.23	0.21	0.22	0.09	0.57	0.15	1.00
x_1	0.56	0.71	0.10	0.20	0.24	0.12	0.39	0.03	0.63
$\bar{I}_{CHR}$	0.17	0.13	0.25	0.32	0.27	0.23	0.67	0.25	0.13
$\bar{I}_{ORB}$	0.61	0.61	0.48	0.60	0.52	0.34	0.57	0.45	0.82
ξ	0.88	0.75	0.98	0.84	0.98	0.95	0.75	0.99	0.22
RCI	0.44	0.33	0.60	0.30	0.58	0.64	0.18	0.62	0.32
DRCI	0.04	0.06	0.24	0.10	0.35	0.35	0.27	0.31	0.71
MCI	0.72	0.59	0.87	0.62	0.89	0.89	0.48	0.88	0.09
RGI	0.33	0.23	0.48	0.28	0.56	0.55	0.30	0.54	0.12
DRGI	0.01	0.09	0.20	0.06	0.21	0.31	0.19	0.24	0.50

Table 6 (continued)

	x_1	$\bar{I}_{CHR}$	$\bar{I}_{ORB}$	ε	RCI	DRCI	MCI	RGI	DRGI
M_1									
N_2									
w									
$\bar{I}_D^E$									
$\bar{I}_D^W$									
z									
$\bar{I}_z$									
χ									
$\bar{I}_\chi$									
x_1	1.00								
$\bar{I}_{CHR}$	0.16	1.00							
$\bar{I}_{ORB}$	0.55	0.02	1.00						
ε	0.14	0.25	0.49	1.00					
RCI	0.23	0.18	0.22	0.45	1.00				
DRCI	0.43	0.25	0.64	0.51	0.79	1.00			
MCI	0.06	0.28	0.09	0.70	0.78	0.59	1.00		
RGI	0.24	0.20	0.37	0.51	0.86	0.89	0.74	1.00	
DRGI	0.43	0.18	0.66	0.22	0.79	0.99	0.55	0.89	1.00

Table 7A. Strong intercorrelations among topological indices[a)]

Eqn.no.	T_i	T_j	a	b	r	s	F	Obs.
1-a	M_1	N_2	5.787	2.895	0.98	1.43	331.23	A
b	"	"	6.552	3.036	0.98	0.84	641.38	B
c	"	"	5.599	2.897	0.97	1.54	373.50	C
2-a	M_1	$\bar{I}_D^W$	-14.585	9.689	0.92	2.52	95.88	A
b	"	"	-32.275	14.591	0.97	1.26	280.09	B
c	"	"	-3.896	8.579	0.91	2.74	102.42	C
3-a	N_2	x_1	-21.503	14.158	0.96	0.58	224.04	A
b	"	"	-46.010	26.014	0.95	0.54	151.63	B
c	"	"	-15.673	10.885	0.71	1.52	23.09	C
4-a	N_2	$\bar{I}_D^W$	-5.141	2.895	0.82	1.26	34.23	A
b	"	"	-11.312	4.517	0.93	0.66	97.40	B
c	"	"	-1.588	2.542	0.80	1.30	40.14	C
5-a	W	Z	6.008	2.383	0.96	5.766	208.34	A
b	"	"	29.123	0.905	0.95	7.856	167.11	B
c	"	"	5.021	1.485	0.96	4.81	298.68	C
6-a	W	$\bar{I}_D^W$	-81.356	31.717	0.93	7.59	113.25	A
b	"	"	-256.838	69.951	0.94	8.54	138.80	B
c	"	"	-60.096	24.749	0.93	6.67	144.30	C
7-a	W	χ	-61.324	55.305	0.98	4.67	326.75	A
b	"	"	-152.671	56.872	0.99	4.17	635.35	B
c	"	"	-52.394	29.337	0.98	4.05	428.71	C
8-a	W	ε	-41.980	0.516	0.97	4.83	304.54	A
b	"	"	-80.365	0.815	0.99	4.07	678.64	B
c	"	"	31.948	0.449	0.98	3.32	652.15	C
9-a	$\bar{I}_D^W$	χ	0.957	1.011	0.95	0.19	157.07	A
b	"	"	1.759	0.750	0.97	0.09	233.60	B
c	"	"	0.623	1.086	0.96	0.19	266.25	C
10-a	$\bar{I}_D^W$	ε	1.404	0.015	0.99	0.10	602.31	A
b	"	"	2.678	0.011	0.98	0.08	443.99	B
c	"	"	1.363	0.017	0.98	0.15	429.87	C
11-a	Z	χ	-25.708	14.019	0.96	2.39	197.40	A
b	"	"	-176.249	57.100	0.94	9.13	134.57	B
c	"	"	-35.295	18.683	0.96	3.46	238.06	C

Table 7A. (continued)

Eqn.no.	T_i	T_j	a	b	r	s	F	Obs.
12-a	Z	ξ	-16.456	o.196	o.92	3.37	9o.26	A
b	"	"	-98.752	o.8oo	o.92	1o.8o	91.33	B
c	"	"	-21.15o	o.279	o.94	4.o1	171.98	C
13-a	%	ξ	o.6o3	o.o14	o.98	o.123	361.83	A
b	"	"	1.3o2	o.o14	o.99	o.o6o	1o65.99	B
c	"	"	o.741	o.o15	o.99	o.o8	1163.32	C
14-a	DRCI	DRGI	o.472	o.936	o.98	1.178	439.75	A
b	"	"	2.552	o.922	o.94	2.34	114.24	B
c	"	"	o.695	o.989	o.99	1.47	1116.14	C

a) Eqns. listed in table were computed for alkanes (A), alkylbenzenes (B), and cyclic structures (C).

Table 7B. Correlation coefficients r between topological indices.

$r(T_i,T_j)$	Alkanes	Alkylbenzenes	Cyclic structures
r(RCI, RGI)	0.97	o.37	o.86
$r(N_2$, RGI)	o.94	o.48	o.23
$r(M_1$, Z_1)	o.93	o.91	o.56
$r(M_1$, RCI)	o.91	o.3o	o.44
$r(M_1$ RGI)	o.9o	o.45	o.33

Table 7 C. Correlation coefficients r between topological indices for alkanes.

$r(T_i,T_j)$	Octane isomers(ref.3)	C_4-C_8 alkane isomers (this paper)
r(B,Q')	o.9o	o.11
$r(B,N_2)$	o.9o	o.96
$r(B,I_b^{\xi})$	o.93	o.o3
r(B, %)	o.93	o.51
$r(C,M_1)$	o.9o	o.73
$r(N_2,w)$	o.85	o.65
$r(N_2,Z)$	o.86	o.51
r(w, %)	o.81	o.98

Table 8. Topological branching equation

T_i	a	b	c	d	r	s	F	r(NCAT)	r(NBP)	r(NSC)
B	-2.417	2.141	-1.497	6.187	0.997	1.461	169.616	0.703	0.757	0.919
C	-0.861	0.062	-0.987	3.235	0.958	0.784	89.964	0.429	0.723	0.948
Q	-	-	-	-	-	-	-	0.392	0.656	0.960
M_1	-	-	-	-	-	-	-	0.917	0.628	0.753
$\bar{I}_D^w$	0.661	0.500	0.025	0.033	0.993	0.075	536.969	0.992	0.467	0.471
χ	-0.189	0.517	0.078	-0.213	0.998	0.032	2.691.417	0.965	0.293	0.211
x_1	1.482	0.054	0.066	0.145	0.969	0.037	122.419	0.723	0.684	0.881
$\bar{I}_C$	0.181	0.246	0.034	-0.291	0.905	0.141	36.020	0.548	-0.237	-0.393
ξ	-49.293	33.244	2.646	-3.904	0.999	0.898	15535.449	0.998	0.437	0.405
RCI	-2.488	2.193	-1.898	5.585	0.949	2.002	71.887	0.711	0.704	0.872
w	-69.608	18.333	1.564	-5.875	0.983	3.908	222.927	0.960	0.311	0.250
Z	-27.704	7.369	1.730	-4.386	0.963	2.291	101.405	0.894	0.208	0.094

Table 9. Alkanes : correlation of boilong temperature with topological indices

T_i	a	b	r	s	F
B	21.538	3.126	0.595	29.089	9.309
C	72.555	3.948	0.294	34.589	1.607
M_1	-35.620	4.684	0.840	19.634	40.749
Q	73.887	6.356	0.247	35.069	1.101
C'	104.574	-58.372	0.426	32.747	3.759
Q'	105.802	-88.160	0.549	30.243	7.339
N_2	4.998	11.633	0.703	25.748	16.578
$\bar{I}_D^E$	-64.536	77.905	0.789	22.214	28.112
W	1.164	1.650	0.957	10.466	186.340
Z	10.793	3.947	0.924	13.845	99.134
$\bar{I}_D^W$	-153.381	57.175	0.975	8.009	330.034
$\bar{I}_Z$	-75.686	105.766	0.763	23.385	23.709
χ	-111.221	61.752	0.989	5.264	786.402
x_1	-219.785	152.678	0.626	28.236	10.928
$\bar{I}_C$	-18.699	70.883	0.647	27.580	12.266
$\bar{I}_{CHR}$	-156.181	253.712	0.450	32.322	4.309
$\bar{I}_{ORB}$	-12.334	37.385	0.636	27.924	11.550

Table 9. Alkanes : correlation of boiling temperature with topological indices (continued)

T_i	a	b	r	s	F
$\overline{I}_\chi$	33.699	36.782	0.582	29.419	8.723
$\mathcal{E}$	-77.114	0.902	0.986	6.052	590.767
RCI	18.237	3.382	0.602	28.887	9.677
DRCI	62.374	1.698	0.287	34.668	1.522
MCI	18.047	0.270	0.824	20.509	35.925
RGI	18.728	3.460	0.605	28.816	9.810
DRGI	62.950	1.651	0.284	34.697	1.491

Table 10. Alkylbenzenes : correlation of boilong temperature with topological indices

T_i	a	b	r	s	F
M_1	-21.412	4.533	0.955	7.461	172.316
N_2	11.400	13.495	0.925	9.586	97.864
w	84.906	0.848	0.881	11.962	56.945
$\bar{I}_D^E$	6.846	75.559	0.647	19.252	11.853
$\bar{I}_D^w$	-53.147	48.349	0.901	11.055	76.690
Z	106.776	0.812	0.837	13.828	38.460
$\bar{I}_Z$	-161.651	179.293	0.729	17.264	18.761
χ	-54.396	50.260	0.909	10.505	78.730
$\bar{I}_\chi$	110.847	35.616	0.591	20.356	8.862
x_1	169.422	0.065	0.095	25.123	0.151
$\bar{I}_{CHR}$	169.425	0.148	0.094	25.126	0.146
$\bar{I}_{ORB}$	125.474	17.470	0.499	21.876	5.459
ε	7.964	0.731	0.920	9.904	90.642
RCI	134.343	1.114	0.289	24.160	1.505
DRCI	180.004	-0.571	0.149	24.956	0.375
MCI	119.839	0.101	0.644	19.301	11.711
DRGI	130.149	1.310	0.395	23.185	3.051
DRGI	182.160	-0.750	0.198	24.738	0.673

Table 11. Cycloalkanes : correlation of boiling temperatures with topological indices

T_i	a	b	r	s	F
M_1	-64.662	4.853	0.790	24.306	37.477
N_2	-17.329	11.733	0.641	30.471	15.664
w	1.803	2.078	0.951	12.319	210.997
$\bar{I}_D^E$	-58.060	87.376	0.852	20.802	59.387
$\bar{I}_D^W$	-139.586	55.521	0.955	11.831	230.664
Z	10.493	3.160	0.939	13.664	167.289
$\bar{I}_Z$	-194.094	178.717	0.891	18.014	86.696
χ	-120.479	65.231	0.991	5.167	1304.910
$\bar{I}_\chi$	76.169	5.565	0.083	39.547	0.157
x_1	80.038	1.934	0.007	39.683	0.001
$\bar{I}_{CHR}$	143.400	-47.130	0.268	38.229	1.745
$\bar{I}_{ORB}$	48.121	19.393	0.401	36.356	4.307
ε	-71.235	0.975	0.976	8.583	458.552
RCI	24.426	2.594	0.658	29.878	17.194
DRCI	63.916	1.380	0.363	36.973	3.420
MCI	14.366	0.325	0.877	19.054	75.101
RGI	34.758	2.341	0.571	32.564	10.915
DRGI	66.398	1.259	0.332	37.440	2.779

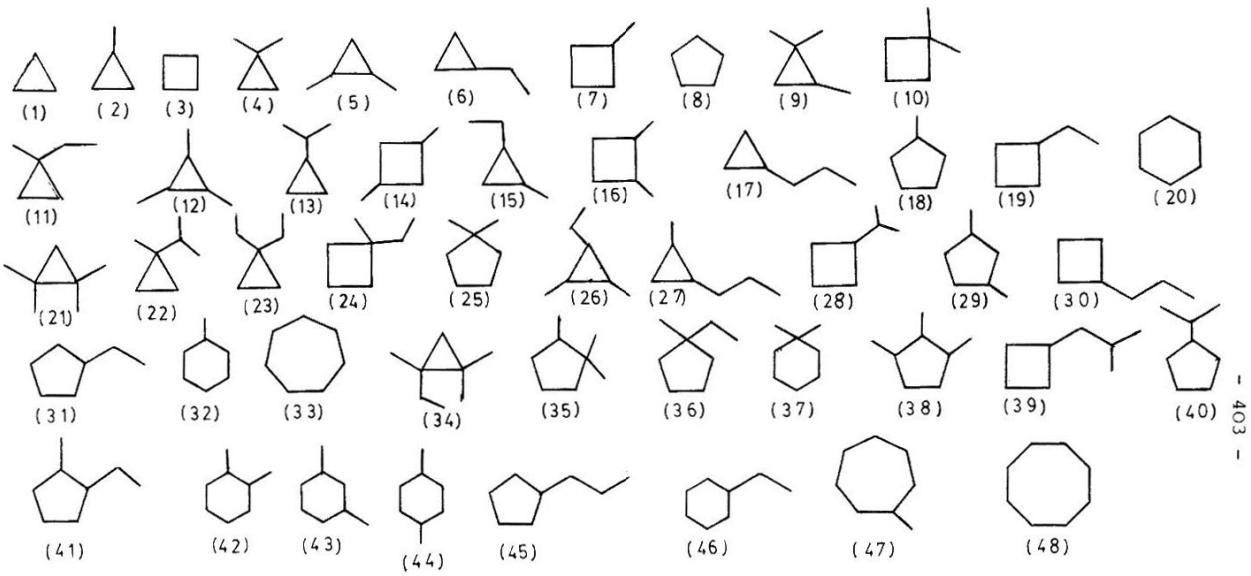


Figure 1. Cyclic structures (the index corresponds to Table 3).

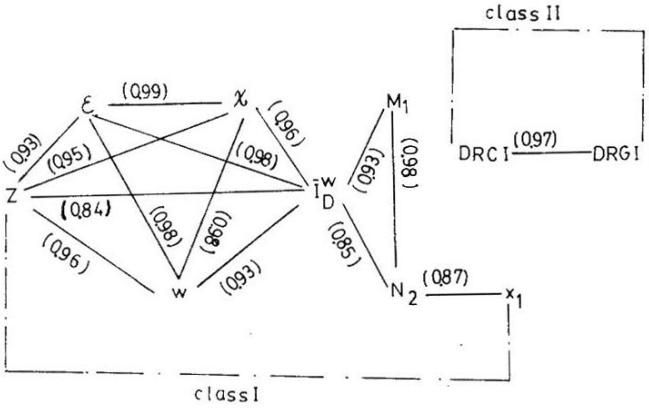


Figure 2. Graph illustrating the strongest intercorrelations among topological indices (the figure in brackets represent the average value of the corresponding correlation coefficients obtained in the three studied series).

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