

TOPOLOGICAL INDICES BASED ON TOPOLOGICAL DISTANCES IN MOLECULAR GRAPHS

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Abstract - Three new distance-based topological indices are described; two of them, D and D_1 (mean distance topological indices, for any graphs, and for acyclic graphs, respectively) have a modest discriminating ability but may be useful for correlations, e. g. with octane numbers. The third index, J (average distance sum connectivity) is the least degenerate single topological index proposed till now. The properties of this promising index J are discussed in more detail.

INTRODUCTION

Topological indices (TI's) are numerical values associated with chemical constitutions for the purpose of correlating chemical structure with various properties: physical properties (boiling points, molar heats of formation and other thermodynamic data), chemical reactivity (octane numbers and other reactivity data) or biological activity. Especially for the latter purpose, namely quantitative structure-activity relationships (QSAR), topological indices seem to hold good promise.

Indeed, according to statistical data, for one year (1978) the cost of pharmaceutical research amounted to 2000 million U. S. dollars, i. e. to 40 million dollars for one product put on the market selected from 4000 tested substances (ref. 1). Any method helping investigators to know which structures are worthy of being synthesized and tested, and which are not, results in enormous savings. Here is one of the main potential uses of TI's, and this explains partly the interest for developing new, better, TI's during the past recent years.

Topological indices have been reviewed repeatedly during the last six years (2-10) in papers, reviews, books or book chapters (some of these are in press). Hence in the present paper the review background will be restricted to a minimum, so as to allow the reader to follow the definition of new distance-based TI's, and to have an overview of their potential usefulness in comparison with previously known topological indices.

GRAPH-THEORETICAL DEFINITIONS (ref. 11)

A constitutional (molecular) graph is the hydrogen-depleted graph whose points (vertices) symbolize atoms, and whose lines (edges) represent covalent bonds. We shall examine only organic structures, assuming for simplicity the vertices to be carbon atoms (therefore an edge represents a pair of shared electrons). If multiple (double or triple) bonds are present, the graph is called a multigraph. We shall neither include in the present discussion electron-deficient compounds where the above correspondence between shared electron pairs and edges no longer holds, nor make any use of directed graphs. Since a graph represents a molecule, all graphs which will be discussed here will be connected graphs, i. e. there will exist successive edges (paths) connecting any two vertices in the graph. The (topological) distance between two vertices is the number of edges in the shortest path between these vertices. Two vertices at distance 1 are called adjacent vertices.

The adjacency matrix \underline{A} of a graph consists of Kronecker δ entries $a_{ij} = 1$ for adjacent vertices, and $a_{ij} = a_{ji} = 0$ otherwise. The distance matrix \underline{D} has as entries d_{ij} the distance between vertices i and j ; the diagonal entries (0) and those for adjacent vertices (1) are the same in \underline{A} and in \underline{D} ,

but all the other zeroes in \underline{A} are replaced in \underline{D} by integers larger than one. The multigraph distance matrix \underline{M} (ref. 12) has fractional entries, resulted from the convention that the topological distance of two adjacent vertices i, j whose bond order is b , is assumed to be $d_{ij} = 1/b$. All these matrices \underline{A} , \underline{D} and \underline{M} characterize completely a graph, and are square symmetrical with respect to the main diagonal.

Graph invariants are properties which do not depend on the arbitrary labeling of vertices. The characteristic polynomial or its eigenvalues are such invariants, and are obtained from \underline{A} by placing x 's on the main diagonal and equating the resulting determinant to zero. Two main invariants for each vertex play a leading part in deriving TI's, namely the vertex degree v_i , the number of lines meeting at vertex i , equal to the sum of entries for the i -th row or column in \underline{A} , and the distance sum or distance degree s_i which is the analogous sum of entries in \underline{D} (or in \underline{M} for multigraphs):

$$v_i = \sum_j a_{ij}$$

$$s_i = \sum_j d_{ij}$$

CLASSIFICATION AND BRIEF REVIEW OF TOPOLOGICAL INDICES

Depending on how a molecular graph is converted into a numerical value, one may classify topological indices according to the following criteria:

I. The numerical basis is provided by:

- the adjacency matrix \underline{A} , or
- the distance matrices \underline{D} (or \underline{M} for multigraphs).

In turn, each of these cases may be subdivided into two groups, according to whether the matrix is processed (i) by means of summing row/columnwise (leading to vertex degrees or to distance sums), or (ii) by means of solving the matrix like a determinant (leading to polynomials or eigenvalues).

II. The above basis set is converted into a TI by operations which:

- (a) do not depend on the adjacencies of the vertex being examined (so-called "inventory" or "book-keeping" operations involving separately the entries for each vertex in one of the matrices);
- (b) depend on the adjacencies or on the whole configuration (so-called "structural" operations involving either several entries of adjacent vertices, or properties such as eigenvalues which depend on the whole matrix). By definition, therefore, (ii) excludes (a).

Many more factors can be taken into account, e. g. whether information theory is, or is not, applied. We shall, however, confine ourselves to the above two criteria, obtaining therefrom Table 1.

TABLE 1. Overview of several TI's according to criteria I and II (for multigraphs, \underline{D} is replaced by \underline{M})

I \ II		(a) Book-keeping operation	(b) Structural operation
$\underline{A}(i)$	Based on vertex degrees	\underline{M} , Zagreb group's TI (13) \underline{F} , First neighbour sum (14,15) \underline{Q} , Quadratic TI (9) \underline{a} \underline{C} , Information content of \underline{F} (16)	χ , Randić's molecular connectivity (6, 17)
$\underline{A}(ii)$	Based on polynomial	-	\underline{Z} , Hosoya's TI (18) x_1 , largest eigenvalue (19) I_Z^1 , information content of \underline{Z} (20)
$\underline{D}(i)$	Based on distance sums	\underline{w} , Wiener's path number (21,22) \underline{B} , centric index (9) \underline{b} I_D^w , inform. content of \underline{w} (20) \underline{c} I_D^E , inform. content of dist.(20)	
$\underline{D}(ii)$	Based on polyn.	-	Hosoya's distance polynomial (23) \underline{d}
Other types		Superindex (linear combination of several TI's (24))	

Notes to Table 1 :

a In addition, normalized and binormalized quadratic indices (9) ;

b In addition, normalized and binormalized centric indices (9) ;

c In addition, mean information content \bar{I} for any informational index I (20) ;

d This distance polynomial, which is not a TI, is believed to characterize graphs up to isomorphism.

It is evident that the distance matrix \underline{D} can be deduced simply from the adjacency matrix, and we have devised a computer program (25) which, being given the adjacencies in graphs or the bond orders b in multigraphs, produces the matrices \underline{A} and \underline{D} (or \underline{M} for multigraphs). Nevertheless, the distance matrices \underline{D} and \underline{M} are richer in information than the adjacency matrix \underline{A} : for instance, the vertex (vertices) with the smallest maximal entry (entries) in \underline{D} or \underline{M} form(s) the classical centre of the respective graph.

One measure of how "poor" is a TI consists in its "degeneracy" : if two or more non-isomorphic graphs have the same TI, the TI is said to be degenerate. It has been recognized from the outset that the simple, book-keeping TI's have a fairly elevated degeneracy. For some time, it was assumed that some structural numerical reduced form of the adjacency matrix might characterize graphs up to isomorphism. It was conjectured that such a form might be the characteristic polynomial or the set of its eigenvalues (26,27), but this conjecture was disproved (28-32) showing that there exist non-isomorphic cospectral graphs which have the same characteristic polynomial.

THREE NEW DISTANCE-BASED TOPOLOGICAL INDICES

Two new book-keeping indices : D and D_1

The distribution of distances i in a graph is indicated by the numbers $2g_i$ of times each distance $i = 1, 2, \dots$ appears in the distance matrix \underline{D} . For instance, the distribution of distances and the distance sums in the three isomers of pentane are indicated in Fig. 1.

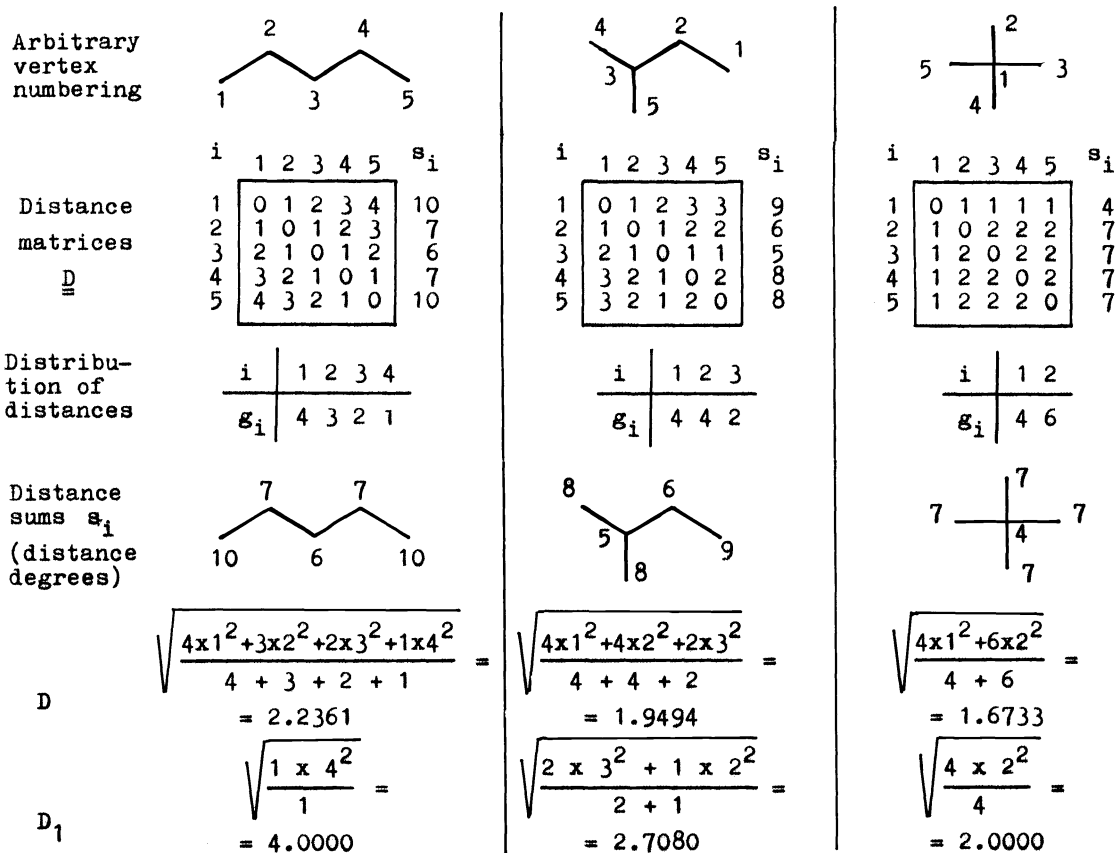


Fig. 1. Calculation of topological indices D and D_1 for pentanes

It is evident that the more branched isomer has a lower average distance sum. After exploring various powers $k = 1$ through 4 in formula (1), we concluded that $k = 2$ gives a convenient TI which we call the mean (square) distance TI and which we denote by D , omitting the exponent ($k = 2$).

$$D^{(k)} = \left(\frac{\sum_i g_i \cdot i^k}{\sum_i g_i} \right)^{1/k} \quad (1)$$

Being of the simple, book-keeping type, $\underline{D}(i)(a)$ -Table 1, this topological index D has a fair discriminating ability, especially for acyclic graphs; however, for polycyclic graphs it has a poorer performance and a higher degeneracy.

For acyclic graphs only, another related TI can be derived by taking into account in formula (1) only distances between endpoints (vertices of degree 1). This TI is called endpoint mean (square) distance TI and is denoted by D_1 . Both D and D_1 decrease with increasing branching, as seen from Fig. 1 and Table 2. The degeneracy of D_1 is a little higher than that of D . Whereas D induces in alkane isomers an ordering similar (but not identical) to that induced by I_D^E , the ordering induced by D_1 resembles that caused by I_D^W . Therefore all these indices, belonging to the same box $\underline{D}(i)(a)$ in Table 1, have comparable performance and degeneracy.

Table 2 presents numerical values for the new TI's (including J which will be discussed in the following §) for all alkanes with 4-8 carbon atoms. In addition, two earlier TI's are included: Randić's molecular connectivity χ (17) and the centric index B (ref. 9) which, despite its high degeneracy, gives a good correlation (ref. 33) with octane numbers. Underlined values indicate degenerate TI's in Table 2. This Table also includes Motor Octane Numbers (MON values), which are known to increase with the branching of the alkane. If one denotes the standard deviation with s , the variance with σ^2 , the correlation coefficient with r , the slope with m , and the intercept with a , then the following linear regressions are obtained from the data of Table 2:

TI	Heptanes ($s = 31.58$; $\sigma^2 = 872.4$)			Octanes ($s = 24.69$; $\sigma^2 = 571.3$)		
	r	m	a	r	m	a
B	0.9876	10.70	-135.44	0.9397	5.57	-63.43
χ	-0.8425	-199.19	709.98	-0.7448	-115.20	491.42
D	-0.9486	-118.45	370.21	-0.9513	-96.65	338.52
D_1	-0.9700	-30.31	182.17	-0.9739	-38.09	221.42
J	0.9140	99.42	-227.71	0.9315	79.70	-184.10

One can see that B , D_1 (and D) have the highest r values, while J (to be introduced in the next §) gives a modest, and χ a poor correlation with MON. What is more, the parameters m and a of the two separate correlations differ less for D_1 (and D) than they do for B , so that the two correlations can be merged into a single one more accurately than for B (where we had to use a weighted indicator variable).

Numerical values of D for cyclic graphs will be presented in Table 4. In conclusion, D_1 has a wider range of variation than D , but its degeneracy is a little higher, and it can be applied only to acyclic systems; both D and D_1 give good correlations with properties such as octane numbers which depend on branching.

A highly discriminating distance-based structural topological index : J

The most conspicuous feature of Table 1 is the blank space left in one box, $\underline{D}(i)(b)$. In a recent publication (12), a new TI belonging to this box was proposed. It is patterned after one of the best TI's known so far, Randić's molecular connectivity χ (χ performed best both for its low degeneracy and for its correlational ability with physical and biochemical properties), but with two differences: (i) the new TI uses distance sums instead of vertex degrees, and (ii) it averages (normalizes) the index against the numbers of edges and cycles. Thus a TI is obtained, which does not vary unpredictably with the number of vertices, edges, or rings. It expresses almost purely the degree of branching (i. e. the "topological shape"). For correlations where the size of the molecule is important, a biparametric correlation may be used, introducing separately the size by means of an appropriate parameter such as the number n of atoms (vertices). Thus the relative weights of the

TABLE 2. Numerical values for TI's of alkanes and Motor Octane Numbers

Alkane	MON	B	χ	D	D_1	J
Butanes						
n-Butane	90.1	8	1.9142	1.8257	3.0000	1.9746
Isobutane	97.6	10	1.7321	1.5811	2.0000	2.3238
Pentanes						
n-Pentane	61.9	9	2.4142	2.2361	4.0000	2.1908
2-Methylbutane	90.3	13	2.2701	1.9494	2.7080	2.5396
2,2-Dimethylpropane	80.2	17	2.0000	1.6733	2.0000	3.0236
Hexanes						
n-Hexane	26.0	12	2.9142	2.6458	5.0000	2.3840
2-Methylpentane	73.5	14	2.7701	2.3664	3.4641	2.6270
3-Methylpentane	74.3	14	2.8081	2.2657	3.3665	2.7540
2,3-Dimethylbutane	94.4	20	2.6427	2.0817	2.7080	2.9935
2,2-Dimethylbutane	93.4	24	2.5607	2.0000	3.3912	3.1685
Heptanes						
n-Heptane	0.0	13	3.4142	3.0551	6.0000	2.4474
2-Methylhexane	46.4	17	3.2701	2.7946	4.2426	2.6784
3-Methylhexane	55.0	17	3.3081	2.6547	4.0825	2.8320
2,4-Dimethylpentane	83.8	21	3.1259	2.5261	3.4641	2.9532
3-Ethylpentane	65.0	19	3.3461	2.5071	4.0000	2.9922
2,3-Dimethylpentane	88.5	21	3.1807	2.3905	3.2404	3.1440
2,2-Dimethylpentane	95.6	21	3.0607	2.4103	3.1623	3.1542
3,3-Dimethylpentane	86.6	21	3.1213	2.2678	2.7080	3.3606
2,2,3-Trimethylbutane	-	29	2.9434	2.0354	2.6458	3.5412
Octanes						
n-Octane	-	16	3.9142	3.4641	7.0000	2.5301
2-Methylheptane	23.8	18	3.7701	3.2238	5.0332	2.7158
3-Methylheptane	35.0	18	3.8081	3.0706	4.8305	2.8620
4-Methylheptane	39.0	18	3.8081	3.0178	4.7610	2.9126
2,5-Dimethylhexane	55.7	24	3.6259	2.9761	4.2426	2.9278
3-Ethylhexane	52.4	22	3.8461	2.8536	4.6904	3.0744
2,4-Dimethylhexane	69.9	24	3.6639	2.8221	3.6742	3.0988
2,2-Dimethylhexane	77.4	24	3.5607	2.8473	3.8079	3.1118
2,3-Dimethylhexane	78.9	24	3.6807	2.7775	3.8297	3.1708
3,4-Dimethylhexane	81.7	24	3.7187	2.6726	3.7417	3.2925
3-Ethyl-2-methylpentane	88.1	26	3.7187	2.6118	3.7417	3.3548
3,3-Dimethylhexane	83.4	24	3.6213	2.6390	3.6286	3.3734
2,2,4-Trimethylpentane	100.0	30	3.4165	2.5912	3.3466	3.3890
2,3,4-Trimethylpentane	95.9	30	3.2500	2.5284	3.2863	3.4642
3-Ethyl-3-methylpentane	88.7	26	3.6280	2.4785	3.5355	3.5832
2,2,3-Trimethylpentane	99.9	30	3.4814	2.4422	3.0984	3.6233
2,3,3-Trimethylpentane	99.4	30	3.5040	2.3905	3.0659	3.6753
2,2,3,3-Tetramethylbutane	-	40	3.5534	2.2039	2.6458	3.9212

TABLE 3. Mean degeneracy of several TI's for all acyclic, monocyclic and bicyclic graphs with n vertices (N, in brackets, is the number of possible graphs with given n). As in ref. (24), for acyclic graphs no restriction was imposed for vertex degrees, but for cyclic graphs these vertex degrees are at most equal to four.

n	(N)	w	Z	\bar{I}_D^W	\bar{I}_Z	\bar{I}_D^E	χ	B	D	D_1	J
Acyclic graphs with vertices of any degree :											
5	(3)	1	1	1	1	1	1	1	1	1	1
6	(5)	1	1	1	1	1	1	1.25	1	1	1
7	(11)	1.22	1	1	1	1	1	1.57	1	1	1
8	(24)	1.15	1.28	1	1	1	1.09	1.85	1	1.04	1
Monocyclic and bicyclic graphs with vertices of degrees 1 - 4 :											
5	(10)	2.5	1.7	2.0	1.4	2.0	1	-	2.0	-	1
6	(29)	3.6	2.6	2.2	1.5	2.4	1.2	-	2.2	-	1
7	(85)	6.0	4.5	2.4	2.2	2.8	1.6	-	...	-	1
8	(250)	10.6	7.7	2.8	2.2	2.5	1.6	-	...	-	1.008

size and shape can be explored.

For each of the adjacent pairs of vertices i, j one computes the product of distance sums $s_i s_j$, and then one obtains the average distance sum connectivity, denoted by J , after formula (2) :

$$J = \frac{q}{\mu + 1} \sum_{i, j \text{ adjac.}} (s_i s_j)^{-1/2} \quad (2)$$

Here the cyclomatic number μ (number of rings in the graph) is $\mu = q - n + 1$, if there are n vertices and q adjacencies in the graph. For multigraphs, instead of \underline{D} one uses \underline{M} ; in simple graphs without multiple bonds, q is the number of edges; in multigraphs, a multiple bond is considered as one adjacency. Numerical values of J for alkanes are presented in Table 2. The alkanes are ordered in Table 2 according to their J values.

The discriminating ability of TI's is expressed by their mean degeneracy, i. e. by the ratio between the number N of graphs with the same number n of vertices, and the number of distinct values for the respective TI. Table 3 demonstrates that J has the lowest degeneracy of all TI's described so far, with the exception of the superindex (24). Since, however, the superindex is a composite TI, one may claim that J is the least degenerate single TI proposed till now.

TABLE 4. Values of D and J for monocyclic six-membered graphs and multigraphs

n	Alkyl group(s)	CYCLOHEXANE		BENZENE
		D	J	J
6	None	1.9494	2.0000	3.0000
7	Methyl	2.1822	2.1229	3.0215
8	Ethyl	2.5355	2.1250	2.8321
	1,2-Dimethyl	2.3299	2.2794	3.1349
	1,3-Dimethyl	2.3830	2.2307	3.0777
	1,4-Dimethyl	2.4495	2.1924	3.0325
9	n-Propyl	2.9439	2.0779	2.6149
	Isopropyl	2.7080	2.2284	2.8483
	1-Ethyl-2-methyl	2.6247	2.2973	3.0065
	1-Ethyl-3-methyl	2.7080	2.2317	2.9369
	1-Ethyl-4-methyl	2.8087	2.1804	2.8816
	1,2,3-Trimethyl	2.4721	2.4017	3.4729
	1,2,4-Trimethyl	2.5604	2.4072	3.1717
	1,3,5-Trimethyl	2.5496	2.3409	3.1657
10	n-Butyl	3.3764	2.0173	2.4265
	Isobutyl	3.1522	2.1313	2.5873
	s-Butyl	3.0000	2.2396	2.7470
	t-Butyl	2.8087	2.3892	2.9661
	1,2-Diethyl	2.8636	2.3401	2.9640
	1,3-Diethyl	3.0000	2.2465	2.8563
	1,4-Diethyl	3.1588	2.1739	2.7973
	1-Methyl-2-n-propyl	3.0000	2.2514	2.8112
	1-Methyl-3-n-propyl	3.0984	2.1848	2.7463
	1-Methyl-4-n-propyl	3.2146	2.1322	2.6938
	1-Isopropyl-2-methyl	2.7809	2.3860	3.0330
	1-Isopropyl-3-methyl	2.8790	2.3199	2.9551
	1-Isopropyl-4-methyl	2.9963	2.2599	2.8938
	1,2-Dimethyl-3-ethyl	2.7528	2.4245	2.1431
	1,2-Dimethyl-4-ethyl	2.8944	2.3300	3.1229
	1,3-Dimethyl-2-ethyl	2.7162	2.4504	3.1695
	1,3-Dimethyl-4-ethyl	2.8597	2.3524	3.0700
	1,3-Dimethyl-5-ethyl	2.8441	2.3474	3.0617
	1,4-Dimethyl-2-ethyl	2.8166	2.3447	3.0907
	1,2,3,4-Tetramethyl	2.6373	2.5159	3.3422
1,2,3,5-Tetramethyl	2.6667	2.4873	3.3106	
1,2,4,5-Tetramethyl	2.7039	2.4620	3.2825	

It is easy to explain why J which is similar to χ is much less degenerate than χ : vertex degrees in organic constitutional hydrogen-depleted graphs vary between 1 and 4, hence all products of two vertex degrees for edges in

Randić's formula leading to χ have one of the ten possible combinations. By contrast, there is no limit to the distance sums, therefore there is an infinity of possible products in formula (2).

Unlike the two preceding new indices, J increases with increasing branching. This may be seen both in Table 2 and in Table 4. The latter Table contains numerical values for D and J in the case of six-membered monocyclic systems with side-chains of 0-4 carbon atoms. For J , two results are presented, with a saturated six-membered ring (bond order $b = 1$ for the C-C bonds), and a benzene ring with delocalized electrons ($b = 1.5$ for the ring bonds).

Hundreds of J values were computed by means of a pocket calculator; a computer program was also developed for this purpose as a development of the previously mentioned program (25). For instance, for the isomeric pentenes, J values are: 3.0249 (1-pentene); 3.2780 (2-pentene); 3.5322 (3-methyl-1-butene); 3.5592 (2-methyl-1-butene); and 3.9290 (2-methyl-2-butene), reflecting both positional and skeletal isomerism.

For an alkane consisting of 2-4 linear branches emerging from a centre, the main program (as applied on a simple TI-51-III calculator) is the following: RCL 1 + 2 = STO 1 + RCL 2 = STO 3 x RCL 2 = \sqrt{x} 1/x = SUM 4 RCL 3 STO 2 - RCL 5 = 1/x Reset. The initial data are input in 1, 2, and 5, while the final value is obtained by RCL 4; this value is then multiplied by the number of branches and by q in order to obtain J . A linear alkane may be either V or U: V-alkane (two branches, one central point): -1 STO 1; $k(k+1)$ STO 2; $k(2k+1)$ STO 5, and $J = 4k \times RCL 4$ (linear alkane with $2k+1$ vertices); U-alkane (two branches, one central bond): 0 STO 1; $4k^2$ STO 2; $2k(4k-1)$ STO 5, and $J = (2 \times RCL 4 + 0.25k^2)(4k-1)$, linear alkane with $4k$ vertices. The same program gives J for branched structures (Y- or X-shaped alkanes): Y-alkane (three branches, one central point): $k-1$ STO 1; $1.5k(k+1)$ STO 2; $0.5k(7k+3)$ STO 5, and $J = 9k \times RCL 4$; X-alkane (four branches, one central point): $2k-1$ STO 1; $2k(k+1)$ STO 2; $k(5k+2)$ STO 5, and $J = 16k \times RCL 4$.

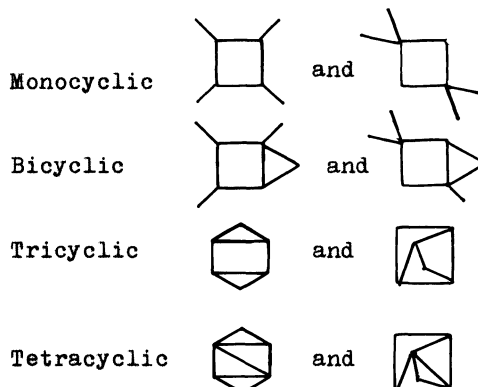
It can be demonstrated that for linear saturated or unsaturated chains of n carbon atoms, the asymptotic J values are those indicated in the last row of Table 5. Similarly, the asymptotic values are: for a Y-alkane, $J = 4.1033 = (18/\sqrt{5})\arctan(\sqrt{5}/4)$; for an X-alkane, $J = 5.1480 = 16\arctan(1/3)$. On the other hand, for highly branched alkanes J increases without limit; thus for graphs with vertices of degrees 4 and 1 we have the series: $F1 = CMe_4$, $F2 = C(CMe_3)_4$, $F3 = C(CtBu_3)_4$, etc.; for graphs with vertices of degrees 3 and 1 we have series $G1 = HCMe_3$; $G2 = HC(CHMe_2)_3$; $G3 = HC(CHiPr_2)_3$, etc. The corresponding J values are presented below:

	1	2	3	4	5
Series F	3.0236	6.3656	12.8513	27.5179	59.6697
Series G	2.3238	3.9835	6.0281	9.1270	14.3308

The degeneracy of J is of two kinds: (i) an apparent one, due to the averaging term $q/(\mu+1)$ in formula (2), among non-isomeric structures, e. g. all $2k$ -membered cycloalkanes have $J = 2$, all localized [4m]annulenes have $J = 8/3$ and all delocalized [4m]annulenes have $J = 3$, irrespective of the ring size; (ii) a true one for isomeric systems: the smallest alkanes with degenerate J are one pair out of the 355 constitutionally isomeric dodecanes; for the smallest mono- and bicyclic systems (shown below) with the same J , $n = 8$; the smallest tri- and tetracyclic systems with degenerate J have six vertices and are also shown below.

TABLE 5. Asymptotic behaviour of J for linear carbon chains C_n

n	U-Alkane	C o n j u g a t e d	
		polyene	polyyne
4	1.9747	2.2731	3.1375
8	2.5301	3.4052	3.8503
12	2.7272	3.6512	4.1167
40	3.0144	4.0206	4.5240
80	3.0777	4.1042	4.6171
160	3.1095	4.1461	4.6486
240	3.1202	4.1543	4.6804
∞	3.1416 = π	4.1888 = $4\pi/3$	4.7124 = $3\pi/2$



In conclusion, index J appears very promising owing to its low degeneracy and to the possibility of taking into account both multiple bonding (as discussed here) and the presence of heteroatoms (to be discussed in a future paper).

The relations among various TI's, their correlational ability and their physical meaning are discussed in several papers (ref. 34).

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