

DESIGN OF TOPOLOGICAL INDICES. PART 2.<sup>1</sup>  
DISTANCE MEASURE CONNECTIVITY INDICES.

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The use of distance measure in defining a highly selective, connectivity-based spectrum of topological indices, denoted by  $DN^k$  is presented. They are obtained by a distance measure method, using a spectrum of fourteen connectivity topological indices. The newly defined topological indices have no degenerate value for a set of 661 alkanes between butane and dodecane. The statistical characteristics and the ordering of structures induced by the values of the indices are also considered.

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A great number of methods from mathematics and computer science have been largely investigated for the elucidation of the causal relationships between chemical structure and physico-chemical properties. Pattern Recognition (PARC) <sup>2</sup> methods are especially useful for the classification of chemical structures into distinct classes on the basis of characteristic features. A set of characteristic features of a chemical structure is considered as an abstract pattern which contains information about physico-chemical properties, chemical reactivity or biological activity of the investigated chemical structure.

We have to mention here that PARC methods try to find relationships between the pattern and a chemical property without using chemical knowledge.

A largely used classification method in PARC is the distance measure in pattern space, briefly described in what follows.

Let  $X(x_1, x_2, \dots, x_n)$ ,  $Y(y_1, y_2, \dots, y_n)$  and  $Z(z_1, z_2, \dots, z_n)$  be three points in an n-dimensional space. Any function  $D(X, Y)$  which satisfies the following relationships:

$$\begin{aligned} D(X, X) &= 0 \\ D(X, Y) &> 0 \quad \text{for } X \neq Y \\ D(X, Y) &= D(Y, X) \\ D(X, Z) + D(Z, Y) &\geq D(X, Y) \end{aligned} \tag{1}$$

has the quality of a distance.

The most frequently used distance measurements form the general Minkowski distance:

$$D_H = \sum_{i=1}^n [(x_i - y_i)^k]^{1/k} \quad (2)$$

For  $k=1$  we obtain the Manhattan distance ("city block distance") in analogy with the shortest distance between two points in a city with rectangular streets:

$$D_{Mh} = \sum_{i=1}^n |x_i - y_i| \quad (3)$$

and  $k=2$  gives the most often used Euclidean distance:

$$D_E = \sum_{i=1}^n (x_i - y_i)^2 \quad (4)$$

Classifications of chemical structures by distance measurements in pattern space were used for the recognition of the structure of molecules from mass spectra<sup>3</sup> and infrared spectra.<sup>4</sup> The distance measure method was also applied in studies concerning aromaticity, photoreactivity, thermal reactivity and intermolecular forces.<sup>5</sup>

Another method used in establishing correlations between structure and physico-chemical properties is to express the bonding topology of the molecular graph by a mathematical expression which may be a matrix, a polynomial or a numerical index.<sup>6-11</sup> Numerical indices developed in this way are called topological indices (TI's).

Although in their origins TI's were developed for the purpose of obtaining correlations with a great variety of physicochemical

properties of chemical substances, namely QSPR (Quantitative Structure-Property Relationships), their range of applications has extended to bibliographical classification of chemical compounds and QSAR (Quantitative Structure-Activity Relationships).

A general problem of topological indices is that they are more or less degenerate, i.e. two or more nonisomorphic structures may lead to the same value for a given topological index. The discriminating ability or structural selectivity of a TI is inversely related to its degeneracy. A study on the structural selectivity of six TI's : Wiener's number  $W$ , the Zagreb group (Gutman, Ruscic, Trinajstic, Wilcox) TI denoted by  $M_1$ , Hosoya's index  $Z$ , Randic's connectivity index  $\chi$ , the information on distance index  $I_D^E$  and Balaban's average distance sum connectivity index  $J$ , reveals that  $J$  has the greatest selectivity.<sup>12</sup> Of course, high selectivity, although strongly desirable, is not sufficient to obtain good results in QSPR and QSAR if the values of indices do not properly reflect structural information in conjunction with the property under investigation.

The Randic connectivity index<sup>8</sup> was defined as:

$$\chi = \sum_m (v_i v_j)^{-1/2} \quad (5)$$

where  $v_i$  and  $v_j$  denote the degrees of the two endpoints of an edge in the molecular graph  $G$ , and the summation is extended over all  $m$  edges.

A generalized connectivity index was suggested by extending the summation in eq. (5) over all possible

connected subgraphs with  $m$  edges of four types : path,  
cluster, path/cluster and chain:<sup>9</sup>

$${}^m X_t = \sum_{j=1}^{n_m} \prod_{i=1}^r (v_i)_j^{-1/2} \quad (6)$$

where  $n_m$  is the number of connected subgraphs of type  $t$  with  $m$  edges and  $r$  is the number of vertices of the subgraph. In the case of path, cluster and path/cluster subgraphs,  $r=m+1$  and for a chain-type subgraph  $r=m$ .

A further extension of the connectivity index was suggested in order to take into account the presence in the molecule of atoms of different chemical nature as well as the presence of single, double, triple and aromatic bonds. The vertex degree  $v_i$  is replaced by the atom connectivity  $\Delta_i^v$ :<sup>10</sup>

$$\Delta_i^v = Z_i^v - H_i \quad (7)$$

where  $Z_i^v$  and  $H_i$  are the number of valence electrons of atom  $i$  and the number of hydrogen atoms attached to this atom, respectively. In order to obtain valence delta-values ( $\Delta_i^v$ ) for second and third level atoms and halogens, a slightly different definition was proposed:<sup>11</sup>

$$\Delta_i^v = \frac{Z_i^v - H_i}{Z_i - Z_i^v} \quad (8)$$

where the significance of  $Z_i^v$  and  $H_i$  is the same as in equation (7) and  $Z_i$  is the count of all electrons of atom  $i$ . The connectivity

index is given by:

$${}^m X_t^v = \sum_{j=1}^{n_m} \prod_{i=1}^r (\Delta_i^v)_j^{-1/2} \quad (9)$$

The generalized connectivity indices have found numerous applications in establishing QSPR for alkanes. Good correlations were obtained for the heat of atomization, heat of formation, boiling point, molar refraction, molar magnetic susceptibilities, heat of vaporization, solubility.<sup>9</sup>

### TOPOLOGICAL INDICES $DN^k$

The mechanism of constructing a TI, considered earlier,<sup>13</sup> was revealed to be a two-stage process, viz. the assignment and the operational stages, respectively. The assignment stage consists in finding a local vertex invariant (LOVI). In the operational stage the LOVI's are mathematically manipulated in order to produce a number which represents the TI. For the generalized connectivity index  ${}^m X_t$ , the LOVI is selected to be the vertex degree and the operational stage consists in a summation over all subgraphs of connectivity contributions of the subgraphs.

We introduce here a new spectrum of highly selective TI's as a result of another operational stage using as the basis of computations a spectrum of connectivity indices  ${}^m X_t$ , based on the method of distance measure; we denote these indices by  $DN^k$ :

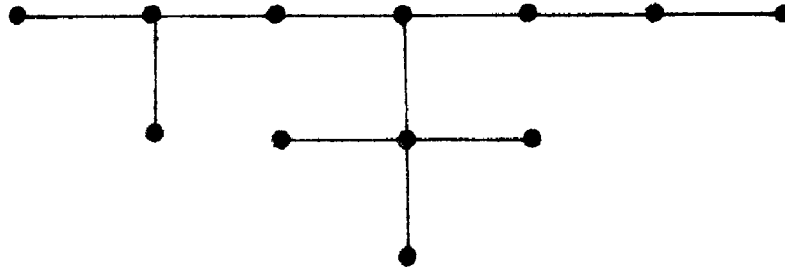
$$DM^k = \sum_{i=1}^{14} \left[ \left( \overset{m}{X}_{t,i} - \overset{m}{X}_{t,r} \right)^k \right]^{1/k} \quad (10)$$

where  $\overset{m}{X}_{t,i}$  and  $\overset{m}{X}_{t,r}$  represents the corresponding connectivity indices of the molecular and reference structure, respectively, and the summation is done over all fourteen connectivity terms up to the sixth order ( $m=6$ ) and  $k=1,3$ . The reference molecular graph is considered to be that of methane, in whose case all  $\overset{m}{X}_{t,r}$  are equal to zero. By its definition, this type of TI is reminiscent of the superindex.<sup>14</sup> In FIGURE 1 is presented the computation of  $DM^k$  TI's for 4-tB-2-M-C<sub>7</sub>.

We have investigated some basic properties of the new TI's  $DM^k$  for a population consisting of 661 alkane isomers between butane and dodecane. The alkane class of chemical compounds was chosen due to the rapidly increasing number of isomers which allows comparisons between isomers with subtle structural differences. The set was limited to dodecane due to the small interest in investigating higher alkane isomers, reflected in the small amount of data on various physico-chemical properties. For the set of 661 alkane isomers no degenerate value was detected.

In TABLE 1 are presented values of TI's  $DM^k$  for the 147 alkane isomers between butane and decane. The abbreviations used in the nomenclature of alkanes are: M=methyl, E=ethyl, P=propyl, iP=iso-propyl, tB=tert-butyl and a linear chain of n carbon atoms is symbolized by C<sub>n</sub>.

Some statistics are given in TABLES 2-6 for the whole set of 661 alkane isomers between butane and dodecane and for the sets of 35



$${}^0\chi = 9.77602 \quad {}^1\chi = 5.37523 \quad {}^2\chi = 5.48117$$

$${}^3\chi_p = 2.61780 \quad {}^3\chi_c = 1.91861 \quad {}^4\chi_p = 1.82191$$

$${}^4\chi_c = 0.28868 \quad {}^4\chi_{pc} = 2.07886 \quad {}^5\chi_p = 1.49367$$

$${}^5\chi_c = 0.43301 \quad {}^5\chi_{pc} = 2.36317 \quad {}^6\chi_p = 0.23570$$

$${}^6\chi_c = 0.14434 \quad {}^3\chi_{pc} = 3.67297$$

$$DH^1 = \sum_{i=1}^{14} \chi_{t,i} = 37.70115$$

$$DH^2 = \sum_{i=1}^{14} [\chi_{t,i}]^{1/2} = 13.94043$$

$$DH^3 = \sum_{i=1}^{14} [\chi_{t,i}]^{1/3} = 11.08072$$

$$DH^4 = \sum_{i=1}^{14} [\chi_{t,i}]^{1/4} = 10.28268$$

$$DH^5 = \sum_{i=1}^{14} [\chi_{t,i}]^{1/5} = 9.99367$$

FIGURE 1. The computation of  $DH^k$  TI's for 4-t8-2-N-C<sub>7</sub>.



TABLE 1. Values of the TI's  $DM^k$  for alkane isomers  $C_4$  through  $C_{10}$ .

No.	Name	$DM^1$	$DM^2$	$DM^3$	$DM^4$	$DM^5$
1	$C_4H_{10}$	6.82843	4.07076	3.63268	3.50180	3.45268
2	$C_4$ 2-M- $C_3$	7.61880	4.37387	3.83417	3.67240	3.61471
3	$C_5H_{12}$	8.94975	5.02701	4.43021	4.24947	4.17977
4	$C_5$ 2-M- $C_4$	9.98960	5.26852	4.59278	4.39928	4.33074
5	2,2-M <sub>2</sub> - $C_3$	12.00000	6.12372	5.12041	4.78246	4.64067
6	$C_6H_{14}$	11.15685	5.99576	5.23310	5.00010	4.90870
7	$C_6$ 2-M- $C_5$	12.37312	6.22647	5.39444	5.14933	5.05843
8	3-M- $C_5$	12.55852	6.24659	5.38987	5.14463	5.05627
9	2,2-M <sub>2</sub> - $C_4$	15.07107	6.86289	5.73880	5.41341	5.29451
10	2,3-M <sub>2</sub> - $C_4$	13.95214	6.62242	5.60300	5.31770	5.21903
11	$C_7H_{16}$	13.42462	6.97257	6.03945	5.75273	5.63891
12	$C_7$ 2-M- $C_6$	14.76562	7.19466	6.19899	5.90056	5.78707
13	3-M- $C_6$	15.08212	7.20870	6.19075	5.89492	5.78480
14	3-E- $C_5$	15.36658	7.25435	6.19705	5.89658	5.78615
15	2,2-M <sub>2</sub> - $C_5$	17.94975	7.81372	6.53066	6.16006	6.02112
16	2,3-M <sub>2</sub> - $C_5$	16.94921	7.57322	6.38401	6.05477	5.93981
17	2,4-M <sub>2</sub> - $C_5$	16.36313	7.54215	6.40512	6.07560	5.95274
18	3,3-M <sub>2</sub> - $C_5$	18.48528	7.88594	6.50882	6.12932	5.99923
19	2,2,3-M <sub>3</sub> - $C_4$	20.54701	8.46943	6.85240	6.37878	6.20511
20	$C_8H_{18}$	15.61028	7.95382	6.84817	6.50676	6.37006
21	$C_8$ 2-M- $C_7$	17.02015	8.16964	7.00646	6.65346	6.51690
22	3-M- $C_7$	17.42935	8.18587	6.99937	6.64828	6.51478
23	4-M- $C_7$	17.56044	8.19717	6.99968	6.64827	6.51494
24	3-E- $C_6$	17.91494	8.22740	7.00082	6.64815	6.51565
25	2,2-M <sub>2</sub> - $C_6$	20.51561	8.75210	7.32066	6.90480	6.74622
26	2,3-M <sub>2</sub> - $C_6$	19.60890	8.52990	7.18120	6.80400	6.66787
27	2,4-M <sub>2</sub> - $C_6$	19.20822	8.49687	7.18043	6.80789	6.67080
28	2,5-M <sub>2</sub> - $C_6$	18.60840	8.47418	7.19967	6.82303	6.67933
29	3,3-M <sub>2</sub> - $C_6$	21.42983	8.83181	7.29276	6.87327	6.72557
30	3,4-M <sub>2</sub> - $C_6$	20.00839	8.60561	7.19309	6.80405	6.66684
31	3-E-2-M- $C_5$	20.10744	8.61035	7.18685	6.80099	6.66587
32	3-E-3-M- $C_5$	22.13693	9.03071	7.34684	6.88412	6.72587
33	2,2,3-M <sub>3</sub> - $C_5$	24.14856	9.39424	7.57885	7.07839	6.90390
34	2,2,4-M <sub>3</sub> - $C_5$	22.80578	9.34954	7.63329	7.13473	6.94471
35	2,3,3-M <sub>3</sub> - $C_5$	24.49869	9.54702	7.64187	7.10049	6.90990
36	2,3,4-M <sub>3</sub> - $C_5$	22.07279	9.03695	7.41989	6.98234	6.83206
37	2,2,3,3-M <sub>4</sub> - $C_4$	29.75000	11.00852	8.45704	7.65464	7.32502

TABLE 1. (Continued).

No.	Name	DM <sup>1</sup>	DM <sup>2</sup>	DM <sup>3</sup>	DM <sup>4</sup>	DM <sup>5</sup>
	C <sub>9</sub> H <sub>20</sub>					
38	C <sub>9</sub>	17.81111	8.93865	7.65860	7.26185	7.10190
39	2-M-C <sub>8</sub>	19.15960	9.14907	7.81589	7.40758	7.24763
40	3-M-C <sub>8</sub>	19.63434	9.16570	7.80947	7.40269	7.24561
41	4-M-C <sub>8</sub>	19.85814	9.17512	7.80862	7.40243	7.24574
42	3-E-C <sub>7</sub>	20.26217	9.20291	7.81016	7.40250	7.24652
43	4-E-C <sub>7</sub>	20.46331	9.21844	7.80990	7.40194	7.24640
44	2,2-M <sub>2</sub> -C <sub>7</sub>	22.71384	9.69154	8.11706	7.65272	7.47306
45	3,3-M <sub>2</sub> -C <sub>7</sub>	23.89581	9.77848	8.09048	7.62313	7.45389
46	4,4-M <sub>2</sub> -C <sub>7</sub>	24.27449	9.85039	8.10692	7.62796	7.45594
47	2,3-M <sub>2</sub> -C <sub>7</sub>	21.89196	9.49158	7.98721	7.55667	7.39730
48	2,4-M <sub>2</sub> -C <sub>7</sub>	21.62238	9.48662	7.99251	7.56244	7.40113
49	2,5-M <sub>2</sub> -C <sub>7</sub>	21.20796	9.43959	7.98444	7.55983	7.39974
50	2,6-M <sub>2</sub> -C <sub>7</sub>	20.59842	9.42199	8.00267	7.57418	7.40796
51	3,4-M <sub>2</sub> -C <sub>7</sub>	22.57392	9.56926	7.99165	7.55354	7.39531
52	3,5-M <sub>2</sub> -C <sub>7</sub>	21.95915	9.50164	7.98150	7.55301	7.39575
53	3-E-2-M-C <sub>6</sub>	22.74302	9.57620	7.98845	7.55237	7.39524
54	3-E-3-M-C <sub>6</sub>	25.10292	9.99240	8.12868	7.62461	7.45050
55	4-E-2-M-C <sub>6</sub>	22.12826	9.51664	7.98174	7.55340	7.39640
56	3-E-4-M-C <sub>6</sub>	23.18683	9.67321	8.00961	7.55653	7.39627
57	2,2,3-M <sub>3</sub> -C <sub>6</sub>	26.88478	10.32016	8.35562	7.81829	7.62804
58	2,2,4-M <sub>3</sub> -C <sub>6</sub>	25.72740	10.25209	8.36344	7.83605	7.64225
59	2,2,5-M <sub>3</sub> -C <sub>6</sub>	24.59251	10.14575	8.37688	7.86131	7.66134
60	2,3,3-M <sub>3</sub> -C <sub>6</sub>	27.48250	10.45963	8.39217	7.82371	7.62582
61	3,3,4-M <sub>3</sub> -C <sub>6</sub>	28.03870	10.62413	8.43764	7.83174	7.62448
62	2,4,4-M <sub>3</sub> -C <sub>6</sub>	26.32512	10.34058	8.36583	7.82400	7.63170
63	2,3,4-M <sub>3</sub> -C <sub>6</sub>	25.16898	10.08645	8.22887	7.72698	7.55497
64	2,3,5-M <sub>3</sub> -C <sub>6</sub>	23.90616	9.88340	8.19818	7.73202	7.56312
65	3,3-E <sub>2</sub> -C <sub>5</sub>	26.01713	10.26930	8.22328	7.65772	7.46271
66	3-E-2,4-M <sub>2</sub> -C <sub>5</sub>	25.48212	10.16756	8.24897	7.73310	7.55742
67	3-E-2,3-M <sub>2</sub> -C <sub>5</sub>	28.56041	10.78609	8.50079	7.85603	7.63327
68	3-E-2,2-M <sub>2</sub> -C <sub>5</sub>	27.78762	10.52467	8.39863	7.82197	7.62442
69	2,2,3,3-M <sub>4</sub> -C <sub>5</sub>	34.31891	12.04613	9.17576	8.31011	7.97684
70	2,2,4,4-M <sub>4</sub> -C <sub>5</sub>	30.44023	11.65191	9.11569	8.33002	8.01423
71	2,2,3,4-M <sub>4</sub> -C <sub>5</sub>	30.24957	11.17576	8.75092	8.06560	7.82374
72	2,3,3,4-M <sub>4</sub> -C <sub>5</sub>	31.35641	11.47089	8.88594	8.12645	7.84904

TABLE 1. (Continued).

No.	Name	DM <sup>1</sup>	DM <sup>2</sup>	DM <sup>3</sup>	DM <sup>4</sup>	DM <sup>5</sup>
	C <sub>10</sub> H <sub>22</sub>					
73	C <sub>10</sub>	20.01193	9.92572	8.47029	8.01771	7.83427
74	2-M-C <sub>9</sub>	21.36714	10.13338	8.62679	8.16264	7.97905
75	3-M-C <sub>9</sub>	21.78617	10.14846	8.62093	8.15800	7.97714
76	4-M-C <sub>9</sub>	22.07552	10.15850	8.62018	8.15775	7.97726
77	5-M-C <sub>9</sub>	22.16822	10.16382	8.62032	8.15774	7.97728
78	2,2-M <sub>2</sub> -C <sub>8</sub>	24.81999	10.64846	8.91848	8.40280	8.20118
79	2,3-M <sub>2</sub> -C <sub>8</sub>	24.06698	10.46091	8.79527	8.31037	8.12753
80	2,4-M <sub>2</sub> -C <sub>8</sub>	23.89010	10.45508	8.79845	8.31531	8.13106
81	2,5-M <sub>2</sub> -C <sub>8</sub>	23.60678	10.42583	8.79376	8.31416	8.13057
82	2,6-M <sub>2</sub> -C <sub>8</sub>	23.18264	10.40213	8.79213	8.31331	8.12982
83	2,7-M <sub>2</sub> -C <sub>8</sub>	22.68408	10.39315	8.80978	8.32685	8.13756
84	3,3-M <sub>2</sub> -C <sub>8</sub>	26.06631	10.72254	8.89190	8.37493	8.18329
85	3,4-M <sub>2</sub> -C <sub>8</sub>	24.83083	10.53084	8.79828	8.30735	8.12574
86	3,5-M <sub>2</sub> -C <sub>8</sub>	24.34717	10.48318	8.78966	8.30658	8.12618
87	3,6-M <sub>2</sub> -C <sub>8</sub>	23.78137	10.44390	8.78975	8.30780	8.12639
88	4,4-M <sub>2</sub> -C <sub>8</sub>	26.71276	10.79542	8.90243	8.37746	8.18464
89	4,5-M <sub>2</sub> -C <sub>8</sub>	25.11330	10.55749	8.79845	8.30621	8.12534
90	3-E-C <sub>8</sub>	22.41251	10.18394	8.62161	8.15778	7.97804
91	4-E-C <sub>8</sub>	22.75588	10.19922	8.62052	8.15708	7.97792
92	2,2,3-M <sub>3</sub> -C <sub>7</sub>	29.08342	11.22327	9.13998	8.56287	8.35391
93	2,2,4-M <sub>3</sub> -C <sub>7</sub>	28.05714	11.19871	9.16114	8.58528	8.37006
94	2,2,5-M <sub>3</sub> -C <sub>7</sub>	27.10765	11.04539	9.12346	8.57334	8.36494
95	2,2,6-M <sub>3</sub> -C <sub>7</sub>	26.26410	11.01103	9.15583	8.60301	8.38489
96	2,3,3-M <sub>3</sub> -C <sub>7</sub>	29.85621	11.37078	9.17286	8.56576	8.35066
97	3,3,4-M <sub>3</sub> -C <sub>7</sub>	30.66136	11.53969	9.20671	8.56713	8.34680
98	3,3,5-M <sub>3</sub> -C <sub>7</sub>	29.13318	11.31418	9.14407	8.55331	8.34607
99	3,3,6-M <sub>3</sub> -C <sub>7</sub>	27.88043	11.13462	9.12128	8.56002	8.35456
100	2,4,4-M <sub>3</sub> -C <sub>7</sub>	29.07751	11.37966	9.19395	8.58424	8.36382
101	3,4,4-M <sub>3</sub> -C <sub>7</sub>	30.90894	11.58714	9.21826	8.57001	8.34761
102	2,3,4-M <sub>3</sub> -C <sub>7</sub>	27.64751	11.02861	9.02053	8.47417	8.28256
103	2,3,5-M <sub>3</sub> -C <sub>7</sub>	26.57008	10.87985	8.99496	8.47216	8.28383
104	2,3,6-M <sub>3</sub> -C <sub>7</sub>	25.62781	10.77823	8.99238	8.48127	8.29077
105	2,4,5-M <sub>3</sub> -C <sub>7</sub>	26.78416	10.90358	8.99605	8.47180	8.28389
106	2,4,6-M <sub>3</sub> -C <sub>7</sub>	25.64155	10.82830	9.01621	8.49608	8.29987
107	3,4,5-M <sub>3</sub> -C <sub>7</sub>	28.15810	11.15391	9.05370	8.48142	8.28354
108	3-E-2-M-C <sub>7</sub>	25.04946	10.53028	8.79357	8.30580	8.12557
109	3-E-3-M-C <sub>7</sub>	27.50197	10.92189	8.92121	8.37376	8.17941

TABLE 1. (Continued).

No.	Name	DM <sup>1</sup>	DM <sup>2</sup>	DM <sup>3</sup>	DM <sup>4</sup>	DM <sup>5</sup>
110	3-E-4-M-C <sub>7</sub>	25.68925	10.64597	8.81351	8.30818	8.12585
111	3-E-5-M-C <sub>7</sub>	24.81607	10.52855	8.79272	8.30514	8.12538
112	3-E-6-M-C <sub>7</sub>	24.00000	10.43927	8.78441	8.30659	8.12654
113	4-E-2-M-C <sub>7</sub>	24.63584	10.50349	8.79255	8.30824	8.12735
114	4-E-3-M-C <sub>7</sub>	25.75930	10.64386	8.81150	8.30782	8.12587
115	4-E-4-M-C <sub>7</sub>	28.00197	11.00060	8.93485	8.37558	8.17959
116	4-P-C <sub>7</sub>	23.00655	10.21685	8.62231	8.15743	7.97812
117	4-iP-C <sub>7</sub>	25.40198	10.57325	8.79896	8.30666	8.12594
118	2,2,3,3-M <sub>4</sub> -C <sub>6</sub>	37.26561	12.89461	9.86278	8.98100	8.65585
119	2,2,4,4-M <sub>4</sub> -C <sub>6</sub>	33.92246	12.57776	9.79473	8.97267	8.66343
120	2,2,5,5-M <sub>4</sub> -C <sub>6</sub>	30.82107	12.03627	9.67511	8.97033	8.68891
121	2,2,3,4-M <sub>4</sub> -C <sub>6</sub>	33.31078	12.19834	9.54246	8.79551	8.53532
122	2,2,3,5-M <sub>4</sub> -C <sub>6</sub>	31.34085	11.78067	9.43108	8.77884	8.54299
123	2,2,4,5-M <sub>4</sub> -C <sub>6</sub>	30.58415	11.73366	9.43281	8.78793	8.55085
124	2,3,3,4-M <sub>4</sub> -C <sub>6</sub>	34.82191	12.57600	9.69677	8.85677	8.55724
125	2,3,3,5-M <sub>4</sub> -C <sub>6</sub>	32.47364	12.00048	9.48326	8.78394	8.53749
126	3,3,4,4-M <sub>4</sub> -C <sub>6</sub>	38.69543	13.44154	10.12324	9.10048	8.70714
127	2,3,4,4-M <sub>4</sub> -C <sub>6</sub>	34.06521	12.46106	9.64954	8.83575	8.54843
128	2,3,4,5-M <sub>4</sub> -C <sub>6</sub>	30.41994	11.66699	9.31851	8.67458	8.45424
129	3-E-2,2-M <sub>2</sub> -C <sub>6</sub>	30.48033	11.45571	9.17952	8.56379	8.34965
130	3-E-2,3-M <sub>2</sub> -C <sub>6</sub>	31.55197	11.74018	9.26854	8.58533	8.35152
131	3-E-2,4-M <sub>2</sub> -C <sub>6</sub>	28.58562	11.22622	9.06648	8.48296	8.28352
132	3-E-2,5-M <sub>2</sub> -C <sub>6</sub>	27.10464	10.94854	9.00526	8.47534	8.28582
133	3-E-3,4-M <sub>2</sub> -C <sub>6</sub>	32.04063	11.95056	9.35677	8.62027	8.36471
134	3-E-4,4-M <sub>2</sub> -C <sub>6</sub>	31.61798	11.79031	9.28443	8.59014	8.35303
135	3-E-4,5-M <sub>2</sub> -C <sub>6</sub>	28.37154	11.16887	9.05033	8.47865	8.28235
136	3-E-5,5-M <sub>2</sub> -C <sub>6</sub>	28.70456	11.25413	9.14581	8.56573	8.35623
137	3-E-3,5-M <sub>2</sub> -C <sub>6</sub>	30.02379	11.50524	9.19385	8.56378	8.34677
138	3,3-E <sub>2</sub> -C <sub>6</sub>	28.93763	11.23770	9.00674	8.39712	8.18646
139	3,4-E <sub>2</sub> -C <sub>6</sub>	26.32239	10.76658	8.84050	8.31541	8.12876
140	3-iP-2-M-C <sub>6</sub>	28.18207	11.11838	9.04128	8.48043	8.28513
141	2,2,3,3,4-M <sub>5</sub> -C <sub>5</sub>	42.21763	14.41131	10.69097	9.50037	9.01246
142	2,2,3,4,4-M <sub>5</sub> -C <sub>5</sub>	39.68173	13.99388	10.52846	9.42363	8.97431
143	3-E-2,2,3-M <sub>3</sub> -C <sub>5</sub>	38.86701	13.44801	10.11571	9.09464	8.70363
144	3-E-2,2,4-M <sub>3</sub> -C <sub>5</sub>	34.02821	12.48650	9.68147	8.86589	8.57032
145	3-E-2,3,4-M <sub>3</sub> -C <sub>5</sub>	35.71442	12.88210	9.83714	8.92329	8.58781
146	3,3-E <sub>2</sub> -2-M-C <sub>5</sub>	32.76944	12.17784	9.44863	8.66004	8.38220
147	3-iP-2,4-M <sub>2</sub> -C <sub>5</sub>	31.40982	11.99926	9.45440	8.73297	8.47956

nonanes, 75 decanes, 159 undecanes and 355 dodecanes, consisting in the lower, upper and average values, standard deviation, relative width of the interval of values, defined as in eq. (11) and the

$$R_w = \frac{V_{\text{upper}} - V_{\text{lower}}}{V_{\text{average}}} \quad (11)$$

distribution of the values of the corresponding TI in ten equal intervals between the lower upper value of the TI. In order to express quantitatively the distribution of the values of a TI, the informational energy content<sup>15</sup> was computed:

$$E = \sum p_i^2 \quad (12)$$

where

$$p_i = \frac{N_i}{N} \quad (13)$$

whose  $N_i$  and  $N$  are the number of isomers in the  $i$ -th interval and the total number of isomers, respectively. For an even distribution of the values of a TI,  $E=0.1$ , and the more uneven the distribution, the closer to 1 is the information energy content.

The most apparent features in TABLES 2-6 are that the populations of  $DM^k$  indices are overlapping for consecutive numbers of carbon atoms, and the standard deviation and relative width of the interval of values increase in the same direction. This feature reveals that the values are spread over a larger field as the number of carbon atoms increases, thus even if the structural differences are less pronounced the indices discriminate well the set of structures.

TABLE 7 contains the values of information energy content of the distribution of  $DM^k$  in ten equal intervals for the classes of isomers

TABLE 2. Statistics for the set of 661 C<sub>4</sub>-C<sub>12</sub> alkanes of the values of TI's DM<sup>k</sup>.

TI	Lower value	Upper value	Average value	Standard deviation	Relative width of the interval of values
DM <sup>1</sup>	6.82843	59.38371	32.74990	58.32095	1.60475
DM <sup>2</sup>	4.07076	20.29166	12.71322	4.40355	1.27391
DM <sup>3</sup>	3.63268	14.94078	10.20309	1.98213	1.10830
DM <sup>4</sup>	3.50180	13.07701	9.47444	1.45499	1.01064
DM <sup>5</sup>	3.45268	12.18046	9.20150	1.27673	0.94852

Intervals										
TI	1	2	3	4	5	6	7	8	9	10
DM <sup>1</sup>	6	12	35	97	198	174	89	33	13	4
DM <sup>2</sup>	4	10	17	55	132	277	119	33	11	3
DM <sup>3</sup>	4	6	14	31	74	182	286	51	9	4
DM <sup>4</sup>	4	6	8	19	41	136	282	148	13	4
DM <sup>5</sup>	3	5	10	17	33	76	161	331	21	4

TABLE 3. Statistics for the set of 35 C<sub>9</sub> alkanes of the values of TI's DM<sup>k</sup>.

TI	Lower value	Upper value	Average value	Standard deviation	Relative width of the interval of values
DM <sup>1</sup>	17.81111	34.31891	24.38361	14.50162	0.67700
DM <sup>2</sup>	8.93865	12.04613	10.00126	0.56307	0.31071
DM <sup>3</sup>	7.65860	9.17576	8.20269	0.12876	0.18496
DM <sup>4</sup>	7.26185	8.33002	7.69098	0.06073	0.13889
DM <sup>5</sup>	7.10190	8.01423	7.50359	0.04279	0.12159

Intervals										
TI	1	2	3	4	5	6	7	8	9	10
DM <sup>1</sup>	2	5	8	4	6	3	3	2	1	1
DM <sup>2</sup>	6	6	6	5	5	3	0	1	2	1
DM <sup>3</sup>	5	1	11	6	6	2	0	1	1	2
DM <sup>4</sup>	1	5	9	5	3	8	0	1	1	2
DM <sup>5</sup>	1	5	0	13	3	8	1	1	1	2

TABLE 4. Statistics for the set of 75 C<sub>10</sub> alkanes of the values of TI's DH<sup>k</sup>.

TI	Lower value	Upper value	Average value	Standard deviation	Relative width of the interval of values
DH <sup>1</sup>	20.01193	42.21763	28.29778	21.73949	0.784/1
DH <sup>2</sup>	9.92572	14.41131	11.26055	0.88844	0.39835
DH <sup>3</sup>	8.47029	10.69097	9.13417	0.19371	0.24312
DH <sup>4</sup>	8.01771	9.50037	8.52595	0.08152	0.17390
DH <sup>5</sup>	7.83427	9.01246	8.30245	0.05220	0.14191

Intervals										
TI	1	2	3	4	5	6	7	8	9	10
DH <sup>1</sup>	5	11	15	14	12	8	4	2	3	1
DH <sup>2</sup>	8	21	18	8	8	6	2	2	0	2
DH <sup>3</sup>	8	19	16	15	6	5	2	2	0	2
DH <sup>4</sup>	8	14	9	25	4	7	4	2	0	2
DH <sup>5</sup>	1	7	22	11	17	4	7	4	0	2

TABLE 5. Statistics for the set of 159 C<sub>11</sub> alkanes of the values of TI's DH<sup>k</sup>.

TI	Lower value	Upper value	Average value	Standard deviation	Relative width of the interval of values
DH <sup>1</sup>	22.21276	54.37500	32.36131	29.79951	0.99385
DH <sup>2</sup>	10.91443	18.17751	12.57235	1.38487	0.57770
DH <sup>3</sup>	9.28294	13.20660	10.09848	0.32516	0.38854
DH <sup>4</sup>	8.77419	11.48336	9.38314	0.13309	0.28873
DH <sup>5</sup>	8.56706	10.67394	9.11676	0.07728	0.23110

Intervals										
TI	1	2	3	4	5	6	7	8	9	10
DH <sup>1</sup>	11	32	42	33	20	9	8	3	0	1
DH <sup>2</sup>	36	51	33	18	11	4	4	1	0	1
DH <sup>3</sup>	36	61	32	16	5	5	3	0	0	1
DH <sup>4</sup>	9	76	42	18	7	3	3	0	0	1
DH <sup>5</sup>	9	36	62	36	8	4	3	0	0	1

TABLE 6. Statistics for the set of 335 C<sub>12</sub> alkanes of the values of TI's DH<sup>k</sup>.

TI	Lower value	Upper value	Average value	Standard deviation	Relative width of the interval of values
DH <sup>1</sup>	24.41358	59.38371	36.32847	37.12236	0.96261
DH <sup>2</sup>	11.90437	20.29166	13.87807	1.90189	0.60436
DH <sup>3</sup>	10.09633	14.94078	11.06665	0.48889	0.43775
DH <sup>4</sup>	9.53115	13.07701	10.24626	0.20890	0.34606
DH <sup>5</sup>	9.30018	12.18046	9.93676	0.11987	0.28986

Intervals

TI	1	2	3	4	5	6	7	8	9	10
DH <sup>1</sup>	14	66	87	75	56	25	16	12	2	2
DH <sup>2</sup>	63	119	78	47	21	13	8	3	1	2
DH <sup>3</sup>	63	166	66	30	14	9	2	2	2	1
DH <sup>4</sup>	61	145	97	27	13	6	2	1	2	1
DH <sup>5</sup>	22	155	116	40	11	5	2	1	2	1

TABLE 7. The informational energy content of the distribution of DH<sup>k</sup>.

Isomers	DH <sup>1</sup>	DH <sup>2</sup>	DH <sup>3</sup>	DH <sup>4</sup>	DH <sup>5</sup>
C <sub>4</sub> -C <sub>12</sub>	0.20482	0.25854	0.28450	0.27984	0.32781
C <sub>9</sub>	0.13796	0.14122	0.18694	0.17224	0.22449
C <sub>10</sub>	0.14311	0.17867	0.17404	0.18756	0.18293
C <sub>11</sub>	0.18010	0.21617	0.25145	0.31696	0.26134
C <sub>12</sub>	0.17389	0.21512	0.29416	0.27851	0.31518



examined in TABLES 2-6. As a rule, with increasing the number of carbon atoms the distribution becomes more and more uneven. The most evenly distributed is  $DM^1$  and the most unevenly distributed are  $DM^4$  and  $DM^5$ .

TABLE 8 presents the intercorrelation matrix of the TI's  $DM^k$  for the set of 661 isomers. It results that all TI's are strongly intercorrelated, especially  $DM^2$ ,  $DM^3$  and  $DM^3$ ,  $DM^4$ ,  $DM^5$ . The intercorrelation coefficients indicate that all TI's express approximately the same type of structural information and they are not worthy to be used as independent variables in a multiparametric regression equation.

As previously mentioned, the main goal in developing a TI is its capacity to be a reliable parameter in QSPR and QSAR. Because TI's  $\chi^0$ ,  $\chi^1$  and  $\chi^2$  are largely used as parameters in correlational equations, we have computed the correlation matrix between the above mentioned connectivity indices and  $DM^k$  and the results are presented in TABLE 9. Taking into consideration that the correlation coefficients are rather high, especially for  $DM^3$ ,  $DM^4$  and  $DM^5$ , we expect that they could be used as good correlational parameters.

There is another important feature of graph invariants: they can be used to characterize and to order the molecular structures according to their branching. The rules of branching were recently defined and tested using informational graph invariants.<sup>16</sup>

An example of ordering of a structural population using  $DM^k$  is presented in TABLE 10. All 62 heptane, octane and nonane isomers are ordered in ascending order according to the corresponding  $DM^k$  values. The order induced is in the increasing grade of branching, with small

TABLE 8. Intercorrelation matrix of TI's  $DM^k$ .

TI	$DM^1$	$DM^2$	$DM^3$	$DM^4$	$DM^5$
$DM^1$	1.000	0.976	0.921	0.874	0.844
$DM^2$		1.000	0.982	0.954	0.932
$DM^3$			1.000	0.993	0.982
$DM^4$				1.000	0.998
$DM^5$					1.000

TABLE 9. Correlation matrix between TI's

$X^0, X^1, X^2$  and  $DM^k$ .

TI	$DM^1$	$DM^2$	$DM^3$	$DM^4$	$DM^5$
$X^0$	0.799	0.893	0.955	0.982	0.992
$X^1$	0.514	0.664	0.778	0.838	0.867
$X^2$	0.807	0.833	0.843	0.837	0.829

TABLE 10. Ordering of all isomers of heptane, octane and decane by DM<sup>k</sup>.

No.	DM <sup>1</sup>	DM <sup>2</sup>	DM <sup>3</sup>	DM <sup>4</sup>	DM <sup>5</sup>
	C <sub>7</sub> H <sub>16</sub>				
1	C <sub>7</sub>	C <sub>7</sub>	C <sub>7</sub>	C <sub>7</sub>	C <sub>7</sub>
2	2-M-C <sub>6</sub>	2-M-C <sub>6</sub>	3-M-C <sub>6</sub>	3-M-C <sub>6</sub>	3-M-C <sub>6</sub>
3	3-M-C <sub>6</sub>	3-M-C <sub>6</sub>	3-E-C <sub>5</sub>	3-E-C <sub>5</sub>	3-E-C <sub>5</sub>
4	3-E-C <sub>5</sub>	3-E-C <sub>5</sub>	2-M-C <sub>6</sub>	2-M-C <sub>6</sub>	2-M-C <sub>6</sub>
5	2,4-M <sub>2</sub> -C <sub>5</sub>	2,4-M <sub>2</sub> -C <sub>5</sub>	2,3-M <sub>2</sub> -C <sub>5</sub>	2,3-M <sub>2</sub> -C <sub>5</sub>	2,3-M <sub>2</sub> -C <sub>5</sub>
6	2,3-M <sub>2</sub> -C <sub>5</sub>	2,3-M <sub>2</sub> -C <sub>5</sub>	2,4-M <sub>2</sub> -C <sub>5</sub>	2,4-M <sub>2</sub> -C <sub>5</sub>	2,4-M <sub>2</sub> -C <sub>5</sub>
7	2,2-M <sub>2</sub> -C <sub>5</sub>	2,2-M <sub>2</sub> -C <sub>5</sub>	3,3-M <sub>2</sub> -C <sub>5</sub>	3,3-M <sub>2</sub> -C <sub>5</sub>	3,3-M <sub>2</sub> -C <sub>5</sub>
8	3,3-M <sub>2</sub> -C <sub>5</sub>	3,3-M <sub>2</sub> -C <sub>5</sub>	2,2-M <sub>2</sub> -C <sub>5</sub>	2,2-M <sub>2</sub> -C <sub>5</sub>	2,2-M <sub>2</sub> -C <sub>5</sub>
9	2,2,3-M <sub>3</sub> -C <sub>4</sub>	2,2,3-M <sub>3</sub> -C <sub>4</sub>	2,2,3-M <sub>3</sub> -C <sub>4</sub>	2,2,3-M <sub>3</sub> -C <sub>4</sub>	2,2,3-M <sub>3</sub> -C <sub>4</sub>
	C <sub>8</sub> H <sub>18</sub>				
1	C <sub>8</sub>	C <sub>8</sub>	C <sub>8</sub>	C <sub>8</sub>	C <sub>8</sub>
2	2-M-C <sub>7</sub>	2-M-C <sub>7</sub>	3-M-C <sub>7</sub>	3-M-C <sub>7</sub>	3-M-C <sub>7</sub>
3	3-M-C <sub>7</sub>	3-M-C <sub>7</sub>	4-M-C <sub>7</sub>	4-M-C <sub>7</sub>	4-M-C <sub>7</sub>
4	4-M-C <sub>7</sub>	4-M-C <sub>7</sub>	3-E-C <sub>6</sub>	3-E-C <sub>6</sub>	3-E-C <sub>6</sub>
5	3-E-C <sub>6</sub>	3-E-C <sub>6</sub>	2-M-C <sub>7</sub>	2-M-C <sub>7</sub>	2-M-C <sub>7</sub>
6	2,5-M <sub>2</sub> -C <sub>6</sub>	2,5-M <sub>2</sub> -C <sub>6</sub>	2,4-M <sub>2</sub> -C <sub>6</sub>	3-E-2-M-C <sub>5</sub>	3-E-2-M-C <sub>5</sub>
7	2,4-M <sub>2</sub> -C <sub>6</sub>	2,4-M <sub>2</sub> -C <sub>6</sub>	2,3-M <sub>2</sub> -C <sub>6</sub>	2,3-M <sub>2</sub> -C <sub>6</sub>	3,4-M <sub>2</sub> -C <sub>6</sub>
8	2,3-M <sub>2</sub> -C <sub>6</sub>	2,3-M <sub>2</sub> -C <sub>6</sub>	3-E-2-M-C <sub>5</sub>	3,4-M <sub>2</sub> -C <sub>6</sub>	2,3-M <sub>2</sub> -C <sub>6</sub>
9	3,4-M <sub>2</sub> -C <sub>6</sub>	3,4-M <sub>2</sub> -C <sub>6</sub>	3,4-M <sub>2</sub> -C <sub>6</sub>	2,4-M <sub>2</sub> -C <sub>6</sub>	2,4-M <sub>2</sub> -C <sub>6</sub>
10	3-E-2-M-C <sub>5</sub>	3-E-2-M-C <sub>5</sub>	2,5-M <sub>2</sub> -C <sub>6</sub>	2,5-M <sub>2</sub> -C <sub>6</sub>	2,5-M <sub>2</sub> -C <sub>6</sub>
11	2,2-M <sub>2</sub> -C <sub>6</sub>	2,2-M <sub>2</sub> -C <sub>6</sub>	3,3-M <sub>2</sub> -C <sub>6</sub>	3,3-M <sub>2</sub> -C <sub>6</sub>	3,3-M <sub>2</sub> -C <sub>6</sub>

TABLE 10. (Continued).

No.	DM <sup>1</sup>	DM <sup>2</sup>	DM <sup>3</sup>	DM <sup>4</sup>	DM <sup>5</sup>
12	3,3-M <sub>2</sub> -C <sub>6</sub>	3,3-M <sub>2</sub> -C <sub>6</sub>	2,2-H <sub>2</sub> -C <sub>6</sub>	3-E-3-M-C <sub>5</sub>	3-E-3-M-C <sub>5</sub>
13	2,3,4-M <sub>3</sub> -C <sub>5</sub>	3-E-3-M-C <sub>5</sub>	3-E-3-M-C <sub>5</sub>	2,2-H <sub>2</sub> -C <sub>6</sub>	2,2-H <sub>2</sub> -C <sub>6</sub>
14	3-E-3-M-C <sub>5</sub>	2,3,4-M <sub>3</sub> -C <sub>5</sub>	2,3,4-M <sub>3</sub> -C <sub>5</sub>	2,3,4-M <sub>3</sub> -C <sub>5</sub>	2,3,4-M <sub>3</sub> -C <sub>5</sub>
15	2,2,4-M <sub>3</sub> -C <sub>5</sub>	2,2,4-M <sub>3</sub> -C <sub>5</sub>	2,2,3-M <sub>3</sub> -C <sub>5</sub>	2,2,3-M <sub>3</sub> -C <sub>5</sub>	2,2,3-M <sub>3</sub> -C <sub>5</sub>
16	2,2,3-M <sub>3</sub> -C <sub>5</sub>	2,2,3-M <sub>3</sub> -C <sub>5</sub>	2,2,4-M <sub>3</sub> -C <sub>5</sub>	2,3,3-M <sub>3</sub> -C <sub>5</sub>	2,3,3-M <sub>3</sub> -C <sub>5</sub>
17	2,3,3-M <sub>3</sub> -C <sub>5</sub>	2,3,3-M <sub>3</sub> -C <sub>5</sub>	2,3,3-M <sub>3</sub> -C <sub>5</sub>	2,2,4-M <sub>3</sub> -C <sub>5</sub>	2,2,4-M <sub>3</sub> -C <sub>5</sub>
18	2,2,3,3-M <sub>4</sub> -C <sub>4</sub>	2,2,3,3-M <sub>4</sub> -C <sub>4</sub>	2,2,3,3-M <sub>4</sub> -C <sub>4</sub>	2,2,3,3-M <sub>4</sub> -C <sub>4</sub>	2,2,3,3-M <sub>4</sub> -C <sub>4</sub>
1	C <sub>9</sub> H <sub>2</sub> O				
2	C <sub>9</sub>	2-M-C <sub>8</sub>	4-M-C <sub>8</sub>	4-E-C <sub>7</sub>	3-M-C <sub>8</sub>
3	3-M-C <sub>8</sub>	3-M-C <sub>8</sub>	3-M-C <sub>8</sub>	4-M-C <sub>8</sub>	4-M-C <sub>8</sub>
4	4-M-C <sub>8</sub>	4-M-C <sub>8</sub>	4-E-C <sub>7</sub>	3-E-C <sub>7</sub>	4-E-C <sub>7</sub>
5	3-E-C <sub>7</sub>	3-E-C <sub>7</sub>	3-E-C <sub>7</sub>	3-M-C <sub>8</sub>	3-E-C <sub>7</sub>
6	4-E-C <sub>7</sub>	4-E-C <sub>7</sub>	2-M-C <sub>8</sub>	2-M-C <sub>8</sub>	2-M-C <sub>8</sub>
7	2,6-M <sub>2</sub> -C <sub>7</sub>	2,6-M <sub>2</sub> -C <sub>7</sub>	3,5-M <sub>2</sub> -C <sub>7</sub>	3-E-2-M-C <sub>6</sub>	3-E-2-M-C <sub>6</sub>
8	2,5-M <sub>2</sub> -C <sub>7</sub>	2,5-M <sub>2</sub> -C <sub>7</sub>	4-E-2-M-C <sub>6</sub>	3,5-M <sub>2</sub> -C <sub>7</sub>	3,4-M <sub>2</sub> -C <sub>7</sub>
9	2,4-M <sub>2</sub> -C <sub>7</sub>	2,4-M <sub>2</sub> -C <sub>7</sub>	2,5-M <sub>2</sub> -C <sub>7</sub>	4-E-2-M-C <sub>6</sub>	3,5-M <sub>2</sub> -C <sub>7</sub>
10	2,3-M <sub>2</sub> -C <sub>7</sub>	2,3-M <sub>2</sub> -C <sub>7</sub>	2,3-M <sub>2</sub> -C <sub>7</sub>	3,4-M <sub>2</sub> -C <sub>7</sub>	3-E-4-M-C <sub>6</sub>
11	3,5-M <sub>2</sub> -C <sub>7</sub>	3,5-M <sub>2</sub> -C <sub>7</sub>	3-E-2-M-C <sub>6</sub>	3-E-4-M-C <sub>6</sub>	4-E-2-M-C <sub>6</sub>
12	4-E-2-M-C <sub>6</sub>	4-E-2-M-C <sub>6</sub>	3,4-M <sub>2</sub> -C <sub>7</sub>	2,3-M <sub>2</sub> -C <sub>7</sub>	2,3-M <sub>2</sub> -C <sub>7</sub>
13	3,4-M <sub>2</sub> -C <sub>7</sub>	3,4-M <sub>2</sub> -C <sub>7</sub>	2,4-M <sub>2</sub> -C <sub>7</sub>	2,5-M <sub>2</sub> -C <sub>7</sub>	2,5-M <sub>2</sub> -C <sub>7</sub>
14	2,2-M <sub>2</sub> -C <sub>7</sub>	3-E-2-M-C <sub>6</sub>	2,6-M <sub>2</sub> -C <sub>7</sub>	2,4-M <sub>2</sub> -C <sub>7</sub>	2,4-M <sub>2</sub> -C <sub>7</sub>

variations between indices.

Following the rules of branching, we have determined that the ordering of structures induced by  $DM^k$  closely parallels these rules, with few exceptions concerning  $DM^3$ ,  $DM^4$  and  $DM^5$ .

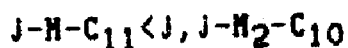
The precision of only five decimal places of the reported data in TABLE 1 becomes insufficient in a comparison concerning the rules of branching for trees applied to dodecane isomers, so in TABLE 11 selected values of  $DM^k$  are presented with nine decimal figures.

After a careful inspection of the values of  $DM^k$  in TABLE 11 one can observe a clustering tendency for higher terms, i.e. for  $DM^4$  and  $DM^5$ . For example,  $DM^4$  for 1,1- $M_2$ - $C_{10}$  ranges between 9.88400 and 9.90723 and for J,1- $M_2$ - $C_{10}$  ranges between 9.81621 and 9.83513.

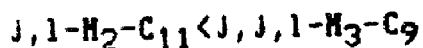
The following rules of branching are commented as defined in ref.16:

1. The influence of the total number of branches.

Rule 1.1. In a tree having a constant number of vertices, the branching increases when the number of branches attached to a given vertex increases owing to the chain decrease:



for  $J=2,3,4,5$  and  $k=1,2,3,4,5$



for  $J=2, 1=3,4,5,6,7,8$

$J=3, 1=2,4,5,6,7,8$

TABLE II. Selected values of DM<sup>k</sup> for dodecane isomers.

No.	Name	1 DM	2 DM	3 DM	4 DM	5 DM
	C <sub>12</sub> H <sub>26</sub>					
1	C <sub>12</sub>	24.413582088	11.904365753	10.096331102	9.531148172	9.300178393
2	2-H-C <sub>11</sub>	25.768791693	12.107421704	10.251531692	9.674752701	9.443413486
3	3-H-C <sub>11</sub>	26.194542605	12.123035169	10.246736580	9.670580166	9.441698937
4	4-H-C <sub>11</sub>	26.434894580	12.131560130	10.246055632	9.670302868	9.441802379
5	5-H-C <sub>11</sub>	26.537430900	12.134280336	10.245801669	9.670251139	9.441815838
6	6-H-C <sub>11</sub>	26.602979976	12.136213821	10.245808630	9.670248135	9.441817747
7	2,2-H <sub>2</sub> -C <sub>10</sub>	29.232363935	12.585379671	10.529313742	9.907232937	9.660193088
8	2,3-H <sub>2</sub> -C <sub>10</sub>	28.431844671	12.415697643	10.416377077	9.820485520	9.589962340
9	2,4-H <sub>2</sub> -C <sub>10</sub>	28.264798019	12.409103692	10.418991162	9.824846969	9.593142854
10	2,5-H <sub>2</sub> -C <sub>10</sub>	28.139722858	12.391813750	10.415662889	9.823945838	9.592733489
11	2,6-H <sub>2</sub> -C <sub>10</sub>	27.939382289	12.378269610	10.414378471	9.823802877	9.592707833
12	2,7-H <sub>2</sub> -C <sub>10</sub>	27.757323180	12.373601331	10.414648653	9.823863691	9.592697624
13	2,8-H <sub>2</sub> -C <sub>10</sub>	27.552728657	12.363937556	10.414022692	9.823210585	9.592033890
14	2,9-H <sub>2</sub> -C <sub>10</sub>	27.124001418	12.355432373	10.429085149	9.835132363	9.598884134
15	3,3-H <sub>2</sub> -C <sub>10</sub>	30.394736852	12.651010044	10.505699872	9.882652128	9.644479305
16	3,4-H <sub>2</sub> -C <sub>10</sub>	29.173279841	12.475651533	10.418076343	9.817498633	9.588348975
17	3,5-H <sub>2</sub> -C <sub>10</sub>	28.847864542	12.439068478	10.410793072	9.816909249	9.588786903
18	3,6-H <sub>2</sub> -C <sub>10</sub>	28.505863045	12.416006390	10.409606336	9.817180993	9.588860082
19	3,7-H <sub>2</sub> -C <sub>10</sub>	28.223633860	12.400478583	10.408220068	9.816859812	9.588726464
20	3,8-H <sub>2</sub> -C <sub>10</sub>	27.948208127	12.393522572	10.411205778	9.818109681	9.588943001
21	4,4-H <sub>2</sub> -C <sub>10</sub>	31.010853733	12.704048140	10.511596292	9.884003864	9.645488870
22	4,5-H <sub>2</sub> -C <sub>10</sub>	29.565461148	12.495561235	10.416511803	9.816211914	9.587996499
23	4,6-H <sub>2</sub> -C <sub>10</sub>	29.023119662	12.458963349	10.413576407	9.817625806	9.589240348
24	4,7-H <sub>2</sub> -C <sub>10</sub>	28.599228386	12.423371108	10.409081823	9.816852190	9.588961631
25	5,5-H <sub>2</sub> -C <sub>10</sub>	31.342960323	12.718806114	10.511739150	9.883844275	9.645473137
26	5,6-H <sub>2</sub> -C <sub>10</sub>	29.647349943	12.499121086	10.416791578	9.816370659	9.588089473
27	3-E-C <sub>10</sub>	26.784266639	12.156002110	10.247393821	9.670277829	9.442579796
28	4-E-C <sub>10</sub>	27.082815814	12.167809019	10.246180751	9.669611822	9.442476547
29	5-E-C <sub>10</sub>	27.223553407	12.171470417	10.245961958	9.669597243	9.442510732

TABLE 11. (Continued).

No.	Name	1 DM	2 DM	3 DM	4 DM	5 DM
30	2, 2, 3-M3-C9	33.396475297	13.104032602	10.732962695	10.061076682	9.809919424
31	2, 2, 4-M3-C9	32.528439086	13.082063346	10.749911517	10.080286281	9.823993533
32	2, 2, 5-M3-C9	31.802746277	12.985625553	10.729425084	10.074911661	9.821990552
33	2, 2, 6-M3-C9	31.275693160	12.933846054	10.722471025	10.073907098	9.821821920
34	2, 2, 7-M3-C9	30.962461721	12.914910540	10.718796595	10.071461915	9.820014475
35	2, 2, 8-M3-C9	30.592323821	12.919728384	10.751452432	10.097749289	9.837230678
36	2, 3, 3-M3-C9	34.129092556	13.222728239	10.754098548	10.059976925	9.805616967
37	3, 3, 4-M3-C9	35.010962915	13.357748441	10.773686818	10.057386416	9.801162876
38	3, 3, 5-M3-C9	33.706578981	13.197040092	10.734075217	10.051917864	9.803436633
39	3, 3, 6-M3-C9	32.770329487	13.063702457	10.707366288	10.046308198	9.801972837
40	3, 3, 7-M3-C9	32.167752218	13.019161629	10.704963158	10.046455015	9.801674756
41	3, 3, 8-M3-C9	31.695078325	12.978042227	10.711841456	10.058623823	9.810725396
42	2, 4, 4-M3-C9	33.682497095	13.228697481	10.780706881	10.057924509	9.816337834
43	3, 4, 4-M3-C9	35.432403963	13.405070545	10.784939588	10.058457112	9.801042718
44	4, 4, 4-M3-C9	35.718484353	13.436550823	10.765001656	10.062209873	9.801292494
45	4, 4, 6-M3-C9	34.203543615	13.297063593	10.713330703	10.047306813	9.807349661
46	4, 4, 7-M3-C9	33.191769879	13.106014405	10.720183884	10.061816451	9.802398576
47	4, 4, 8-M3-C9	32.429750931	13.035017234	10.739080772	10.061816451	9.812914947
48	2, 5, 5-M3-C9	33.131870847	13.133281931	10.760440006	10.065662796	9.813739895
49	3, 5, 5-M3-C9	34.303086203	13.298275527	10.795849533	10.059329607	9.805746172
50	4, 5, 5-M3-C9	35.893549960	13.472867418	10.795849533	10.061902386	9.802366701
51	2, 3, 4-M3-C9	32.075893452	12.922702123	10.621811975	9.977746374	9.741913333
52	2, 3, 5-M3-C9	31.222264056	12.817359416	10.604398336	9.977255424	9.743626111
53	2, 3, 6-M3-C9	30.596491163	12.753696033	10.596480427	9.976302457	9.743386964
54	2, 3, 7-M3-C9	30.197254246	12.741519503	10.600230124	9.977798171	9.743544084
55	2, 3, 8-M3-C9	29.756703054	12.700051337	10.603676545	9.986228177	9.749652398
56	3, 4, 5-M3-C9	32.873985817	13.049380325	10.645040528	9.980032739	9.741148692
57	3, 4, 6-M3-C9	31.816540544	12.891244650	10.609216278	9.972440321	9.739861016
58	3, 4, 7-M3-C9	31.112065201	12.824747070	10.605409227	9.974312979	9.740828682
59	3, 4, 8-M3-C9	30.551902538	12.756060470	10.597034988	9.976311677	9.743304924
60	4, 5, 6-M3-C9	33.104065289	13.075883879	10.647366361	9.979266216	9.740616234

TABLE 11. (Continued).

No.	Name	1 DM	2 DM	3 DM	4 DM	5 DM
61	4, 5, 7-H3-C9	31.967917984	12.913023335	10.613602390	9.973470185	9.740135867
62	2, 5, 6-H3-C9	31.102515851	12.796312145	10.599858079	9.976560849	9.743686202
63	2, 4, 5-H3-C9	31.576911782	12.855443972	10.609638194	9.978271906	9.744136321
64	2, 4, 6-H3-C9	30.750798663	12.802736023	10.612687958	9.985312955	9.748894985
65	2, 4, 7-H3-C9	30.209900220	12.727016939	10.595814474	9.980304173	9.746774509
66	2, 4, 8-H3-C9	29.669179281	12.700334408	10.612845702	9.996037420	9.756594925
67	2, 5, 7-H3-C9	30.361278673	12.744598034	10.598208602	9.980675252	9.746853536
68	2, 5, 8-H3-C9	29.678895553	12.703474930	10.612098567	9.995162309	9.755971527
69	3, 5, 7-H3-C9	31.063102921	12.813194152	10.597608504	9.972575036	9.741164965
70	3-E-2-H-C9	29.337252397	12.476180120	10.414110293	9.816148577	9.588231621
71	3-E-3-H-C9	31.767896722	12.815810061	10.524565261	9.879159454	9.640413674
72	3-E-4-H-C9	30.111079749	12.571006600	10.427005576	9.817003956	9.588305182
73	3-E-5-H-C9	29.461697314	12.499450214	10.413585410	9.814689468	9.587839885
74	3-E-6-H-C9	28.962118242	12.452175282	10.408898910	9.814492434	9.587866488
75	3-E-7-H-C9	28.533002649	12.432910790	10.410952444	9.816045602	9.588373727
76	3-E-8-H-C9	28.112181042	12.390652545	10.407032063	9.817153870	9.589143471
77	4-E-2-H-C9	29.064370427	12.452312381	10.412287924	9.818138603	9.589836823
78	4-E-3-H-C9	30.163613375	12.565270292	10.425194195	9.816859946	9.588408776
79	4-E-4-H-C9	32.517896901	12.879209091	10.529409591	9.878231405	9.639870981
80	4-E-5-H-C9	30.468077805	12.597862171	10.427745020	9.816341575	9.588101712
81	4-E-6-H-C9	29.661117111	12.511538548	10.414532319	9.814814251	9.588005197
82	4-E-7-H-C9	29.014650915	12.450782071	10.408487996	9.814685650	9.588032079
83	4-E-8-H-C9	28.440139387	12.403876907	10.407044219	9.817378542	9.589558192
84	5-E-2-H-C9	28.771897827	12.421538239	10.408247924	9.817520301	9.589615311
85	5-E-3-H-C9	29.563759897	12.495672762	10.412736330	9.814824943	9.587987775
86	5-E-4-H-C9	30.517606612	12.591516838	10.426363303	9.816157587	9.588086589
87	5-E-5-H-C9	32.746450136	12.901063749	10.533023042	9.879080291	9.640138044
88	4-P-C9	27.419565576	12.184931559	10.246752837	9.669631684	9.442629570
89	5-P-C9	27.494754749	12.188250782	10.246556347	9.669523573	9.442615318
90	4, 4-E2-C8	34.156221653	13.160586619	10.595686725	9.893349444	9.643746065
91	4-H-4-P-C8	33.164343606	12.973747912	10.550153374	9.883175721	9.641332701



$$j=4, l=2,3,5,6,7$$

$$\text{and } k=1,2,3,4,5$$

$$J-E-C_{10} < J-E-J-M-C_9$$

$$\text{for } J=3,4,5 \text{ and } k=1,2,3,4,5$$

Rule 1.2. A tree is always more branched than a chain having the same number of vertices:

this is evident after an inspection of TABLE 11.

Rule 1.3. In a tree having a constant number of vertices, the branching increases when the number of branches connected to a given vertex increases owing to the decrease in length of a long branch attached to the same vertex:

$$J-E-C_{10} < J, J-M-C_{10}$$

$$\text{for } J=3,4,5 \text{ and } k=1,2,3,4,5$$

$$J-P-C_9 < J-E-J-M-C_9$$

$$\text{for } j=4,5 \text{ and } k=1,3,4,5$$

Rule 1.4. Among the trees having the same number of vertices and different number of branches of the same size attached to different vertices, the greater the number of branches, the greater the branching:

$$i-M-C_{11} < i, j-M_2-C_{10} < i, j, l-M_3-C_9$$

$$\text{for all } i \neq j \neq l \text{ and } k=1,2,3,4,5$$

## 2. The influence of the chain length.

Rule 2.1. The branching decreases when at a constant number of

vertices the chain length increases at the cost of some branch length decrease:

$$i-E-C_{10} > i-M-C_{11} \quad \text{for } i=3,4,5 \text{ and } k=1,2,3,5$$

$$i-P-C_9 > i-E-C_{10} \quad \text{for } i=4,5 \text{ and } k=1,2,3,5$$

### 3. The influence of the branch length.

Rule 3.1. In graphs having a constant number of vertices, the branching decreases when some branch increases its length at the cost of the decrease of the length of another branch having the same or smaller size than the first branch:

$$4,4-E-C_8 > 4-M-4-P-C_8 \quad \text{for } k=1,2,3,4,5$$

### 4. The influence of the branch position.

Rule 4.1. In graphs having a constant number of vertices as well as a constant number and length of branches, the branching increases with the displacement of the branch from the terminal to the middle vertex of the chain:

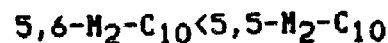
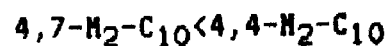
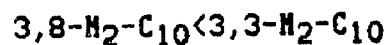
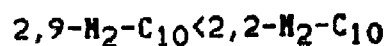
$$2-M-C_{11} < 3-M-C_{11} < 4-M-C_{11} < 5-M-C_{11} < 6-M-C_{11} \quad \text{for } k=1,2$$

$$3-E-C_{10} < 4-E-C_{10} < 5-E-C_{10} \quad \text{for } k=1,2$$

$$4-P-C_9 < 5-P-C_9 \quad \text{for } k=1,2$$

5. The influence of the number of branches attached to a given vertex.

Rule 5.1. In a tree having a constant number of vertices and branches, the branching increases when a branch is displaced from one vertex to another branched one, having equivalent position in the chain (thereby instead of two vertices with degree  $v$  we obtain two vertices with degrees  $v+1$  and  $v-1$ , respectively):



for  $k=1,2,3,4,5$

#### CONCLUDING REMARKS

The analysis of the spectrum of indices  $DM^k$  is favourable, being the basis of further studies. The calculation of the indices, based on a spectrum of connectivity indices, is straightforward and the computer time needed is very small. The new indices have no degenerate value for the set of 661 alkane isomers between butane and dodecane, thus eliminating one of the main drawbacks of connectivity indices. Moreover, they express in a proper way the structural information contained in the molecular graph and we expect that they could be used as good correlational parameters. Work is in progress in this direction.

$DM^1$  has the largest range of variation for a given set of isomeric alkanes, and the largest overlap with other sets.

$DM^1$  and  $DM^2$  order alkanes according to generally accepted increasing branching (2-Me < 3-Me < 4-Me... alkanes), unlike  $DM^3$ - $DM^5$ .

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