Extension of the *Z* Matrix to Cycle-Containing and Edge-Weighted Molecular Graphs†

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The Hosoya ***Z*** matrix is originally defined only for trees. Due to a multitude of possibilities to connect pairs of vertices in a general connected undirected graph, the ***Z*** matrix could be generalized in different ways. A possibility to resolve this problem is discussed. For edge-weighted graphs, the $\boldsymbol{Z}_{ew}$ matrix based on the novel *Z** index is defined. In analogy to path numbers invariants ${}^kZ$, $k = 1, 2, ...$, are introduced, and their correlation with boiling points of saturated hydrocarbons is studied.

INTRODUCTION

It is well-known that molecular topology (molecular connectivity) determines a large number of molecular properties[1−6] and that it can be represented by a molecular graph.[7,8] Since a graph is essentially a non-numerical mathematical object, and most molecular properties are recorded by means of a single number, it is necessary to quantify the information contained in the graph in order to perform topology−property−activity studies. These studies are in the focus of interest of contemporary chemistry.[9,10]

The representation of a molecule (or molecular graph) by a single number (a molecular index[7,8]) entails a considerable loss of information concerning the molecular structure. To diminish the loss of information an intensive search for novel indices which would improve the graph-theoretical characterization of molecular structure has been undertaken in several directions.[11,12] One direction of investigations is the creation of novel graph matrices and generalization of the existing graph matrices whose selected invariants could be used as novel molecular descriptors.[13−19]

Recently, Randić has put forward a novel graph matrix, the Hosoya ***Z*** matrix, the construction of which is related to the construction of the Hosoya *Z* index.[19,20] The ***Z*** matrix is originally defined for simple connected undirected acyclic graphs (trees). Randić also introduced two new molecular indices, the path numbers ${}^1Z$ and ${}^2Z$ from the ***Z*** matrix. The modeling of boiling points of hydrocarbons with ${}^1Z$ and ${}^2Z$ has shown their usefulness as predictor variables in topology−property studies.[19] The path numbers, ${}^mZ$, of a connected undirected graph were also introduced and studied analytically.[21]

A great number of molecules of interest contain heteroatoms. The representation of such molecules by simple molecular graphs is inadequate since these graphs do not contain information on the nature of atoms and chemical bonds. To overcome this deficiency of the topological description it is necessary to supply the molecular graph with such information. This can be done by means of weighted graphs,[7,8,22−28] which are quite common in applications of graph theory. A special class of weighted graphs are edge-weighted graphs.

Inasmuch as the invariants of the ***Z*** matrix are interesting and useful graph-theoretical indices, it is desirable to generalize the ***Z*** matrix so as to be defined not only for tree graphs but also for all simple connected undirected graphs as well as edge-weighted graphs.

DEFINITIONS

***Z* Index.** The *Z* index, $Z = Z(G)$, of a connected undirected graph *G* is defined by[20]

$$Z = \sum_{k=0}^{[N/2]} a(G,k) \tag{1}$$

where $a(G,k)$ is the number of *k*-matchings of *G*, *N* is the number of vertices of *G*, and $[N/2]$ represents the integer part of $N/2$. By definition $a(G,0) = 1$, whereas $a(G,1)$ is equal to the number of edges of *G*. In addition to these expressions, the formulas for computing a certain number of higher $a(G,k)$'s also exist.[21,29] The $a(G,k)$'s appear as coefficients in the *Z*-counting polynomial, $Q(G;x)$, of *G*[20]

$$Q(G) = Q(G;x) = \sum_{k=0}^{[N/2]} a(G,k)x^k \tag{2}$$

The polynomial can be computed by a recursive relation[2]

$$Q(G;x) = Q(G\text{-}e;x) + xQ(G\text{-}[e];x) \tag{3}$$

where *G*-*e* and *G*-[*e*] represent spanning subgraphs of *G* obtained by removing an edge and the edge and its incident edges from *G*, respectively. Clearly, the *Z* index can be obtained from the polynomial for $x = 1$

$$Z = Q(G;1) \tag{4}$$

***Z** Index.** An edge-weighted graph, G_{ew}, is created by assigning certain real numbers to the edges of a graph *G*. One can define the graph polynomial $Q^*(G_{ew};x)$ of G_{ew} as

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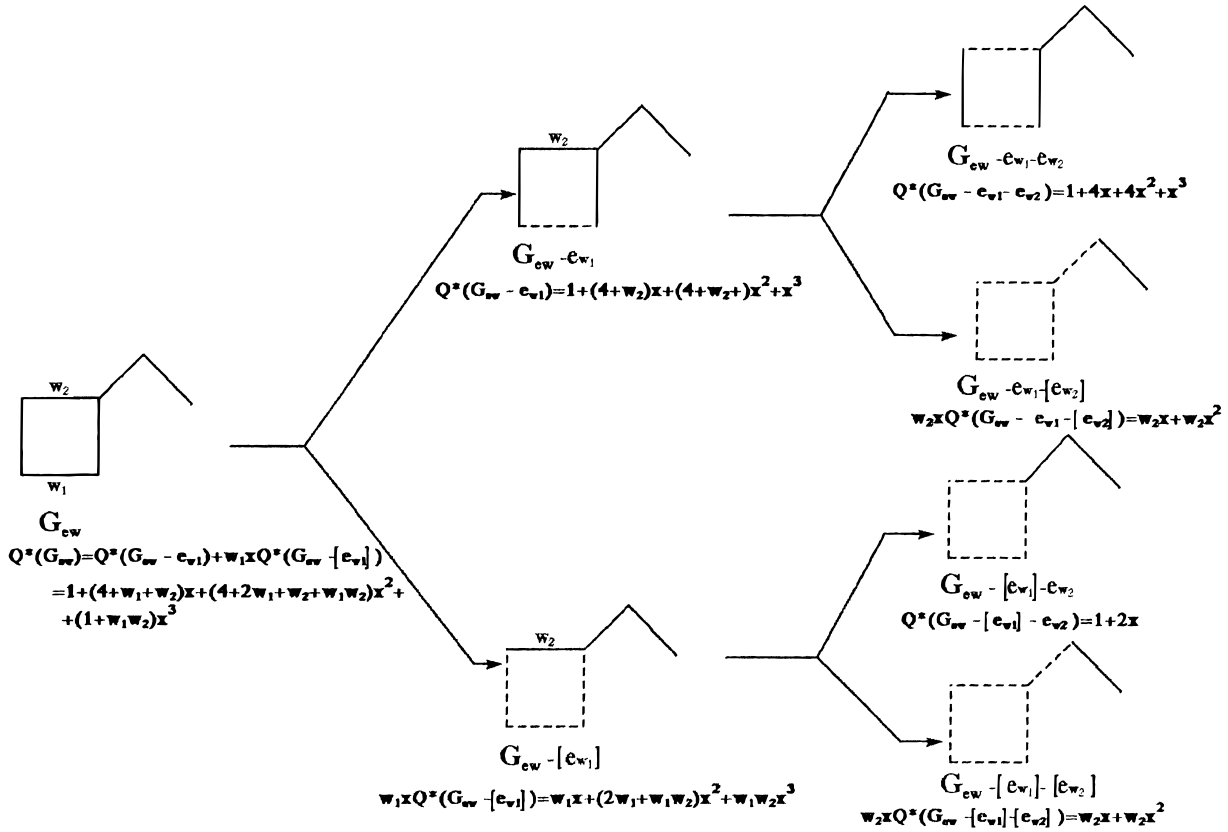

Figure 1. A graph G_{ew} with two weighted-edges and the construction of its $Q^*(G_{ew};x)$ polynomial. The broken lines represent erased bonds.

$$Q^*(G_{ew}) = Q^*(G_{ew};x) = \sum_{k=0}^{[N/2]} a^*(G_{ew},k)x^k \qquad (5)$$

where the coefficients $a^*(G_{ew},k)$ are given by

$$a^*(G_{ew},k) = \sum_{\boldsymbol{E}_k} \prod_{e_i \in E_k} w_{e_i} \qquad (6)$$

The weight of the edge e_i is denoted by w_{e_i}, the product runs over all edges in a k-tuple (k-matching) E_k of G_{ew}, and $\boldsymbol{E}_k$ is the set of all such k-matchings. Obviously, for 1-matchings one has

$$a^*(G_{ew},1) = \sum_{e_i} w_{e_i} \qquad (7)$$

and by definition

$$a^*(G_{ew},0) = 1 \qquad (8)$$

The $Q^*(G_{ew})$ polynomial can be also computed recursively.[29,30] The recursive relation given by eq 3 can be used but in a modified form[30]

$$Q^*(G_{ew};x) = Q^*(G_{ew} - e_w;x) + wxQ^*(G_{ew} - [e_w];x) \qquad (9)$$

where e_w is an edge with weight w. An example of the construction of the $Q^*(G_{ew})$ polynomial for an edge-weighted graph is given in Figure 1.

We will put forward a novel topological index, $Z^* = Z^*(G_{ew})$, of an edge-weighted graph, which is equal to the sum of the coefficients of the corresponding $Q^*(G_{ew};x)$ polynomial

$$Z^* = \sum_{k=0}^{[N/2]} a^*(G_{ew},k) \qquad (10)$$

Clearly, Z^* is equal to the value of the $Q^*(G_{ew};x)$ polynomial for $x = 1$

$$Z^* = Q^*(G_{ew};1) \qquad (11)$$

In distinction from the Z index, the Z^* index has in general noninteger values, because the edge-weights are real numbers. If the weights of all edges in a graph are the same and equal to 1, then eq 9 is reduced to eq 3, and Z^* becomes equal to the Hosoya Z index.

Hosoya *Z* Matrix. The original Hosoya $\boldsymbol{Z}$ matrix is defined only for a tree graph, T. Its matrix element z_{ij} is equal to the Z index of the spanning subgraph T-p obtained from T by the removal of all edges along the path p connecting the vertices i and j. The $\boldsymbol{Z}$ matrix of a labeled tree with N vertices is the square $N \times N$ symmetric matrix, $z_{ij} = z_{ji}$, with $z_{ii} = 0$ by definition. The finding of the elements of the $\boldsymbol{Z}$ is illustrated for 2,2,3-trimethylbutane in Figure 2.

GENERALIZATION OF *Z* MATRIX

Cycle-Containing Graphs. To associate a matrix with a graph, one has to design a procedure or algorithm that assigns to each pair of graph vertices a number in a unique, mathematically well defined way. This is not too hard a task if only the adjacent vertices are taken into account, but it is not always easy to find a convenient way to define the matrix elements corresponding to nonadjacent vertices.

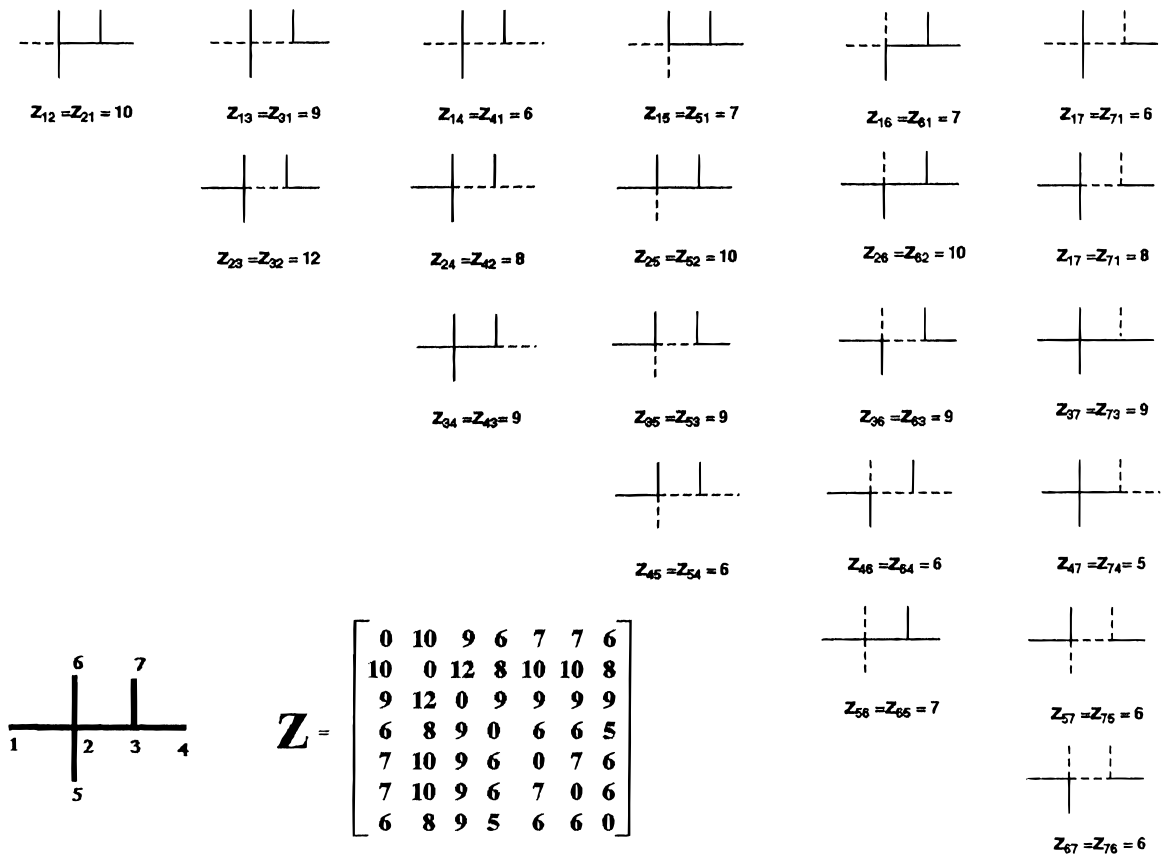

Figure 2. Construction of the elements of the ***Z*** matrix for 2,2,3-trimethylbutane. The broken lines represent erased bonds.

Let *G* be a simple connected undirected graph. Then *G* is either acyclic or *G* contains ring(s). Suppose that *W* is the set of pairs of vertices of *G*, and *P* is the set of paths connecting them. For a tree graph, *T*, there exists a function associating sets *W* and *P* in such a way that every element of each set is uniquely paired with a member of the other. In other words in a tree graph there is one and only one path connecting a given pair of vertices. If *G* contains ring(s) then between any two vertices of *G* there is at least one path connecting them. Clearly, the number of paths in a connected graph is either greater than (*G* contains ring(s)) or equal to (*G* is *T*) the number of pairs of vertices in the graph.

Constrain for the moment the consideration to the sets W_a and P_e, the elements of which are pairs of adjacent vertices and edges of *G*, respectively. For all simple connected graphs there exists a one-to-one correspondence between the elements of the sets. The entries of the ***Z*** matrix, corresponding to the elements of W_a can be defined by means of the erasure of edges of *G*, and if we define the other entries of ***Z*** to be zero, a sparse Hosoya matrix, $\boldsymbol{Z}_0$, is obtained.

The uniqueness of paths in a tree graph enables the construction of its complete Hosoya ***Z*** matrix by a straight generalization of the above procedure. If the constructional procedure is not restricted to the removal of edges of *T*, as we do in the construction of the $\boldsymbol{Z}_0$ matrix, but paths of length ≥ 2 are also taken into account, then the complete Hosoya ***Z*** matrix will be created.

A multitude of possibilities to connect pairs of vertices in a graph containing ring(s) prevents the construction of ***Z*** by the straight generalization of $\boldsymbol{Z}_0$ and at the same time offers a chance to define quite a few different general Hosoya ***Z*** matrices. It is desirable that a general ***Z*** matrix is defined in such a way that its constructional procedure is reduced to the constructional procedure for a tree graph if *G* does contain ring(s). Hence, one should notice that for a tree graph the following holds: (i) if the vertices *i* and *j* are adjacent, then the path p_{ij} connecting them is equal to the edge, e_{ij}, incident with *i* and *j*. The correponding ***Z*** matrix element is given by $z_{ij} = Z(T - e_{ij})$; (ii) the larger the distance between *i* and *j* the smaller z_{ij}; and (iii) all subgraphs used in the calculation of the entries of ***Z*** are spanning subgraphs of *T*. If we choose that (i) also holds for cycle-containing graphs, this suggests that we take the shortest paths (geodesics[31]) into account, defining the general ***Z*** matrix by means of them. In particular if there is only one geodesic, g_{ij}, connecting the vertices *i* and *j* of *G*, then we define the corresponding ***Z*** matrix element as

$$z_{ij} = Z(G - g_{ij}) \tag{12}$$

In certain cases in spite of the presence of ring(s) in *G* eq 12 makes the construction of the complete Hosoya ***Z*** matrix possible. To wit, if *G* contains one or more odd rings and no even cycle(s) and if the rings have no common edges but can have common vertices, then each pair of vertices of *G* is connected by one and only one geodesic.

If *G* contains even ring(s), then there exists pairs of vertices connected with more than one geodesic. The search for an expression for a matrix element corresponding to such a pair of vertices gives rise to the question how to treat "degenerate" geodesics. A possibility is to impose a certain condition on the geodesics and break their "degeneracy". Thereafter one chooses a specific geodesic and calculates the corresponding matrix element by means of eq 12. This method of construction of z_{ij} seems attractive because it offers us a

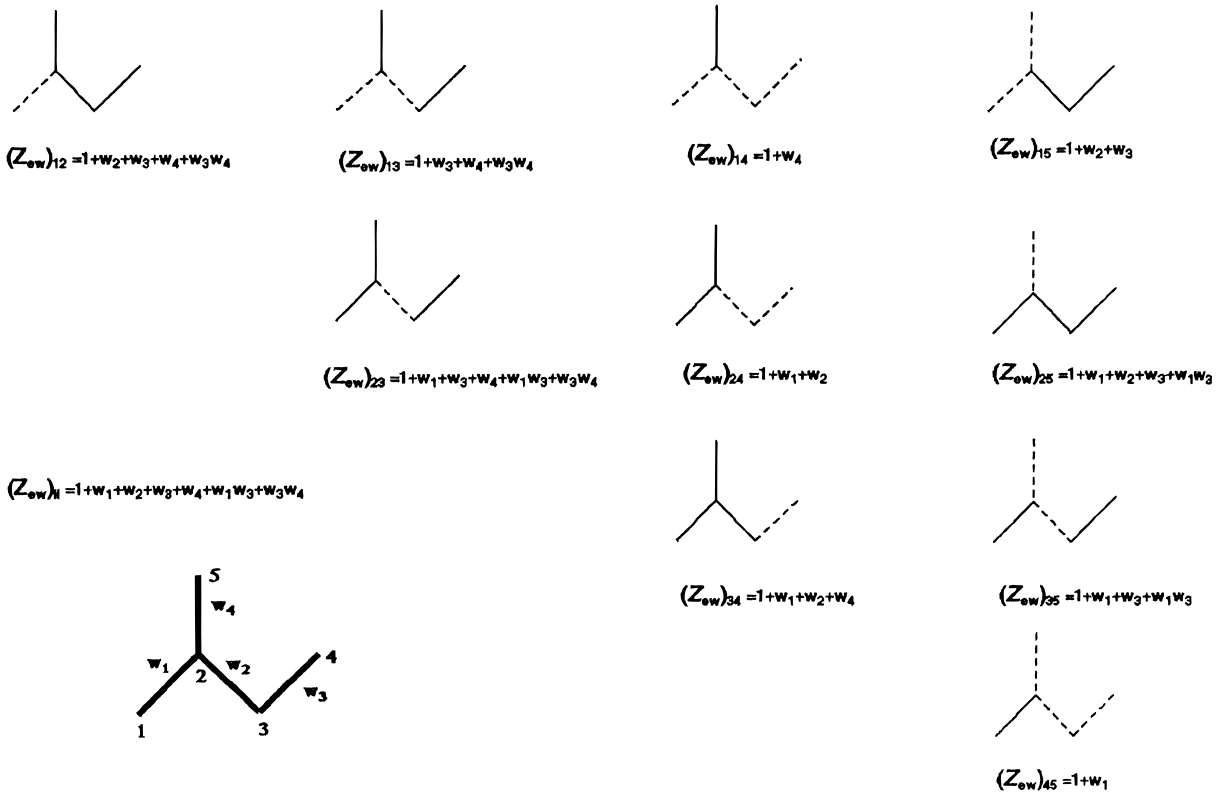

Figure 3. The calculation of the entries of the $\boldsymbol{Z}_{ew}$ matrix of an edge-weighted tree. The broken lines represent erased bonds.

chance to create quite a few different $\boldsymbol{Z}$ matrices. Unfortunately, the method is "nondemocratic" in relation to degenerate geodesics since it is based on a selection of a privileged geodesic. Intuitively, we feel that all degenerate geodesics, and not just a specific one, need to be incorporated in the expression for z_{ij}. A formula for z_{ij} satisfying the conditions (i)−(iii) as well as the condition of "democracy" reads

$$z_{ij} = \left(\sum_{g_{ij} \in P_{g_{ij}}} Z(G - g_{ij}) \right) / |P_{g_{ij}}| \qquad (13)$$

where $Z(G - g_{ij})$ is the Z index of a spanning subgraph of G obtained by the removal of all edges along a geodesic, g_{ij}, connecting the vertices i and j, the sum goes over all members of the set of geodesics, $P_{g_{ij}}$, connecting i and j, and the denominator is the cardinality (the number of elements) of the set $P_{g_{ij}}$. If the vertices i and j are connected by just one geodesic, then eq 13 is reduced to eq 12. In case of $i = j$, the geodesic connecting i and j has no edges, and we define the corresponding matrix element as $z_{ii} = Z(G)$, which is in harmony with eqs 12 and 13. Note that here we deviate from the original definition of Randić where all diagonal elements of $\boldsymbol{Z}$ are equal zero.

In general, the erasure of different geodesics (all edges along them) connecting a given pair of vertices of G results in the creation of different spanning subgraphs with different Z values. It is known that there exists a general trend of the lowering of the Z value by increasing the degree of branching.[20,32] The deviation from the trend is possibly due to degeneracy of the Z index. Inasmuch as z_{ij} is defined as the arithmetic average, eq 13, a matrix element corresponding to the pair of nonadjacent vertices connecting with two or more geodesics reflects the "average" branching of the spanning subgraphs associated with these vertices.

Edge-Weighted Graphs. Edge-weighted graphs are of considerable importance in application of graph theory in many fields,[27] particularly in chemistry if a molecule contains heteroatom(s) or atoms of one kind connected with bonds of different types.[8,26] By analogy with the $\boldsymbol{Z}$ matrix of a simple connected graph, one can also define the $\boldsymbol{Z}_{ew}$ matrix, $\boldsymbol{Z}_{ew} = \boldsymbol{Z}_{ew}(G_{ew})$, of an edge-weighted graph, G_{ew}. The $\boldsymbol{Z}_{ew}$ matrix can be created by a procedure similar to that described for the $\boldsymbol{Z}$ matrix. The procedure is based on the $Q^*(G_{ew})$ polynomial, eqs 5−8, and the Z^* index, eq 10. The general $\boldsymbol{Z}_{ew}$ matrix element, $(\boldsymbol{Z}_{ew})_{ij}$, is defined as

$$(\boldsymbol{Z}_{ew})_{ij} = \left(\sum_{g_{ij} \in P_{g_{ij}}} Z^*(G_{ew} - g_{ij}) \right) / |P_{g_{ij}}| \qquad (14)$$

where $Z^*(G_{ew} - g_{ij})$ is the Z^* index of a spanning graph of G_{ew} obtained by erasure of all edges along a geodesic, g_{ij}, connecting the vertices i and j. The length of a path in G_{ew} is measured by the number of bonds incorporated in it. Diagonal elements of $\boldsymbol{Z}_{ew}$ are defined by $(\boldsymbol{Z}_{ew})_{ii} = Z^*(G_{ew})$. An example of the construction of the $\boldsymbol{Z}_{ew}$ matrix entries of an edge-weighted tree is given in Figure 3. One should note that if weights of all edges in G_{ew} are the same and equal to 1, then the $\boldsymbol{Z}_{ew}$ matrix becomes equal to the $\boldsymbol{Z}$ matrix of the corresponding nonweighted graph.

The approach presented here is a generalization of the method of D. J. Klein[33] where a rather general permanental as well as a determinantal formula applicable to a restricted set of graphs are given together with a corresponding computational scheme.

MODELING BOILING POINTS WITH ^1Z, ^2Z, AND ^3Z INDICES

A justification for the introduction of a novel graph matrix or for the generalization of the existing one is that it enables

Table 1. Boiling Points (bp) of All the Saturated Monocyclic Hydrocarbons with up to Six Carbon Atoms

no.	compound	bp (°C)
1	cyclopropane	−32.8
2	methylcyclopropane	0.7
3	cyclobutane	12.7
4	1,1-dimethylcyclopropane	20.6
5	1,2-dimethylcyclopropane	32.6[a]
6	ethylcyclopropane	35.9
7	methylcyclobutane	36.3
8	cyclopentane	49.3
9	1,1,2-trimethylcyclopropane	52.4[b]
10	1,1-dimethylcyclobutane	56.0
11	1-ethyl-1-methylcyclopropane	56.8
12	1,2,3-trimethylcyclopropane	62.9[c]
13	isopropylcyclopropane	58.3
14	1,3-dimethylcyclobutane	59.0[c]
15	1-ethyl-2-methylcyclopropane	62.8[d]
16	1,2-dimethylcyclobutane	64.0[a]
17	propylcyclopropane	69.2
18	methylcyclopentane	71.8
19	ethylcyclobutane	70.6
20	cyclohexane	80.7

[a] Mean value of the boiling points of cis and (d,l) trans isomers. [b] Boiling point of racemic mixture. [c] Mean value of the boiling points of cis and trans isomers. [d] Mean value of the boiling points of (d,l) cis and (d,l) trans isomers.

to define at least one matrix invariant which can be used as a molecular index. We introduce, by analogy with previously mentioned path numbers,[19] the invariants of the general ***Z*** matrix

$$ {}^{k}Z = \sum {}^{k}z_{ij} \qquad (15) $$

where the superscript *k*, associated with elements of the ***Z*** matrix, denotes that the corresponding vertices (*i*,*j*) of *G* are connected by geodesic(s) of lengths *k*. Randić put forth a set of 13 desirable attributes for topological indices.[34] Among them particularly important is the requirement that an index shows good correlation with at least one molecular property. Modeling performances of ${}^{1}Z-{}^{3}Z$ indices were tested on boiling points (bp) of 20 saturated monocyclic hydrocarbons listed in Table 1. The bp data were taken from the ref 20. We focused our attention to the ${}^{k}Z$ indices up to the third order, because numerical values of indices higher than ${}^{3}Z$ are predominantly zeros, due to the small size of the compounds.

We have investigated the modeling abilities of the indices on the whole set of the monocyclic hydrocarbons where molecular size is variable and on its subset of 12 isomeric cycloalkanes (compounds 9−20) whose size in the sense of the number of atoms is constant. The obtained models were compared with the models based on the first three path molecular connectivity indices, ${}^{1}\chi-{}^{3}\chi$, the members of a frequently used family of topological descriptors in QSPR and QSAR studies.[35,36] The results of the analysis are summarized in Table 2. It is seen that molecular connectivity indices are more successful predictor variables than ${}^{k}Z$ indices, when the whole set of cycloalkanes is considered. The opposite is true in case of the isomeric set, where the size effect is eliminated. Another interesting result of the analysis is that the combination of ${}^{1}\chi$ and ${}^{3}Z$ is the "best" two-parameter model. Hence, it appears that the family of the structurally related ${}^{k}Z$ indices can be considered promising, especially in modeling of isomeric series as well as in using them as additional descriptors in a multiparametric fit of molecular properties.

Table 2. Selected Regression Equations for the Whole Set ($n = 20$) of the Saturated Monocyclic Hydrocarbons and Its Subset of Isomers ($n = 12$) with Six Carbon Atoms

no. of compounds	models	R^2	*s*
$n = 20$	${}^{1}Z$	0.914	8.43
	${}^{1}Z$, $1/{}^{1}Z$	0.979	4.27
	${}^{1}\chi$	0.984	3.69
	${}^{1}\chi$, ${}^{2}\chi$, ${}^{3}\chi$	0.990	3.08
	${}^{1}\chi$, ${}^{3}Z$	0.991	2.87
$n = 12$	${}^{1}Z$	0.928	2.28
	${}^{1}\chi$	0.845	3.34

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