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Double Invariants

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Abstract

We outline a new route to construction of structural invariants for molecules viewed as molecular graphs or as 3-dimensional objects. To a graph G, or a structure S, we associate a matrix M(G) or M(S) respectively, the elements of which are qualified molecular subgraphs or substructures. In the case of molecular graphs the new invariants are derived by selecting a matrix invariant of M and a graph invariant for subgraph elements of M. In the case of molecular structure the new invariants are derived by selecting a matrix invariant of M and a structure invariant for the substructures that represent elements of M. We have illustrated the approach on smaller graphs. In this article we consider matrices based on the following definition: The matrix elements are given by the induced subgraph G_{ij} of G that contains all *the shortest paths* between the vertices i, j.

"But it is often a very difficult and complicated question to decide in what part of the theory the improvement has to be made."

Max Planck

1 Introduction

Structure-property and structure-activity relationship remain one of the central topics of theoretical chemistry. The first step in such studies is to select suitable molecular descriptors. If the property of interest is bond additive, or if the property is a function of molecular connectivity alone, i.e., can be viewed as a result of "through-bond" interaction between the atoms involved, graphs offer an adequate molecular model. If however, the dominant description depends on "through-space" interactions modeling will require descriptors that are sensitive on molecular geometry.

In the past two decades considerable progress was made in designs of mathematical and chemical descriptors for molecular graphs [1]. These descriptors are referred to as topological indices. Apparently over hundred topological descriptors have been proposed to encode different features of molecular graphs. In contrast, descriptors for 3-dimensional structure are few, although this topic has received some attention recently. There is a continuing need for novel molecular descriptors since present descriptors fail to satisfactorily describe some molecular properties [2]. When several descriptors are used simultaneously in multiple regression analysis (MRA) one can often obtain satisfactory results. It has been found in most of the reported studies that topological indices outperform the traditional QSAR descriptors, like log P, etc. [3]. On the other hand, the long standing concern about the instability of the regression equation in MRA has finally been resolved [4]. The cause of the instability is interdependence of molecular descriptors, and the same applies as well to the traditional QSAR descriptors. Often topological indices are highly interrelated so that inclusion of an additional descriptor, even if making a small contribution to decrease of the standard error of prediction, can dramatically change the coefficients of the regression equation for descriptors already used. With use of orthogonalized descriptors this serious limitation of MRA has been lifted. This makes MRA

again as one of the first tools of choice in structure-property and structure-activity studies.

We are interested here in novel *methodology* that generates structural invariants rather than design of novel descriptors. Of particular interest to us are descriptors that (1) can be generalized to lead to a novel basis for describing molecular graphs (structures); and that (2) can be generalized to 3-dimensional structures. Both these desirable features have been for the most part overlooked in the past. Historically, the early topological indices, the Hosoya index Z [5], the connectivity index χ [6], the Balaban's index J [7], were used as a single descriptor in simple regression analysis. Later they have been combined with other indices in MRA, often in *ad hoc* manner. However, the connectivity index χ could be generalized to set of descriptors that have similar structural origin[8]. The so called higher order connectivity indices $^{m}\chi$ facilitates comparisons when several molecular properties are characterized by the same descriptors [9]. Only recently generalizations of other leading topological indices has received attention [10]. These efforts resulted in generalized Hosoya index [11] and generalized Wiener numbers [12], the latter based on Wiener number [13], which deservingly received considerable attention in the literature [14].

2 Matrices associated with graphs

For a long time the adjacency matrix was the only matrix associated with graphs [15]. Then emerged Distance matrix in which the element d_{ij} gives the shortest distance between vertices i and j [16]. Laplacean matrix, which has been known in linear algebra, received recently some attention [17]. Conceptually similar to Distance matrix of graphs is the Euclidean matrix for structures in 3-D space. In the former interatomic separations are measured "through-bond," by counting the number of bonds separating atoms, while in the latter interatomic separations are measured "through-space," using Euclidean metric.

Construction of novel matrices for graphs (and 3-D structures) offers a new route to design of molecular descriptors [18]. Several novel matrices were introduced recently: the Extended distance matrix, (ED) [19], the Electrotopological matrix (ET) [20], the Wiener matrix (W) [21], the Resistance Distance matrix (RD) [22], the Hosoya matrix (H) [23] and

Generalized Hosoya matrix (GH) [11], the Restricted Random Walk matrix (RR) [24], the Distance/Distance matrix (DD) [25], and Detour matrix (DT) [26].

In this article we will introduce another *class* of matrices for graphs. The approach is sufficiently general that it also extends to matrices representing 3-D chemical structures. In contrast to all the matrices already mentioned, the entries of which are numbers, the elements of the new class of matrices are not numbers but matrices themselves. For the particular case considered here the new matrix elements are submatrices of the matrix considered to characterize the structure. We refer to this class of matrices as Generalized Graph matrices, or briefly GG matrices. The GG matrices are a source of a multitude of novel structural invariants. There are several choices that one has to made before extracting such novel molecular descriptor:

(1) Select the algorithm for construction of elements gg_{ij} of GG matrix (that are matrices themselves);

(2) Select the matrix to characterize the graph, such as A, D, ED, ET, W, RD, H, GH, RR, DD, DT, and others;

(3) Select an invariant of gg_{ij}; (this converts the elements of GG matrix to numbers);

(4) Select an invariant of GG matrix.

Because of the last two steps we have referred to the whole class of the so derived invariants as *double invariants*. The new invariants are derived by combining the two choices for selection of invariants. Each of the four steps is totally independent of others, which allow combinatorial explosion of novel invariants.

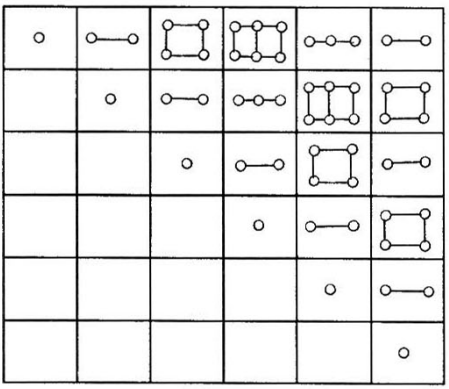
3 GG matrix based on minimal distances

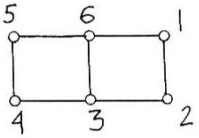
We will consider a particular algorithm for construction of GG matrix for graphs. Motivation for this particular choice originates with some unsatisfactory features of graph Distance matrix. As is well-known in acyclic graphs (trees) there is a unique path between any pair of vertices. However, in cyclic graphs there may be several shortest paths between a pair of vertices Although the elements of D matrix are well defined (by the *length* of the shortest paths), they do not reflect the distinction between the presence of a single or several multiple shortest paths.

To obtain a matrix M to be associated with a graph G one should define to each pair of vertices i, j a numerical value m_{ij}. In the case of adjacency matrix m_{ij} =1 if the vertices i, j are adjacent and zero otherwise. In the distance matrix, as already mentioned, m_{ij} is determined by the shortest length between the vertices. Other graph matrices are obtained by selecting other functions that can be defined for pair of vertices of a graph. For example, m_{ij} element of the RR matrix is defined as the probability that a random walk initiated at vertex *i* will end at vertex *j* [24]. The corresponding RR matrix is non symmetrical since the probabilities of random walk from i to j and from j to i are in general different.

Here we will consider distances between vertices of cyclic graphs. Instead of selecting the length, or frequency of shortest paths, that figure so dominantly in D and RR matrices respectively, we will select the subgraph that contains *the shortest paths* between vertices *i* and *j*.

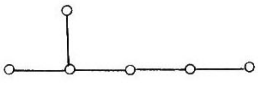
The GG matrix is necessarily symmetric. On the main diagonal it has paths of length zero, i.e., the diagonal entries correspond to individual vertices. Without a loss of generality we can assume diagonal elements to be zero, unless otherwise specified. Below is GG matrix for graph of bicyclo[2.2.0]hexane:

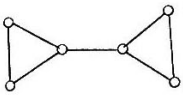




As we see from the example shown the matrix elements between adjacent vertices are paths of length one. Othe entries include paths of length two, 4-cycle and even the whole graph G.

As a consequence of the definition the elements of GG matrix can only be bipartite subgraphs of G, because in odd cycles there is always a unique shortest path between a pair of vertices, hence the induced subgraph is a path. Therefore the GG elements for acyclic graphs and graphs having only odd cycles are paths p_k (paths of length k, k=1 to k_{max}). Another interesting feature of the GG matrix considered is the presence of graph G as one of its elements. This is clearly not always the case and never happens for acyclic graphs except for straight (unbranched) chains. Below we show GG matrix for two simple graphs, one acyclic and the other having only odd cycles



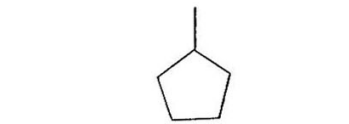


$$\begin{pmatrix} 0 & P_1 & P_2 & P_3 & P_4 & P_2 \\ & 0 & P_1 & P_2 & P_3 & P_1 \\ & & 0 & P_1 & P_2 & P_2 \\ & & & 0 & P_1 & P_3 \\ & & & & 0 & P_4 \\ & & & & & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & P_1 & P_1 & P_2 & P_3 & P_3 \\ & 0 & P_1 & P_2 & P_3 & P_3 \\ & & 0 & P_1 & P_2 & P_2 \\ & & & 0 & P_1 & P_1 \\ & & & & 0 & P_1 \\ & & & & & 0 \end{pmatrix}$$

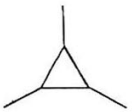
In Table 1 and Table 2 at the end of this section we show GG matrices for several cyclic graphs. Because these graphs contain even cycles they have as induced subgraphs cyclic components. Since GG matrices are symmetric only elements above the main diagonal are shown. The last two graphs of Table 2 include graph G also as one of its matrix element. Even, at this stage, before we choose matrix form for G, choose subgraph invariant, and choose matrix invariant, we can *classify* graphs. For example, classification can be

based on whether their elements are only paths p_k or not. An alternative classification can be based on whether they contain G itself as an element or not.

Table 1 GG matrix for several cyclic graphs



$$\begin{pmatrix} 0 & p_1 & p_2 & p_3 & p_3 & p_2 \\ & 0 & p_1 & p_2 & p_2 & p_1 \\ & & 0 & p_1 & p_2 & p_2 \\ & & & 0 & p_1 & p_2 \\ & & & & 0 & p_1 \\ & & & & & 0 \end{pmatrix}$$

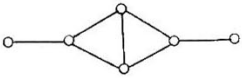


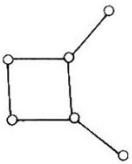
$$\begin{pmatrix} 0 & p_1 & p_2 & p_1 & p_2 & p_2 \\ & 0 & p_1 & p_1 & p_2 & p_2 \\ & & 0 & p_1 & p_2 & p_1 \\ & & & 0 & p_1 & p_2 \\ & & & & 0 & p_1 \\ & & & & & 0 \end{pmatrix}$$

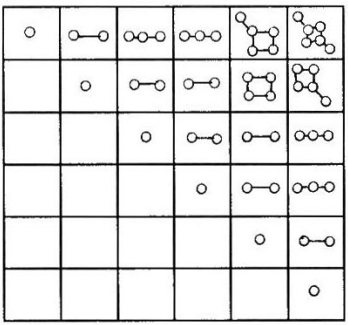
$$\begin{pmatrix} 0 & p_1 & p_2 & c_6 & p_2 & p_1 \\ & 0 & p_1 & p_2 & p_2 & p_1 \\ & & 0 & p_1 & p_2 & p_2 \\ & & & 0 & p_1 & p_2 \\ & & & & 0 & p_1 \\ & & & & & 0 \end{pmatrix}$$

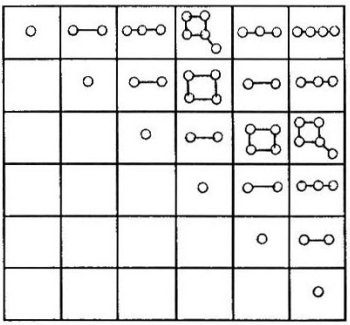
$$\begin{pmatrix} 0 & p_1 & p_1 & c_6 & p_2 & p_1 \\ & 0 & p_1 & p_2 & c_4 & p_1 \\ & & 0 & p_1 & p_1 & c_4 \\ & & & 0 & p_1 & p_2 \\ & & & & 0 & p_1 \\ & & & & & 0 \end{pmatrix}$$

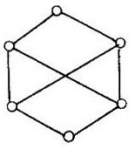
Table 2 GG matrix for additional cyclic graphs

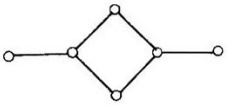


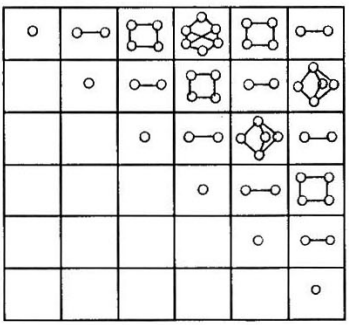


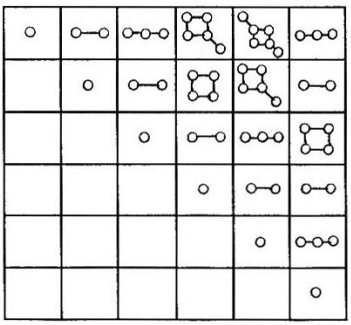










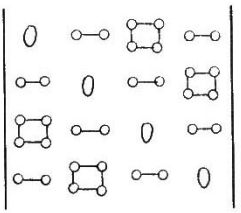


4 Selection of Invariants

Invariants of GG matrix, once matrix form for G is selected, will depend on the selection of invariants of the subgraphs G_{ij} as well as on the choice of matrix invariant of GG. For example, we may choose to characterize subgraphs by one of many topological indices and then continue with a choice of matrix invariant, e.g., determinant of GG, the leading eigenvalue of GG, etc. In general all invariants will be described as a double function of the type $F_iF_j(GG)$, i.e., $F_i\{F_j(GG)\}$. This presumes that the operations F_i and F_j are compatible, that is that the domain of F_i is in the range of F_j (and *vice versa* when the order of operators is exchanged). As will be illustrated shortly the operations F_i and F_j do not commute, i.e., generally $F_i\{F_j(GG)\} \neq F_j\{F_i(GG)\}$.

In some situations after construction of GG matrix we can continue to generate expression for topological index *without* expressing numerically GG matrix elements. For example, if we are interested in matrix determinant we can manipulate matrix elements expressed as subgraphs without specifying subgraph invariant. Consider a simple graph C_4, for which the determinant of GG matrix is:

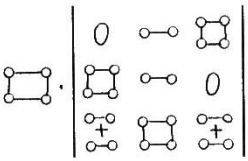
$$\begin{vmatrix} 0 & p_1 & c_4 & p_1 \\ p_1 & 0 & p_1 & c_4 \\ c_4 & p_1 & 0 & p_1 \\ p_1 & c_4 & p_1 & 0 \end{vmatrix}$$



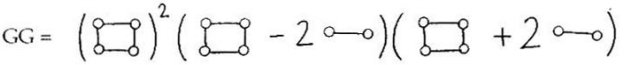
By first subtracting the second column from the last column and then adding the second row to the last row we obtain a determinant which can be expanding along the elements of the last column giving

$$c_4 \begin{vmatrix} 0 & p_1 & c_4 \\ c_4 & 0 & p_1 \\ 2p_1 & c_4 & 2p_1 \end{vmatrix}$$

or



By expanding the 3x3 determinant we can finally write:

det GG = 

The invariant det GG is a simple function of the invariants of $^{c}4$ and p_1. Each time we select an invariant of $^{c}4$ and p_1 we obtain a "double" invariant of GG. For instance we may select determinant of the subgraphs as the second invariant. Since det ($^{c}4$) = 0, and this is one of the factors of det GG, we obtain immediately that det det GG = 0. Alternatively one could first find the determinants of all the subgraphs in GG and introduce these as matrix elements of GG:

$$\begin{vmatrix} 0 & -1 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 \end{vmatrix}$$

and find the determinant of that matrix. The result, of course, is the same. The above determinant has two columns (rows) the same and must be zero necessarily.

5 Selection of Double Invariants

The det (det GG) is a simple illustration of an invariant obtained from the novel GG matrix, the elements of which are various subgraphs of the original structure. Using the expression: det GG = (c_4)^2 (c_4 - $2p_1$) (c_4 + $2p_1$), we can construct additional descriptors by considering other graph invariants or topological indices for the components p_1 and c_4. We illustrate several such choices in Table 3. We can represent descriptors listed in Table 3 as K(det GG), χ(det GG), $^{2}\chi$(det GG), $^{3}\chi$(det GG), Z(det GG), W(det GG), etc. Often we can also consider descriptors obtained by reversing the order of selection of the invariants, that is, we may consider descriptors det (K(GG)), det (χ(GG)), det ($^{2}\chi$(GG)), det ($^{3}\chi$(GG)), det (Z(GG)), det (W(GG)), etc. In general det (F(GG)) $\neq$ F(det(GG)).

Table 3 Selection of second invariants when the first invariant is det GG

1st invariant	Symbol	Contributions	2nd invariant
Kekule structures	K	$2 \cdot 0 \cdot 2$	0
Connectivity	χ	$4 \cdot 0 \cdot 4$	0
Connectivity	$^2\chi$	$2 \cdot \sqrt{2} \cdot \sqrt{2}$	4
Connectivity	$^3\chi$	$1 \cdot 1 \cdot 1$	1
Hosoya Index	Z	$43 \cdot 3 \cdot 11$	1617
Hosoya Index	^2Z	$25 \cdot 5 \cdot 5$	625
Wiener index	W	$12 \cdot 2 \cdot 6$	192
Path ID	P_{ID}	$144 \cdot 10 \cdot 14$	2016
Leading eigenvalue	λ	$4 \cdot 0 \cdot 4$	0

In Table 4 we illustrate several matrices derived from the GG matrix for the simple graph of bicyclo[2.2.0]hexane, each based on a different choice of invariant for the components p_1 and c_4. The cases include the determinant, the leading eigenvalue, Wiener index, Hosoya index, the connectivity index and path ID number, i.e., the total number of paths in a graph. Other possibilities may be considered. From the derived matrices a multitude of matrix invariants could then be considered in order to obtain finally various "double" invariants for the bicyclic graph considered.

Table 4 A selection of the first invariants for bicyclo[2.2.0]hexane

Determinant

$$\begin{pmatrix} 0 & -1 & 0 & -1 & 0 & -1 \\ & 0 & -1 & 0 & -1 & 0 \\ & & 0 & -1 & 0 & -1 \\ & & & 0 & -1 & 0 \\ & & & & 0 & -1 \\ & & & & & 0 \end{pmatrix}$$

The leading eigenvalue

$$\begin{pmatrix} 0 & 1 & 2 & 1+\sqrt{2} & \sqrt{2} & 1 \\ & 0 & 1 & \sqrt{2} & 1+\sqrt{2} & 2 \\ & & 0 & 1 & 2 & 1 \\ & & & 0 & 1 & 2 \\ & & & & 0 & 1 \\ & & & & & 0 \end{pmatrix}$$

Wiener matrix

$$\begin{pmatrix} 0 & 1 & 8 & 25 & 4 & 1 \\ & 0 & 1 & 4 & 25 & 8 \\ & & 0 & 1 & 8 & 1 \\ & & & 0 & 1 & 8 \\ & & & & 0 & 1 \\ & & & & & 0 \end{pmatrix}$$

Hosoya matrix

$$\begin{pmatrix} 0 & 2 & 7 & 20 & 3 & 2 \\ & 0 & 2 & 3 & 20 & 7 \\ & & 0 & 2 & 7 & 2 \\ & & & 0 & 2 & 7 \\ & & & & 0 & 2 \\ & & & & & 0 \end{pmatrix}$$

The connectivity index

$$\begin{pmatrix} 0 & 1 & 2 & 2.966 & 1.414 & 1 \\ & 0 & 1 & 1.414 & 2.966 & 2 \\ & & 0 & 1 & 2 & 1 \\ & & & 0 & 1 & 2 \\ & & & & 0 & 1 \\ & & & & & 0 \end{pmatrix}$$

Path identification number

$$\begin{pmatrix} 0 & 1 & 12 & 49 & 3 & 1 \\ & 0 & 1 & 3 & 49 & 12 \\ & & 0 & 1 & 12 & 1 \\ & & & 0 & 1 & 12 \\ & & & & 0 & 1 \\ & & & & & 0 \end{pmatrix}$$

6 Illustrations

In order to illustrate the diversity of topological indices that can be obtained by the novel procedure we have listed in Table 5 a selection of double invariants for graphs having six vertices (illustrated in Fig. 1).

Table 5 Double invariants for graphs of Fig. 1 based on the combination of the determinant and the leading eigenvalue as primary and secondary invariant

Graph	Invariant det det	Invariant eig det	Invariant det eig	Invariant eig eig
1	0	3.0000	0	7.5687
2	-1	2.1584	-9.4020	5.9798
3	15	1.7321	-14.0470	6.3962
4	-1	1.9032	-16.4582	7.1678
5	5	4.5049	-11.1472	6.3233
6	-1	2.1701	1.8938	7.2169
7	0	2.7321	113.1831	7.9194
8	0	4.4495	0	6.5576
9	0	2.2361	1.2024	7.4291
10	0	2.0000	0	7.0000
11	0	2.0000	-106.0387	6.8284
12	0	3.0000	540	7.8990

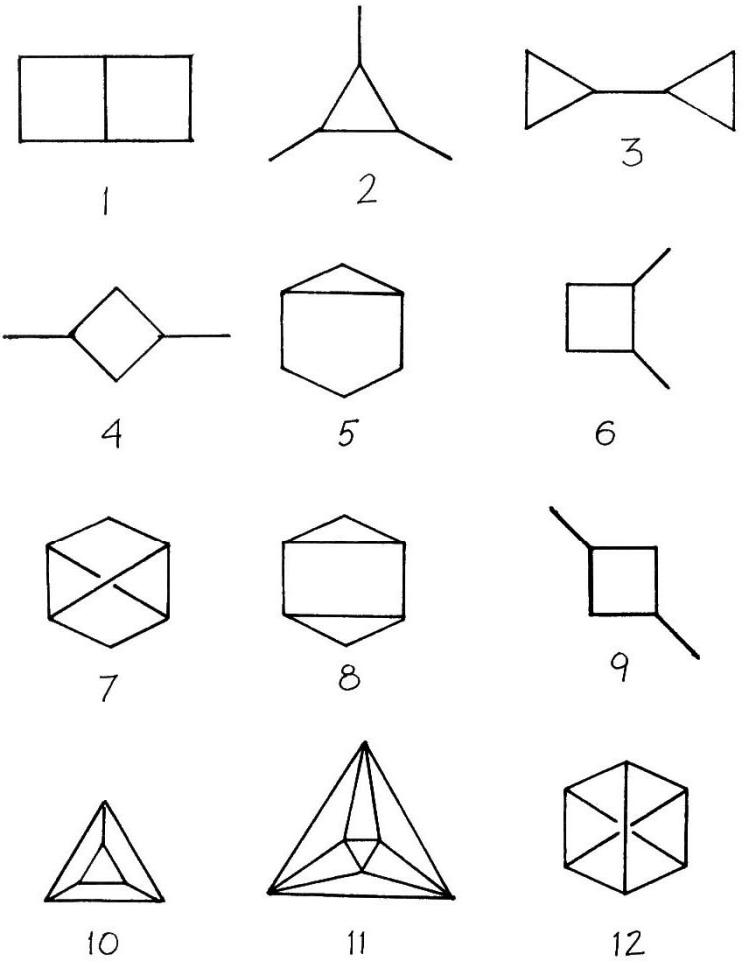


FIG. 1

In order to discern regularities that may emerge for select double invariants one should examine set of structurally closely related graphs, rather than graph of the same size but of diverse structural features. Our prime interest here was to outline the novel approach for construction of mathematical descriptors for chemical structure. However, even though the set of graphs of Fig. 1 is too small and too diverse, some general observations are inescapable. Clearly det det, det eig and eig det invariants are not size-dependent, while it appears that eig eig appears is size dependent. This conclusion is based on the variation of the magnitudes for these invariants for structures of the same size. Apparently the sign of the invariant det eig discriminates between bipartite and non bipartite graphs, leaving the cases det eig = 0 ambiguous, i.e., graphs having det eig 0 could be either bipartite or non bipartite.

7 Concluding Remarks

Although we confined our exposition to molecular graphs it should be emphasized that the outlined approach is applicable to chemical structures viewed as 3-dimensional objects. Instead of generalized graph matrix GG we start with Extended Euclidean matrix EE in which the entries of the matrix are qualified substructures. Again we have four steps

(1) Select the algorithm for construction of elements ee_{ij} of EE matrix (that are matrices themselves);
(2) Select the matrix to represent the graph, e.g., such as matrix based on Euclidean distance, or the distance/distance matrix
(3) Select an invariant of ee_{ij}; (this converts elements of EE matrix to numbers);
(4) Select an invariant of EE matrix.

The EE matrix is analogous to GG matrix. Once a selection of the first structural invariant is made and a numerical form for the matrix is obtained there is no difference between EE and GG in considering choice of the second (matrix) invariants.

There is still one additional generalization that may be of interest when considering application of here outlined procedure for construction of new descriptors. After the selection of the algorithm for construction of the elements of GG or EE matrix, one can consider different functions defined on

matrix matrix elements. For example, the powers of the (i, j) elements generate a sequence of novel descriptors, referred to as "molecular profiles" [27]. In a similar manner GG and EE matrices can generate "GG molecular profiles" and "EE molecular profiles" respectively.

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