Extension of Edge Connectivity Index. Relationships to Line Graph Indices and QSPR Applications

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The concept of edge connectivity index is extended to a series of indices based on adjacency between edges in various fragments of the molecular graph. The analogous concept of vertex adjacency indices of the line graph of the molecular graph is also introduced. Some mathematical relations between both series of indices are found, showing that line-graph-based connectivity indices are linear combinations of edge-based descriptors. The study of eight representative physical properties of alkanes was used to compare the ability of both series of indices to produce significant quantitative structure−property relationship (QSPR) models.

1. INTRODUCTION

Edge adjacency matrix is one of the graph theoretical matrices that can be used for the generation of graph theoretical invariants. This matrix has been explicitly defined in some graph theory books and it has also been identified as the vertex adjacency matrix of the line graph associated with a graph.[1] However, until recently this matrix has scarcely been used to obtain graph theoretical invariants.[2−7]

In 1995, one of the present authors proposed an edge connectivity index analogous to Randic's branching index,[2,3] but calculated by edge degrees instead of vertex degrees. This index was identified as the vertex connectivity index of the line graph associated with a molecular graph.[8] As a consequence, this index is a representative of a general class of graph theoretical descriptors based on the line graph of the molecular graph.[8,9]

The first representative of this class of molecular descriptors appears to be an index introduced by Bertz in the early 1980s.[10] This author seems to be the first who proposed to employ line graphs for modeling physico-chemical properties of organic molecules.[10−12] However, until relatively recently, the application of line graphs for designing quantitative structure−property relations (QSPR) was sporadic in several, mutually unrelated chemical fields. The systematic applications of this novel approach to QSPR have begun with a series of papers by the present authors.[8,9,13]

We wish to emphasize that the line graph of any graph is uniquely determined by the graph itself, and vice versa. The only exceptions to this one-to-one correspondence are the complete graph on three vertexes (K_3) and the complete bipartite graph on 3+1 vertices ($K_{1,3}$), which both have the same line graph that is isomorphic to K_3. If we disregard this single and chemically fully irrelevant case, then we conclude that by shifting from a molecular graph to its line graph no information on molecular connectivity is lost − it is just transformed from one (usual) to another (somewhat less usual) presentation.

One of the necessary attributes of molecular descriptors is the possibility to extend them to "higher" order analogues.[14] This attribute is necessary in many situations in which a single descriptor will not suffice to describe a property and a set of structurally related descriptors can account for that property. Several examples can be mentioned of the improvements obtained in QSPR studies when sets of descriptors were used instead of single ones (e.g., molecular connectivity indices,[15,16] charge indices,[17] and so forth).

In view of the success with which the Randic branching index was extended to higher analogues,[15] we will consider this approach to extend edge connectivity indices. Furthermore, there are some interesting questions related to the relations between edge-based and line-graph-based topological descriptors. Because the edge connectivity index of the graph is identical to the vertex connectivity index of the line graph associated with the corresponding molecular graph,[8] we have the following questions: What are the relationships that exist between the extended edge connectivity indices of graphs and their analogues defined for the line graph?; Which set of indices is better to describe structure-based properties?; and Which set of descriptors contains more specific information about the chemical structure? All these questions will be answered in the present work.

2. EXTENDED EDGE CONNECTIVITY INDICES AND LINE GRAPH CONNECTIVITY INDICES

There are many different ways in which a topological index can be extended to form a basis set of related descriptors. Topological indices can be extended by using the same graph theoretical invariant for larger fragments in the graph, such as the way in which the branching index of Randic was extended to the series of molecular connectivity indices.[15] This extension can be carried out by using linear

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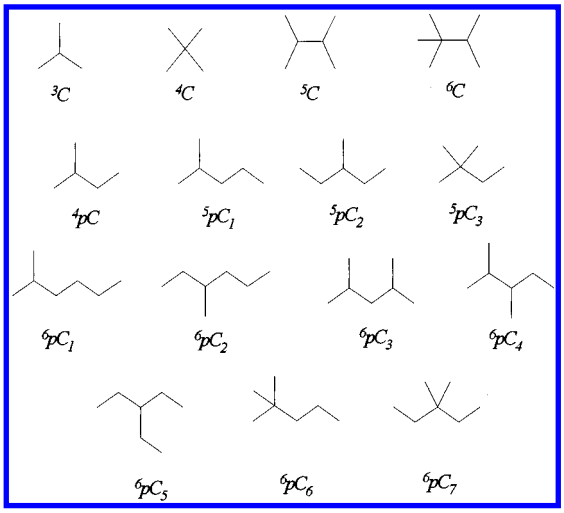

Figure 1. Graphs representing clusters (*C*) and path-clusters (*pC*) used in the extension of edge-based and line-graph-based sets of connectivity indices.

fragments only (i.e., paths of different orders), or by including other kinds of subgraphs, which in the terminology of Kier and Hall,[15] are called clusters, path-clusters, and chains.

Here we apply this scheme to the extension of the edge connectivity index and we also define a new series of topological indices based on the vertex connectivity of the line graph of a molecular graph. The edge connectivity index of a graph G is defined as follows[2]:

$$\epsilon(G) = \sum_{s} [\delta(e_i)\cdot\delta(e_j)]_s^{-0.5} \qquad (1)$$

where $\delta(e_i)$ is the degree of the edge e_i, and the summation is carried out over all pairs of adjacent edges in the graph. As the edge degrees of G are identical to the corresponding vertex degrees of $L(G)$, then $\epsilon(G)$ is identical to the Randic index of the line graph, $\chi(L(G))$.[8]

The extended set of edge connectivity indices can be defined as follows:

$$^{m}\epsilon_t(G) = \sum_{s}\prod_{i} [\delta(e_i)]_s^{-0.5} \qquad (2)$$

where m is the order of the index (i.e., the number of edges in the fragment of type t), the product is carried out over all edges contained in the fragment t, and the sum is over all fragments of this type in the graph. Here, as in the works of Kier and Hall,[15] fragments of type paths, clusters, path-clusters, and chains are used in the definition of the edge connectivity indices. Some of these fragments (namely, those used in the present work) are illustrated in Figure 1.

Another series of topological indices based on the line graph of the molecular graph is defined by using the vertex degrees of the line graph instead of the edge degrees of the graph. These indices are defined as follows:

$$^{m}\chi_t(L(G)) = \sum_{s}\prod_{i} [\delta(v_i)(L(G))]_s^{-0.5} \qquad (3)$$

3. RELATIONSHIPS BETWEEN THE TWO SETS OF INDICES

Considering the aforementioned identity existing between the edge connectivity index of order two of G and the vertex connectivity index of the line graph, the first thing that appears to be interesting to investigate are the relationships between the extended members of these two sets of descriptors. To illustrate these relations we prove the following theorem:

Theorem. Let G be a (molecular) graph and $L(G)$ its line graph. If we denote by $^{k}\epsilon(G)$ ($k \neq 2$) the edge connectivity index of order k in G and by $^{k-1}\chi(L(G))$ the vertex connectivity index of order $k-1$ in $L(G)$, then eq 4 holds

Table 1. Statistical Results of Regression Models to Describe Eight Representative Physical Properties of C_2−C_9 Alkanes with Edge Connectivity Indices of G and Vertex Connectivity Indices of $L(G)$

property	topological indices	R^a	s^b
BP	$^{0}\chi_p(G),^{1}\chi_p(G),^{2}\chi_p(G),^{4}\chi_p(G),^{5}\chi_p(G)$	0.9970	3.70
	$^{0}\chi_p(L(G)),^{1}\chi_p(L(G)),^{2}\chi_p(L(G)),^{5}\chi_p(L(G)),^{4}\chi_c(L(G))$	0.9959	3.76
	$^{2}\epsilon_p(G),^{3}\epsilon_p(G),^{6}\epsilon_p(G),^{5}\epsilon_c(G),^{5}\epsilon_{pc}(G)$	0.9989	2.21**
MV	$^{0}\chi_p(G),^{1}\chi_p(G),^{3}\chi_p(G),^{4}\chi_p(G),^{5}\chi_p(G)$	0.9995	0.54**
	$^{0}\chi_p(L(G)),^{1}\chi_p(L(G)),^{2}\chi_p(L(G)),^{3}\chi_c(L(G)),^{6}\chi_c(L(G))$	0.9988	0.84
	$^{2}\epsilon_p(G),^{3}\epsilon_p(G),^{5}\epsilon_p(G),^{3}\epsilon_c(G),^{5}\epsilon_c(G)$	0.9991	0.76
MR	$^{1}\chi_p(G),^{2}\chi_p(G),^{3}\chi_p(G),^{3}\chi_c(G),^{4}\chi_{pc}(G)$	0.9999	0.04**
	$^{0}\chi_p(L(G)),^{1}\chi_p(L(G)),^{2}\chi_p(L(G)),^{5}\chi_p(L(G)),^{3}\chi_c(L(G))$	0.9999	0.05
	$^{2}\epsilon_p(G),^{3}\epsilon_p(G),^{4}\epsilon_p(G),^{3}\epsilon_c(G),^{5}\epsilon_c(G)$	0.9999	0.07
HV	$^{0}\chi_p(G),^{1}\chi_p(G),^{3}\chi_c(G),^{4}\chi_c(G),^{4}\chi_{pc}(G)$	0.9992	0.22
	$^{0}\chi_p(L(G)),^{1}\chi_p(L(G)),^{3}\chi_p(L(G)),^{3}\chi_c(L(G)),^{4}\chi_c(L(G))$	0.9990	0.25
	$^{2}\epsilon_p(G),^{3}\epsilon_p(G),^{3}\epsilon_c(G),^{4}\epsilon_c(G),^{4}\epsilon_{pc}(G)$	0.9994	0.18**
TC	$^{0}\chi_p(G),^{4}\chi_p(G),^{5}\chi_p(G),^{6}\chi_p(G),^{4}\chi_{pc}(G)$	0.9945	6.18
	$^{0}\chi_p(L(G)),^{1}\chi_p(L(G)),^{6}\chi_p(L(G)),^{3}\chi_c(L(G)),^{6}\chi_c(L(G))$	0.9914	6.71
	$^{2}\epsilon_p(G),^{3}\epsilon_p(G),^{5}\epsilon_p(G),^{6}\epsilon_p(G),^{6}\epsilon_{pc}(G)$	0.9957	5.49**
PC	$^{1}\chi_p(G),^{2}\chi_p(G),^{3}\chi_p(G),^{6}\chi_p(G),^{6}\chi_p(G)$	0.9806	0.88
	$^{0}\chi_p(L(G)),^{2}\chi_p(L(G)),^{3}\chi_c(L(G)),^{4}\chi_c(L(G)),^{6}\chi_c(L(G))$	0.9795	0.74**
	$^{1}\epsilon_p(G),^{3}\epsilon_c(G),^{4}\epsilon_c(G),^{4}\epsilon_{pc}(G),^{5}\epsilon_{pc}(G)$	0.9839	0.80
ST	$^{1}\chi_p(G),^{2}\chi_p(G),^{3}\chi_p(G),^{6}\chi_c(G),^{5}\chi_{pc}(G)$	0.9882	0.31
	$^{0}\chi_p(L(G)),^{3}\chi_p(L(G)),^{4}\chi_c(L(G)),^{5}\chi_c(L(G)),^{5}\chi_{pc}(L(G))$	0.9858	0.34
	$^{2}\epsilon_p(G),^{3}\epsilon_p(G),^{6}\epsilon_c(G),^{5}\epsilon_{pc}(G),^{6}\epsilon_{pc}(G)$	0.9884	0.30**
MP	$^{1}\chi_p(G),^{2}\chi_p(G),^{4}\chi_c(G),^{6}\chi_c(G),^{6}\chi_{pc}(G)$	0.7093	25.5
	$^{2}\chi_p(L(G)),^{3}\chi_p(L(G)),^{4}\chi_p(L(G)),^{3}\chi_c(L(G)),^{4}\chi_c(L(G))$	0.7312	23.9**
	$^{2}\epsilon_p(G),^{4}\epsilon_c(G),^{5}\epsilon_c(G),^{6}\epsilon_c(G),^{6}\epsilon_{pc}(G)$	0.6423	27.8

[a] Regression coefficient of the model. [b] Standard deviation of the regression; the lowest values are double asterisked.

if and only if G is a connected graph whose vertex degrees do not exceed 2.

$$^{k}\epsilon(G) = {}^{k-1}\chi(L(G)) \quad (4)$$

Proof. If G is any graph and $k = 2$, then the paths of order $k - 1$ in $L(G)$ are unique because they correspond to the edges of G ($k = 1$), as a consequence $^{2}\epsilon(G) = {}^{1}\chi(L(G))$. In the case in which G contains at least one vertex with degree $\delta_i \geq 3$, any path of length k in G corresponds to a path of length $k - 1$ in $L(G)$, which is minimal, whereas the reverse is not true. Therefore, in $L(G)$ there will be more than one way to combine k vertices, which correspond to a path of order $k - 1$. In this case, $^{k-1}\chi(L(G))$ will be a combination of several edge connectivity indices that contain the index $^{k}\epsilon(G)$. In other words, eq 4 holds if and only if G is an elemental path or an elemental cycle.

The following is a consequence of the before proved theorem. Let G be a star graph $K_{1,n}$ and K_n its line graph. Then, the maximal length of a path in G (i.e., its diameter because G is a tree) is 2. However, in $L(G)$ there are paths of length up to $n - 1$. In this case, the vertex connectivity index of the path of length p is expressed in terms of the cluster epsilon index of order $p + 1$, by means of the following expression:

$$^{p}\chi(K_n) = 1/2(p+1)p![^{p+1}\epsilon_{C}(K_{1,n})] = [n!/[2(n-p-1)!]](n-1)^{-(p+1)/2} \quad (5)$$

If we consider 4-trees (i.e., graphs representing alkanes), some general relationships can be obtained for all the descriptors previously defined:

$$^{1}\chi_{p}(L(G)) = {}^{2}\epsilon_{p}(G) \quad (6)$$

$$^{2}\chi_{p}(L(G)) = {}^{3}\epsilon_{p}(G) + 3\cdot{}^{3}\epsilon_{C}(G) \quad (7)$$

$$^{3}\chi_{p}(L(G)) = {}^{4}\epsilon_{p}(G) + 12\cdot{}^{4}\epsilon_{C}(G) + 2\cdot{}^{4}\epsilon_{\mathrm{pC}}(G) \quad (8)$$

$$^{4}\chi_{p}(L(G)) = {}^{5}\epsilon_{p}(G) + 4\cdot{}^{5}\epsilon_{C}(G) + 2\cdot{}^{5}\epsilon_{\mathrm{pC1}}(G) + {}^{5}\epsilon_{pC2}(G) + 6\cdot{}^{5}\epsilon_{pC3}(G) \quad (9)$$

$$^{5}\chi_{p}(L(G)) = {}^{6}\epsilon_{p}(G) + 12\cdot{}^{6}\epsilon_{C}(G) + {}^{6}\epsilon_{\mathrm{pC1}}(G) + {}^{6}\epsilon_{pC2}(G) + 4\cdot{}^{6}\epsilon_{pC3}(G) + 2\cdot{}^{6}\epsilon_{\mathrm{pC4}}(G) + 6\cdot{}^{6}\epsilon_{\mathrm{pC6}}(G) + 2\cdot{}^{6}\epsilon_{\mathrm{pC7}}(G) \quad (10)$$

$$^{3}\chi_{C}(L(G)) = 4\cdot{}^{4}\epsilon_{C}(G) + {}^{4}\epsilon_{pC}(G) \quad (11)$$

$$^{4}\chi_{C}(L(G)) = {}^{5}\epsilon_{C}(G) + {}^{5}\epsilon_{pC3}(G) \quad (12)$$

$$^{5}\chi_{C}(L(G)) = 3\cdot{}^{6}\epsilon_{C}(G) + {}^{6}\epsilon_{pC3}(G) + 2\cdot{}^{6}\epsilon_{\mathrm{pC7}}(G) \quad (13)$$

$$^{4}\chi_{pC}(L(G)) = 4\cdot{}^{5}\epsilon_{C}(G) + {}^{5}\epsilon_{pC1}(G) + 2\cdot{}^{5}\epsilon_{\mathrm{pC2}}(G) + 9\cdot{}^{5}\epsilon_{pC3}(G) \quad (14)$$

$$^{5}\chi_{pC}(L(G)) = 32\cdot{}^{6}\epsilon_{C}(G) + {}^{6}\epsilon_{pC1}(G) + {}^{6}\epsilon_{\mathrm{pC2}}(G) + 4\cdot{}^{6}\epsilon_{pC3}(G) + 3\cdot{}^{6}\epsilon_{pC4}(G) + 3\cdot{}^{6}\epsilon_{\mathrm{pC5}}(G) + 10\cdot{}^{6}\epsilon_{\mathrm{pC6}}(G) + 12\cdot{}^{6}\epsilon_{\mathrm{pC7}}(G) \quad (15)$$

Here the number before the type of fragment means the number of the subgraph in Figure 1; for instance, $^{5}\epsilon_{pC1}G$ is the edge connectivity index defined for the path cluster of order five but using only the fragment no. 1 instead of the sum of the three fragments that normally define this path-cluster.

As can be seen from the mathematical relations between the two studied series of graph theoretical descriptors, the edge connectivity indices are more specific than the indices based on vertices of the line graph. The lower specificity of line-graph-based descriptors is expressed by the fact that these descriptors are not independent; that is, they are linear combinations of edge connectivity indices. The linear independence of topological indices has been claimed by Randic[14] as one of the most important attributes that a topological index needs to have to be used in mathematical chemistry.

4. QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIP STUDIES

To compare the ability of the two series of graph theoretical descriptors in QSPR studies we selected the series of 74 alkanes with two to eight carbon atoms, previously used in the seminal work of Needham et al.[18] Eight representative physical properties of this data set were studied[18] by using molecular connectivity indices. The eight mentioned properties are: boiling points (BP), molar volume at 20 °C (MV), molar refraction at 20 °C (MR), heat of vaporization at 25 °C (HV), critical temperature (TC), critical pressure (PC), surface tension at 20 °C (ST) and melting point (MP). Note that in ref 18 some of these data are missing for some of the alkanes. Therefore, the sets on which the calculations have been performed in both ref 18 and this work are not all of equal size.

Our main objective is to obtain the best linear regression models for the description of such physical properties to compare the QSPR ability of both sets of indices. As a reference, we report the best linear regressions with the vertex connectivity indices.[19] In Table 1 we illustrate the statistical parameters of the linear regression models obtained by a stepwise procedure. In Table 1, R is the correlation coefficient and s is the standard deviation of regression. The best models are double asterisked. Thus, the best models for the eight studied physicochemical properties are:

$$\mathrm{BP} = 47.715\ ^{2}\epsilon_{p}(G) + 26.781\ ^{3}\epsilon_{p}(G) - 27.824\ ^{6}\epsilon_{p}(G) + 4.355\ ^{5}\epsilon_{c}(G) - 32.061\ ^{5}\epsilon_{pc}(G) - 85.741$$

$$\mathrm{MV} = 14.633\ ^{0}\chi_{p}(G) + 16.155\ ^{1}\chi_{p}(G) - 7.329\ ^{3}\chi_{p}(G) - 4.453\ ^{4}\chi_{p}(G) - 2.137\ ^{5}\chi_{c}(G) + 22.921$$

$$\mathrm{MR} = 7.026\ ^{1}\chi_{p}(G) + 2.769\ ^{2}\chi_{p}(G) + 0.626\ ^{3}\chi_{p}(G) - 0.416\ ^{3}\chi_{c}(G) - 0.229\ ^{4}\chi_{pc}(G) + 4.127$$

$$\mathrm{HV} = 8.613\ ^{2}\epsilon_{p}(G) + 1.704\ ^{3}\epsilon_{p}(G) - 5.964\ ^{3}\epsilon_{c}(G) + 7.052\ ^{4}\epsilon_{c}(G) + 1.238\ ^{4}\epsilon_{pc}(G) + 8.513$$

$$\mathrm{TC} = 58.887\ ^{2}\epsilon_{p}(G) + 39.336\ ^{3}\epsilon_{p}(G) - 19.737\ ^{5}\epsilon_{p}(G) - 56.499\ ^{6}\epsilon_{p}(G) - 35.546\ ^{6}\epsilon_{\mathrm{pc}}(G) + 40.930$$

$$PC = -1.352\ {}^{0}\chi_p(L(G)) - 5.126\ {}^{2}\chi_p(L(G)) + 10.205\ {}^{3}\chi_c(L(G)) - 12.402\ {}^{4}\chi_c(L(G)) + 6.607\ {}^{6}\chi_c(L(G)) + 43.114$$

$$ST = 1.633\ {}^{2}\epsilon_p(G) + 2.423\ {}^{3}\epsilon_p(G) + 3.206\ {}^{5}\epsilon_c(G) + 1.087\ {}^{5}\epsilon_{pc}(G) - 1.717\ {}^{6}\epsilon_{pc}(G) + 10.685$$

$$MP = 26.92\ {}^{2}\chi_p(L(G)) + 78.28\ {}^{3}\chi_p(L(G)) - 75.94\ {}^{4}\chi_p(L(G)) - 186.86\ {}^{3}\chi_c(L(G)) + 449.63\ {}^{4}\chi_c(L(G)) - 179.82$$

As can be seen from the values of R and s given in Table 1, the edge connectivity indices produce better linear regression models than the indices based on vertex degrees of line graphs for five of the eight studied properties. The improvements of the regressions produced by the use of edge-based indices compared with line-graph-based for these five properties are given as percentages of the change of the respective standard deviations: BP (41%), MV (10%), HV (28%), TC (18%), and ST (12%). Evidently, these improvements are from both statistical and chemical points of view far from insignificant. The line-graph-based descriptors produced better correlation than the edge connectivity indices for the MR (28%), PC (7%), and MP (14%).

The vertex connectivity indices of graphs produced the best models for only two properties; namely, MV and MR. In addition to this, the vertex connectivity index of line graph produced the best models for other two properties; namely, PC and MP. Thus, the edge connectivity indices produced the best regressions for four of the studied properties; they are, BP, HV, TC, and ST. However, for the latter property, the difference between the model obtained using vertex connectivity indices is not highly significant (only 3% improvement in the standard deviation)

We conclude that the edge-based set of descriptors has a better correlating ability than the line-graph-based set of descriptors. Perhaps, this is a consequence of the previously proved fact that the line graph connectivity indices are less independent than the edge ones. This loss of independence of the line graphs descriptors can be interpreted as a lower structural "specificity" producing a decrease in the ability of these indices to describe properties related to more specific structural features of molecules. On the other hand, we need to take into account that the edge connectivity indices produce very good correlations with all the studied properties and for five of these properties this set of descriptors produced better models than the vertex connectivity indices. This point is important because of the well-known broad applicability of vertex connectivity indices in QSPR and quantitative structure−activity relationship (QSAR) studies. As a consequence, the edge connectivity indices represent a novel source for successful structure−property models.

Finally, it should be remarked that the improvements obtained with line graph connectivity indices point to the direction of the search of new descriptors based on line graphs of molecular graphs. One of these directions, that is presently being studied by us, is the extension of the concept of molecular connectivity to iterated line graphs.[20]

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Supporting Information Available: Tables of edge connectivity indices and line graph vertex connectivity indices for the 74 C_2−C_8 alkanes and complete statistical results for each of the regression models (11 pages). Ordering information is given on any current masthead page.

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