# Spectral Moments of the Edge Adjacency Matrix in Molecular Graphs. 1. Definition and Applications to the Prediction of Physical Properties of Alkanes<sup>†</sup>

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A novel graph theoretical invariant based on the spectral moments of the edge adjacency matrix  $(\mathbf{E})$  is proposed. Spectral moments of the  $\mathbf{E}$  matrix are used to describe seven physical properties of alkanes. All the regression models found are very significant from the statistical point of view. The spectral moments are expressed as linear combinations of the different structural fragments of the molecular graph. The use of the substructural approach for the description of seven physical properties of alkanes is also proved. The results obtained are interpreted in term of structural features of molecules.

#### 1. INTRODUCTION

One of the main objectives of graph theoretical representation of molecules is the generation of graph invariants. These quantities, that are independent of the choice of labels for vertices (or edges) in the graph, can be used as molecular descriptors in structure—property studies.<sup>1</sup>

Representation of molecular structures by a set of numbers (graph invariants) reduces the problem of quantitative structure—property relationships (QSPR) to a correlation between two sets of numbers via an algebraic expression. When the graph invariant is a single number such as a topological index, a considerable loss of information appears, and frequently we need to use either a convoluted algebraic expression or a combination of different single descriptors in the correlation.<sup>2</sup>

There are two possible solutions to avoid this loss of information in graph theoretical descriptors. They are (i) generalization of single descriptors to "higher" analogues or (ii) generation of graph invariants as sequences of numbers.<sup>3</sup>

Randić has made important contributions to both approaches. Among his many contributions to chemical graph theory, the initially called branching index<sup>4</sup> and subsequently renamed by Kier *et al.*<sup>5</sup> as the connectivity index has been generalized to a set of "higher" connectivity indices. This approach is the most successful and widespread scheme currently in use in graph theoretical QSPR studies. On the other hand, Randić has considered the sequences of path numbers,<sup>7,8</sup> self -avoiding paths,<sup>10,11</sup> random walks,<sup>12</sup> weighted path numbers,<sup>13,14</sup> and basic graphs<sup>15</sup> as approaches in composing atomic or molecular codes to be used in QSPR, QSAR, and molecular similarity studies.

Both approaches have their strong and weak points: connectivity indices are conceptually simple and easy to compute, but they have limitations when accounting for some specific branching features of molecules. In order to avoid this problem some "path-cluster" and "cluster" indices have been considered.<sup>2</sup> However, the complexity of some of the equations obtained by using these indices is forbidding.<sup>2</sup> On

the other hand, some "accidental" degeneracy has been observed in the connectivity index as a consequence of the exponent -1/2 used in the graph theoretical invariant. In a review on "third generation topological indexes" Balaban has shown that there is a tendency in the construction of novel topological indices with the incorporation of more electronic information about molecules into the graph theoretical invariants.

The essential difficulty of graph invariants based on sequences of numbers is related to the computational complexity of some calculations. For instance, the count of paths in polycyclic structures becomes very involved, and its proliferation in complete graphs increases exponentially with the number of vertices. <sup>18</sup> The enumeration of the recently proposed prime path in large graphs remains also tedious and error prone, which limits its applications in such kind of graphs. <sup>15</sup>

However, chemical graph theory is continuously evolving, and novel approaches have appeared as solutions to those difficulties. Among these recent approaches we will mention the use of edge adjacency relationships <sup>19,20</sup> in the generation of new topological indices related to molecular volume. Such relationships will be applied in the present paper in order to generate a series of molecular descriptors to be used in QSPR and QSAR studies.

### 2. SPECTRAL MOMENTS OF EDGE ADJACENCY MATRIX

Let G = (V, E) be a molecular graph, with  $V = \{v_1, v_2, ...v_n\}$  and  $E = \{e_1, e_2, ...e_m\}$  being the vertex- and edge-sets of G, respectively. Then the vertex-adjacency matrix  $\mathbf{A}$ , commonly known as adjacency matrix, is a square and symmetric matrix, whose nondiagonal entries (i, j) are ones or zeros depending on whether vertices i and j are adjacent or not. The edge-adjacency matrix  $\mathbf{E}$  of G is a square and symmetric matrix whose elements  $e_{ij}$  are 1 if and only if edge i is adjacent to edge j. Two edges are adjacent if they are incidents to a common vertex. The edge-adjacency matrix has been considered and explicitly defined in the chemical graph theory literature.  $^{21,22}$  However, this matrix has received very little attention in both chemical and mathematical literature. Recently, the present author  $^{19}$  has

<sup>†</sup> Dedicated to Professor Milan Randić for his many contributions to Chemical Graph Theory.

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rediscovered the edge-adjacency matrix as an important source of graph theoretical invariants useful in the generation of new molecular descriptors. We also pointed out that the edge-adjacency matrix of a molecular graph G is identical to the vertex-adjacency matrix of the line graph of G.

Spectral moments of E matrix are defined as follows:

$$\mu_k = \operatorname{tr}(\mathbf{E}^k)$$

where  $\mu_k$  is the kth spectral moment of **E** and **tr** is the trace of the matrix. The first spectral moment  $\mu_0$  is the number of edges in the graph, because it is defined as the trace of the identity matrix of order m, where m is the number of edges. On the other hand, the second moment  $\mu_1$  is equal to zero in simple graphs, i.e., graphs having no loops.

The rth spectral moment of the edge adjacency matrix has a simple graph theoretical interpretation. It is the sum of all self-returning walks of length r in the line graph of the molecular graph, beginning and ending with the same vertex.<sup>23</sup>

The analogous concept of spectral moments of vertex-adjacency matrix has been discussed by different authors. <sup>24–26</sup> Several relations between these moments and the structures of alternant molecules has been reported in chemical literature. <sup>24,25</sup> Some of these relations hold for the spectral moments of edge-adjacency matrix too, especially those obtained for simple cycles for which both matrices (**A** and **E**) are the same. A most detailed study of spectral moments of edge matrix for cyclic graphs will appear in a forthcoming paper. <sup>27</sup>

Spectral moments of edge adjacency matrix for all alkanes (4-trees) with 3-9 carbon atoms were calculated. The values of the first 10 spectral moments for such molecules are presented in Table 1.

## 3. DESCRIPTION OF PHYSICAL PROPERTIES OF ALKANES

In order to test the applicability of the spectral moments of edge adjacency matrix in the search of structure—property correlations, we select seven representative physical properties of alkanes: boiling point (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), and surface tension at 20 °C (ST). These properties were examined by Needham *et al.*<sup>28</sup> with molecular modeling techniques by using Wiener indices, connectivity indices and *ad hoc* descriptors. Most of these properties were well correlated (r > 0.99) with connectivity indices and *ad hoc* descriptors.

Using multiple regression by stepwise method with forward search, the first 10 spectral moments were used as independent variables and regressed against the experimental values of the physical properties. The quality of a model was determined by examining the correlation coefficient, standard deviations of regression, Fisher ratios, and the number of variables in the equation. The best linear models found are presented in Table 2.

As can be appreciated from the statistical parameters of the regression equations in Table 2, most of the physical properties are well described by the spectral moments of edge adjacency matrix. However, these equations cannot be considered as optimal. For instance, the standard deviation

in the estimation of boiling points, s = 4.32, is significantly higher than those obtained from the use of other topological and ad hoc descriptors.<sup>28</sup> The use of some topological indices based on matrix-vector multiplication by Balaban and co-workers,<sup>29</sup> has also produced low standard deviations for the description of boiling points of alkanes. These results are encouraged by the fact that as vectors one can select graph theoretical, quantum chemical, or empirical quantities. The high standard deviation obtained for some properties in the present approach can be explained considering that equations in Table 2 are completely linear, and no term accounting for nonlinear dependence among properties and spectral moments was accomplished. The generation of optimal equations for the description of physical properties is not the main objective of the present work. However, in Table 3 we illustrate the improvements produced by the introduction of the square root of  $\mu_0$  in the models to describe boiling points, critical temperatures, and critical pressures. Improvements are significant, especially for boiling points where the standard deviation was reduced to a half of the precedent value.

Almost all equations in Tables 2 and 3 are now statistically similar to those obtained by Needham et al. by using connectivity indices and ad hoc descriptors. This is well appreciated in Table 4 in which the statistical parameters for the best regression equations obtained with the moments of edge-adjacency matrix are compared to those obtained by Needham et al.<sup>28</sup> In this table we can observe that the standard deviations for the models obtained with moments of the E matrix to describe molar refractions, heat of vaporization, and critical pressures of alkanes are the same as those obtained by using molecular connectivity indices. The equations describing molar volume and superficial tensions with the present approach have only slightly higher standard deviations than the best equations found by Needham et al. Only the models found by us to describe boiling points and critical temperatures have significant differences with the precedent models obtained with connectivity or ad hoc descriptors. However, the quality of quantitative structure—property models should not be measured only by statistical criteria. The easy interpretation of equations found in term of structural fragments of the molecules should be included as a very important criterion to select the best model in a QSPR study. Models found in the present work combine very well these two aspects, i.e., they have significant statistical parameters and easy structural interpretation, and as a consequence they can be considered as good QSPR models.

## 4. STRUCTURAL SIGNIFICANCE OF THE PRESENT APPROACH

Topological descriptors have been rationalized by Randić,<sup>3</sup> who proposed a series of desirable attributes that these indices need to have. The first desirable requisite for a novel topological index is its direct structural interpretation. The discovery of the connection existing among topological descriptors and structural concepts will help one to interpret convoluted and complex physical or pharmacological properties in terms of the structure.

The spectral moments of the E matrix can be expressed as linear combinations of the number of times that the different structural fragments appear as subgraphs in the

Table 1. Spectral Moments of Edge Adjacency Matrix for  $C_3-C_9$  Alkanes

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43         3E7         8         16         6         60         60         280         434         1468         2832         819           44         4E7         8         16         6         60         60         286         448         1532         2994         870           45         22MM7         8         20         24         116         270         950         2688         8684         26110         8207           46         23MM7         8         18         12         74         110         408         840         1578         6096         1726           47         24MM7         8         18         12         70         90         324         546         1622         3144         848           49         26MM7         8         18         12         66         80         288         448         1346         2388         649           50         33MM7         8         18         12         78         120         450         966         2774         7302         2081           51         34MM7         8         18         12         74         100         3												6196
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46         23MM7         8         18         12         74         110         408         840         1578         6096         1726           47         24MM7         8         18         12         70         90         336         588         1798         3702         1025           48         25MM7         8         18         12         70         90         324         546         1622         3144         848           49         26MM7         8         18         12         66         80         288         448         1346         2388         649           50         33MM7         8         20         24         124         300         1082         3178         10480         32500         10440           51         34MM7         8         18         12         78         120         450         966         2774         7302         2081           52         35MM7         8         18         12         78         120         456         980         3046         7500         2149           53         44MM7         8         20         24         124         300	44		8	16	6	60			448	1532		8706
47         24MM7         8         18         12         70         90         336         588         1798         3702         1025           48         25MM7         8         18         12         70         90         324         546         1622         3144         848           49         26MM7         8         18         12         76         80         288         448         1346         2388         649           50         33MM7         8         20         24         124         300         1082         3178         10480         32500         10440           51         34MM7         8         18         12         78         120         450         966         2774         7302         2081           52         35MM7         8         18         12         74         100         366         672         2010         4296         1175           53         44MM7         8         20         24         124         300         1094         3220         10670         33180         10690           54         23ME6         8         18         12         74         100<	45	22MM7	8			116	270	950	2688	8684		82070
48	46	23MM7	8	18	12	74	110	408	840	1578		17260
49         26MM7         8         18         12         66         80         288         448         1346         2388         649           50         33MM7         8         20         24         124         300         1082         3178         10480         32500         10440           51         34MM7         8         18         12         78         120         450         966         2774         7302         2081           52         35MM7         8         18         12         74         100         366         672         2010         4296         1175           53         44MM7         8         20         24         124         300         1094         3220         10670         33180         10690           54         23ME6         8         18         12         78         120         456         980         3046         7500         2149           55         24ME6         8         18         12         74         100         372         686         2082         4494         1242           56         33ME6         8         18         12         82         1			8					336				10250
50         33MM7         8         20         24         124         300         1082         3178         10480         32500         10440           51         34MM7         8         18         12         78         120         450         966         2774         7302         2081           52         35MM7         8         18         12         74         100         366         672         2010         4296         1175           53         44MM7         8         20         24         124         300         1094         3220         10670         33180         10690           54         23ME6         8         18         12         78         120         456         980         3046         7500         2149           55         24ME6         8         18         12         74         100         372         686         2082         4494         1242           56         33ME6         8         18         12         82         130         492         1092         3378         8544         2454           58         223MMM66         8         22         30         142								324				8488
51         34MM7         8         18         12         78         120         450         966         2774         7302         2081           52         35MM7         8         18         12         74         100         366         672         2010         4296         1175           53         44MM7         8         20         24         124         300         1094         3220         10670         33180         10690           54         23ME6         8         18         12         78         120         456         980         3046         7500         2149           55         24ME6         8         18         12         74         100         372         686         2082         4494         1242           56         33ME6         8         20         24         132         330         1220         3696         12410         39530         12950           57         34ME6         8         18         12         82         130         492         1092         3378         8544         2454           58         223MMM6         8         22         30         134												6498
52         35MM7         8         18         12         74         100         366         672         2010         4296         1175           53         44MM7         8         20         24         124         300         1094         3220         10670         33180         10690           54         23ME6         8         18         12         78         120         456         980         3046         7500         2149           55         24ME6         8         18         12         74         100         372         686         2082         4494         1242           56         33ME6         8         20         24         132         330         1220         3696         12410         39530         12950           57         34ME6         8         18         12         82         130         492         1092         3378         8544         2454           58         223MMM6         8         22         30         142         370         1324         4088         13730         44350         14660           59         224MMM6         8         22         30         134												104400
53         44MM7         8         20         24         124         300         1094         3220         10670         33180         10690           54         23ME6         8         18         12         78         120         456         980         3046         7500         2149           55         24ME6         8         18         12         74         100         372         686         2082         4494         1242           56         33ME6         8         20         24         132         330         1220         3696         12410         39530         12950           57         34ME6         8         18         12         82         130         492         1092         3378         8544         2454           58         223MMM6         8         22         30         142         370         1324         4088         13730         44350         14660           59         224MMM6         8         22         30         134         320         1084         3080         9798         29570         9269           60         225MMM6         8         22         30         13												20810
54         23ME6         8         18         12         78         120         456         980         3046         7500         2149           55         24ME6         8         18         12         74         100         372         686         2082         4494         1242           56         33ME6         8         20         24         132         330         1220         3696         12410         39530         12950           57         34ME6         8         18         12         82         130         492         1092         3378         8544         2454           58         223MMM6         8         22         30         142         370         1324         4088         13730         44350         1466           59         224MMM6         8         22         30         134         320         1084         3080         9798         29570         9269           60         225MMM6         8         22         30         130         310         1036         2912         9186         27390         8516           61         233MMM6         8         22         30         146												11750
55         24ME6         8         18         12         74         100         372         686         2082         4494         1242           56         33ME6         8         20         24         132         330         1220         3696         12410         39530         12950           57         34ME6         8         18         12         82         130         492         1092         3378         8544         2454           58         223MMM6         8         22         30         142         370         1324         4088         13730         44350         14660           59         224MMM6         8         22         30         134         320         1084         3080         9798         29570         9269           60         225MMM6         8         22         30         130         310         1036         2912         9186         27390         8516           61         233MM66         8         22         30         146         390         1420         4480         15270         50140         16800           62         234MMM6         8         20         18												
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57         34ME6         8         18         12         82         130         492         1092         3378         8544         2454           58         223MMM6         8         22         30         142         370         1324         4088         13730         44350         14660           59         224MMM6         8         22         30         134         320         1084         3080         9798         29570         9269           60         225MMM6         8         22         30         130         310         1036         2912         9186         27390         8516           61         233MMM6         8         22         30         146         390         1420         4480         15270         50140         16800           62         234MMM6         8         20         18         96         180         620         1512         4584         12310         3582           63         235MMM6         8         20         18         88         150         500         1092         3192         7776         2160           64         244MMM6         8         22         30												
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70     2233(M)5     8     26     48     218     690     2600     9240     34030     124100     45640       71     2234(M)5     8     24     36     160     430     1500     4690     15700     51260     17060       72     2244(M)5     8     26     48     194     540     1808     5544     17950     56860     18350												38060
72 2244(M)5 8 26 48 194 540 1808 5544 17950 56860 18350								2600		34030		456400
		` '				160						170600
73 2334(M)5 8 24 36 168 480 1752 5796 20230 69120 23910												183500
	73	2334(M)5	8	24	36	168	480	1752	5796	20230	69120	239100

Table 2. Multiple Regression Equations for the Physical Properties Using the Spectral Moments of Edge Matrix

```
bp (°C) = -76.7187 + 23.992 \ m_0 + 2.5064 \ m_2 - 2.9671 \ m_3 + 0.1492 \ m_5
r = 0.9949 \ s = 4.21 \ F = 1650
MV (cm³) = 38.988 + 27.016 \ m_0 - 4.404 \ m_2 + 2.579 \ m_3 - 0.381 \ m_4 - 0.017 \ m_5
r = 0.9993 \ s = 0.6 \ F = 9659
MR (cm³) = 5.703 + 5.506 \ m_0 - 0.329 \ m_2 + 0.193 \ m_3 - 0.033 \ m_4
r = 0.9999 \ s = 0.05 \ F = 168 \ 569
HV (kJ/mol) = 74.707 + 4.821 \ m_0 - 0.409 \ m_3 + 0.021 \ m_5
r = 0.9988 \ s = 0.2 \ F = 9532
TC (°C) = 77.200 + 12.145 \ m_0 + 12.152 \ m_2 - 10.598 \ m_3 + 1.186 \ m_5 - 0.182 \ m_6
r = 0.9906 \ s = 7.0 \ F = 703
PC (atm) = 48.376 - 6.605 \ m_0 + 1.752 \ m_2 - 1.270 \ m_3 + 0.120 \ m_4 + 0.101 \ m_5 - 0.019 \ m_6
r = 0.9756 \ s = 0.8 \ F = 217
ST (dyn/cm) = 13.054 - 0.779 \ m_0 + 1.058 \ m_2 - 0.853 \ m_3 + 0.049 \ m_4 + 0.052 \ m_5 - 0.006 \ m_6
r = 0.9869 \ s = 0.3 \ F = 380
```

Table 3. Improved Correlations for the Description of Three Physical Properties by Using a Nonlinear Term

```
bp (°C) = -215.72 + 120.09 (m_0)^{0.5} + 1.61 m_2 - 2.098 m_3 + 0.029 m_5
	r = 0.9984 \quad s = 2.48 \quad F = 5194

TC (°C) = -55.41 + 105.66 (m_0)^{0.5} + 7.301 m_2 - 8.970 m_3 + 1.125 m_5 - 0.175 m_6
	r = 0.9944 \quad s = 5.4 \quad F = 1179

PC (atm) = 73.509 - 24.250 (m_0)^{0.5} + 1.575 m_2 - 1.291 m_3 + 0.006 m_4 + 0.179 m_5 - 0.031 m_6
	r = 0.9854 \quad s = 0.6 \quad F = 368
```

**Table 4.** Statistical Parameters for the Models Describing Physical Properties of Alkanes by Using Connectivity Indices, ad Hoc Descriptors and Spectral Moments of Edge-Adjacency Matrix

		nectivity ndices	/	-	nd hoc scriptors		moments of <b>E</b> matrix		
property	no. var.	r	S	no. var.	r	S	no. var.	r	S
bp	5	0.9995	1.86	5	0.9989	2.0	4	0.9984	2.48
MV	5	0.9995	0.5	5	0.9995	0.4	5	0.9993	0.6
MR	5	0.9999	0.05	5	0.9999	0.05	4	0.9999	0.05
HV	5	0.9989	0.2	5	0.9969	0.4	3	0.9988	0.2
TC	5	0.9975	4.1	5	0.9970	4.8	5	0.9944	5.4
PC	5	0.9904	0.6	5	0.9889	0.7	5	0.9854	0.6
ST	5	0.9929	0.2	5	0.9945	0.2	6	0.9869	0.3

molecular graphs. These numbers are commonly known as *embedding frequencies*<sup>30,31</sup> and have been used to describe global properties of organic molecules.<sup>32,33</sup>

In Table 5 we illustrate the equations relating the first eight spectral moments with the number of different fragments in the graph (embedding frequencies). The symbol  $|F_i|$  represents the number of subgraphs of kind i in the molecular graph. The pictorial representations of the subgraphs of different kind are depicted in Figure 1.

In a paper of Barysz et al.,<sup>34</sup> the coefficients of the characteristic polynomial of vertex adjacency **A** matrix were calculated by using a similar substructural approach. However, the approach of Barysz *et al.* was not applied for the interpretation of some structural invariants used in QSPR or QSAR studies. The present approach can be used to find a connection among physical properties of alkanes and structural fragments of the molecules by using a simple method to calculate topological invariants. In Table 6 we depict the correlation equations for description of the seven studied physical properties of alkanes obtained by substituting the spectral moments of **E** matrix by its expression in terms of embedding frequencies. The statistical parameters of these equations are identical to those obtained for equations illustrated in Table 2.

Equations in Table 6 permit an easy interpretation of the physical properties in terms of the molecular structure. In order to show the influence of the individual fragments on the properties, we calculate the mean effect that each subgraph produces on the physical properties. The mean

effects, the average contribution of each fragment on the calculated physical property, are illustrated in Table 7.

The estimates of the relative contributions of molecular mass, branching, and steric factors to the physical properties observed by Needham et al.<sup>28</sup> are similar in global terms to the mean effects of structural fragments illustrated in Table 7. On the other hand, we can appreciate the contribution that each fragment produces on the different properties. For example, the fragment  $F_1$  has a positive contribution to all properties with the exception of critical pressures and surface tensions;  $F_2$  contributes positively to all properties except to those related to molecular volume (molar volume and molar refraction), while  $F_3$  contributes positively only to MV and MR.

The present approach to quantitative structure—property relationship studies is, in some aspects, similar to the Smolenskii's additivity function.<sup>35</sup> Smolenskii's procedure is based on the decomposition of the molecular graph into different fragments. The fragments of a given type then become a variable in a multiple regression model. This approach, like the embedding frequencies, is a powerful tool in QSPR studies. The main disadvantage of the substructural approaches mentioned above is connected to the algorithmic complexity of the computation. These methods need one to generate all subgraphs in the molecular graph and then to check for isomorphism among these subgraphs. It is wellknown that the complexity of such algorithms is nonpolynomial<sup>36</sup> and, of course, the number of operations in the algorithm increases very fast, e.g., exponentially, with the number of vertices in the graph. This is a real limitation of such kinds of algorithms when they are applied to molecules of some structural complexity, such as polycyclic compounds.

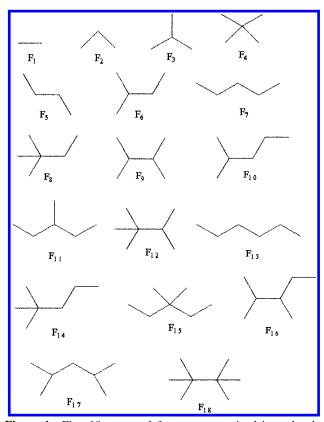
The method based on spectral moments of edge adjacency matrix also has some limitations similar to the Smolenskiitype of approaches.<sup>35</sup> The main drawback of our present approach is related to its performance in QSPR and QSAR studies when it is compared to those approaches that directly use the substructural fragments into correlations. The spectral moments are linear combinations of a series of structural fragments in the molecular graph, but not all of these fragments have a direct influence on the physical

Table 5. The First Eight Spectral Moments of E Matrix as Linear Combinations of the Number of Fragments in the Graph

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\begin{array}{l} \mu_0 = |F_1| \quad \mu_2 = 2 \times |F_2| \quad \mu_3 = 6 \times |F_3| \\ \mu_4 = 2 \times |F_2| + 12 \times |F_3| + 24 \times |F_4| + 4 \times |F_5| \\ \mu_5 = 30 \times |F_3| + 120 \times |F_4| + 10 \times |F_6| \\ \mu_6 = 2 \times |F_2| + 60 \times |F_3| + 480 \times |F_4| + 12 \times |F_5| + 24 \times |F_6| + 6 \times |F_7| + 36 \times |F_8| + 24 \times |F_9| \\ \mu_7 = 126 \times |F_3| + 1680 \times |F_4| + 84 \times |F_6| + 210 \times |F_8| + 112 \times |F_9| + 14 \times |F_{10}| + 14 \times |F_{11}| + 84 \times |F_{12}| \\ \mu_8 = 2 \times |F_2| + 252 \times |F_3| + 5544 \times |F_4| + 28 \times |F_5| + 200 \times |F_6| + 32 \times |F_7| + 1008 \times |F_8| + 464 \times |F_9| + 32 \times |F_{10}| + 40 \times |F_{11}| + 672 \times |F_{12}| + 8 \times |F_{13}| + 48 \times |F_{14}| + 46 \times |F_{15}| + 112 \times |F_{16}| + 536 \times |F_{17}| + 284 \times |F_{18}| \end{array}
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Table 6. Multiple Linear Regression Equations for the Physical Properties as Functions of Molecular Fragments

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\begin{array}{l} bp\ (^{\circ}C) = -76.719 + 23.992|F_1| + 5.01|F_2| - 13.332|F_3| + 17.880|F_4| + 1.492|F_6| \\ mv\ (cm^3) = 38.988 + 27.016|F_1| - 9.570|F_2| + 10.392|F_3| - 11.184|F_4| - 1.524|F_5| - 0.17|F_6| \\ MR\ (cm^3) = 5.703 + 5.506|F_1| - 0.724|F_2| + 1.050|F_3| - 0.797|F_4| - 0.120|F_5| \\ HV\ (kJ/mol) = 74.707 + 4.821|F_1| - 1.813|F_3| + 2.559|F_4| + 0.213|F_6| \\ TC\ (^{\circ}C) = 77.200 + 12.145|F_1| + 23.938|F_2| - 38.947|F_3| + 54.720|F_4| - 2.190|F_5| + 7.484|F_6| - 1.095|F_7| - 6.570|F_8| - 4.380|F_9| \\ PC\ (atm) = 48.376 - 6.606|F_1| + 3.706|F_2| - 4.316|F_3| + 5.710|F_4| + 0.248|F_5| + 0.544|F_6| - 0.116|F_7| - 0.694|F_8| - 0.462|F_9| \\ ST\ (dyn/cm) = 13.054 - 0.779|F_1| + 2.202|F_2| - 3.330|F_3| + 4.536|F_4| + 0.124|F_5| + 0.376|F_6| - 0.036|F_7| - 0.216|F_8| - 0.144|F_9| \end{array}
```



**Figure 1.** First 18 structural fragments contained in molecular graphs of alkanes.

property. For instance, some fragments contained in one spectral moment may have a positive contribution to the physical property, and others may have a negative or null influence on this property. As a consequence, in such cases this spectral moment does not describe linearly the studied property and the use of nonlinear fits are necessary. However, the spectral moments of edge adjacency matrix are very easy to calculate, and they can be combined in appropriate ways in order to produce very good correlations without loss of structural information.

The structural interpretation of spectral moments of the **E** matrix appears to be the most important feature of the present approach. This is the main difference among the models found in the present paper and those obtained by Needham *et al.*<sup>28</sup> According to Mihalic and Trinajstić,<sup>2</sup> some of the QSPR models obtained with the use of higher order connectivity indices and its combinations have a forbidding complexity.

**Table 7.** Mean Effect of the First Six Structural Fragments on the Physical Properties of Alkanes

property	$ F_1 $	$ F_2 $	$ F_3 $	$ F_4 $	$ F_5 $	$ F_6 $
bp	165.98	41.59	-37.62	7.83		7.93
MV	186.87	-79.35	28.58	-4.66	-10.33	-0.87
MR	38.08	-6.00	2.89	-0.33	-0.81	
HV	33.35		-4.99	1.07		1.09
TC	84.02	198.71	-109.91	23.97	-14.90	39.78
PC	-45.70	30.76	-12.18	2.50	1.69	2.89
ST	-5.39	18.26	-9.16	1.89	0.84	1.93

#### 5. CONCLUSIONS

The spectral moments of the edge adjacency matrix are a novel set of topological (graph theoretical) descriptors. These indices have a series of important features that make them useful molecular descriptors to be employed in QSPR and QSAR studies. The decomposition of spectral moments of the E matrix into substructural fragments permits the structural interpretation of the correlation found with them to describe the physical or biological properties of organic compounds. These indices can be used as a set of descriptors in QSPR and QSAR studies in the same way as they were used in the present work. However, spectral moments of the edge adjacency matrix can also be used in combination with pattern recognition techniques and in studies of similarity/dissimilarity features of molecules.

The correlations found by using spectral moments of the **E** matrix for the description of seven representative physical properties of alkanes can be considered as statistically significant. In general, the average contributions of each descriptor to the studied physical properties are similar to the contribution of molecular mass, branching, and steric features of molecules to such properties reported by Needham et al.<sup>28</sup>

The approach described in this paper appears to be a prominent method to find quantitative models for description of physical, thermodynamic, or pharmacological properties with a direct structural interpretation. The applications of the present method to QSAR studies of several classes of organic compounds are now in progress and will be the subject of a future publication.

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