Spectral Moments of the Edge Adjacency Matrix in Molecular Graphs. 3. Molecules Containing Cycles

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A substructural approach to quantitative structure−property relationships based on the spectral moments of the edge adjacency matrix is extended to molecules containing cycles. Spectral moments are expressed as linear combinations of structural fragments of any kind of nonweighted graphs. The boiling points of a series of 80 cycloalkanes was well-described by the present approach. The predictive power of the model was proved by using a test set of another 26 compounds. An equation that expresses the contribution of the different fragments of the molecules to the boiling point was obtained.

1. INTRODUCTION

The edge adjacency matrix, or bond matrix, of molecular graphs has become an interesting source of graph theoretical invariants to be used as molecular descriptors in quantitative structure−property[1,2] (QSPR) and quantitaive structure−activity relationship (QSAR) studies.[3] One of the most recent approaches based on such matrix is the study of its spectral moments. Spectral moments of the edge adjacency matrix have been used to describe seven representative physico-chemical properties of alkanes,[4] boiling points of alkyl halides,[5] antifungal activity of benzyl alcohols,[5] diamagnetic susceptibilities,[6] and chromatographic parameters[7] of organic compounds. In all of the studied cases the quantitative models obtained to describe physical or biological properties were statistically very significant. However, the main advantage of the present approach is concerned not only with its ability to quantitatively describe the properties but also with the "transparency" obtained in the interpretation of the final models.

Spectral moments of the bond matrix have been expressed in terms of structural fragments for both simple[4] and edge-weighted[5] molecular graphs. In both cases the spectral moments are expressed as linear combinations of structural fragments of molecules. This approach permits one to obtain quantitative models that describe a physical or biological property as a function of the easy-to-calculate spectral moments. Then, through a simple substitution of these variables by their expressions in terms of the structural fragment we can find a direct relationship between properties and "molecular structure". This is the final objective of any QSPR or QSAR study. However, when we use very complex graph theoretical descriptors, this relationship is lost.

On some occassions experimental properties are expressed in terms of some parameters which are related to the molecular structure, but they do not permit us to "see" what are the structural features of molecules that influence the studied property. These models permit the prediction of properties for molecules not even synthesized, but we cannot direct this synthesis in a rational way.

In the present work, we extend the approach of spectral moments of the edge adjacency matrix to molecules that contain cycles in their structures. These kinds of molecules are very important from the practical point of view. They represent an important part of the whole field of chemistry, and much of the chemical compounds with applications in chemical and pharmaceutical industries contain cycles in their structures. As a consequence we will find the expressions that relate spectral moments of cyclic graphs to the different subgraphs contained in them. In order to test the QSPR applicability of the present approach, we will study the boiling point of more than 100 cycloalkanes, including polycyclo- and spiroalkanes.

2. SPECTRAL MOMENTS OF THE BOND MATRIX FOR GRAPHS CONTAINING CYCLES

The edge adjacency matrix of graphs is defined in some treatises of graph theory and chemical graph theory.[8,9] This matrix corresponds to the vertex adjacency matrix of the line graph associated with a graph.[10] In the precedent papers of this series[4,5] we have defined the spectral moments of this matrix as follows:

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

where μ_k is the kth spectral moment of the edge adjacency matrix $\mathbf{E}$ and **tr** is the trace, i.e. the sum of diagonal entries, of such matrix. The rth spectral moment of the edge

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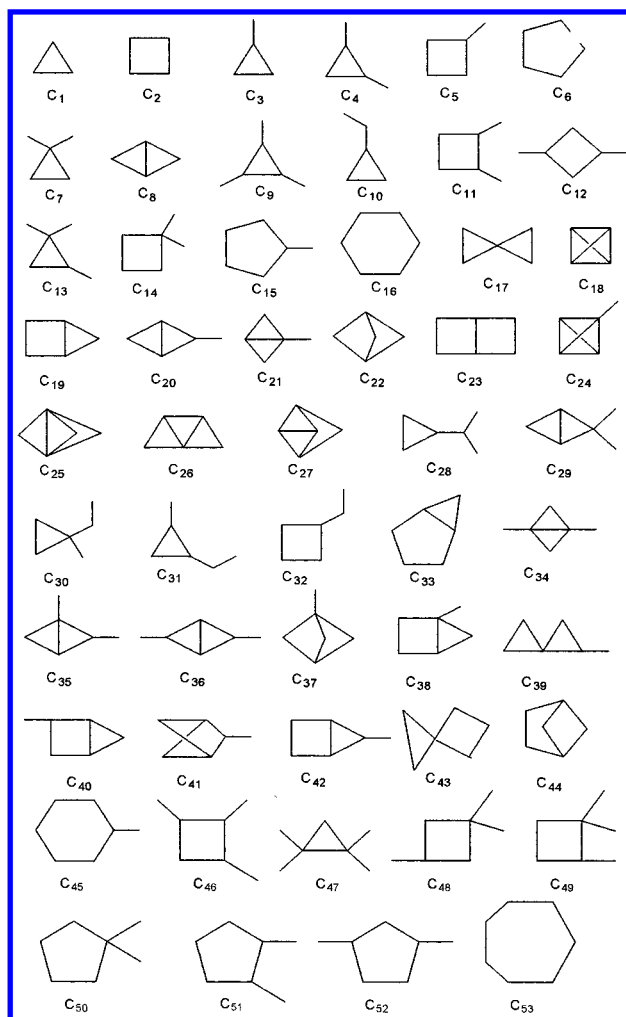
Table 1. Spectral Moments of the Bond Adjacency Matrix Expressed in Terms of Structural Fragments of Molecules Containing Cycles

$\mu_2 = 2|F_2|$

$\mu_3 = 6|F_3| + 6|C_1|$

$\mu_4 = 2|F_2| + 12|F_3| + 24|F_4| + 4|F_5| + 12|C_1| + 8|C_2| + 6|C_3|$

$\mu_5 = 30|F_3| + 120|F_4| + 10|F_6| + 30|C_1| + 40|C_3| + 10|C_4| + 10|C_6| + 20|C_7| + 40|C_8|$

$\mu_6 = 2|F_2| + 60|F_3| + 480|F_4| + 12|F_5| + 24|F_6| + 6|F_7| + 36|F_8| + 24|F_9| + 60|C_1| + 72|C_2| + 144|C_3| + 72|C_4| + 24|C_5| + 192|C_7| + 240|C_8| + + 12|C_9| + 12|C_{10}| + 12_1C_{11}| + 12|C_{12}| + 84|C_{13}| + 24|C_{14}| + 12|C_{15}| + 12|C_{16}| + 24|C_{17}| + 192|C_{18}| + 36|C_{19}| + 36|C_{20}| + 84|C_{21}| + 36|C_{22}|$

$\mu_7 = 126|F_3| + 1680|F_4| + 84|F_6| + 210|F_8| + 112|F_9| + 14|F_{10}| + 14|F_{11}| + 84|F_{12}| + 126|C_1| + 448|C_3| + 392|C_4| + 154|C_5| + 70|C_6| + 1064|C_7| + 1288|C_8| + 84|C_9| + 56|C_{10}| + 56|C_{11}| + 56|C_{12}| + 280|C_{13}| + 140|C_{14}| + 28|C_{15}| + 224|C_{17}| + 2016|C_{18}| + 196|C_{19}| + 336|C_{20}| + 826|C_{21}| + 252|C_{22}| + 28|C_{23}| + 336|C_{24}| + 420|C_{25}| + 238|C_{26}| + 168|C_{27}| + 28|C_{28}| + 84|C_{29}| + 28|C_{30}| + 14|C_{31}| + 14|C_{32}| + 42|C_{33}| + 168|C_{34}| + 70|C_{35}| + 28|C_{36}| + 84|C_{37}| + 70|C_{38}| + 28|C_{39}| + 42|C_{40}| + 28|C_{41}| + 28|C_{42}| + 28|C_{43}| + 28|C_{44}| + 14|C_{45}| + 14|C_{46}| + 56|C_{47}| + 28|C_{48}| + 28|C_{49}| + 28|C_{50}| + 14|C_{51}| + 14|C_{52}| + 14|C_{53}|$
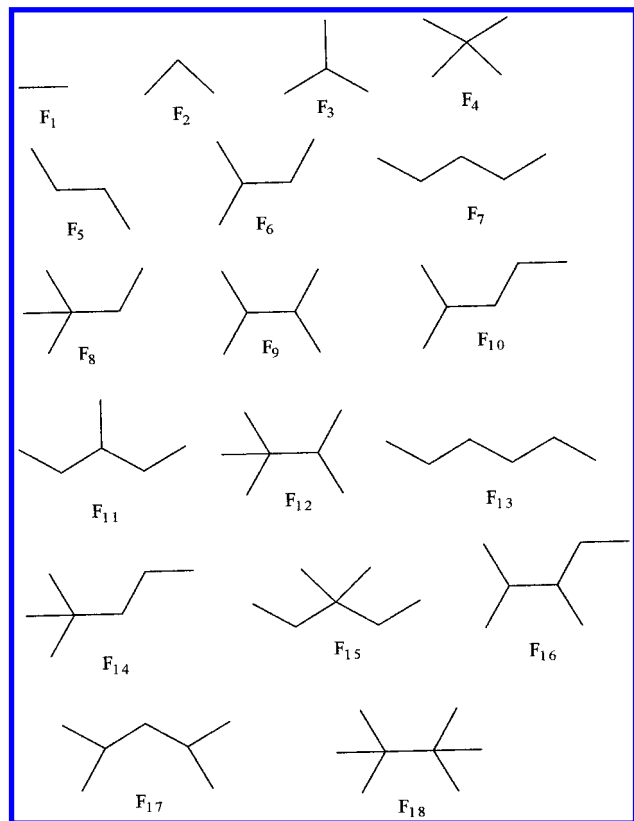
Figure 1. Acyclic subgraphs contained in spectral moments of the bond matrix in Table 1.

Figure 2. Cyclic subgraphs contained in spectral moments of the bond matrix in Table 1.

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 in the same vertex. Using this knowledge, we can express the spectral moments as a linear combination of the numbers of self-returning walks in the line graph, which correspond to certain structural fragments in the molecular graph. This procedure was used to find this kind of relationship for trees representing the molecular structures of alkanes.[4] In Table 1 we give expressions for the first seven spectral moments of the **E** matrix for graphs containing any kind of cycle. Of course, expressions relating moments and structural fragments of graphs for trees are completely contained in these expressions. As a consequence, expressions given in Table 1 can be considered as the general linear combinations of spectral moments in terms of subgraphs for any kind of nonweighted graphs. Acyclic and cyclic fragments appearing in Table 1 are illustrated in Figures 1 and 2, respectively.

3. DESCRIBING AND PREDICTING BOILING POINTS OF CYCLOALKANES

In order to illustrate the possibilities of the present approach in QSPR studies, we have selected the boiling point of 106 cycloalkanes.[11] This data set contains substituted mono- and polycycloalkanes as well as spiro-alkanes. It was randomly divided into two subsets; one contains 80 compounds which were used as a training set, and the other 26 compounds were used as a prediction or test set. By using a stepwise procedure, we obtain the best linear regression model that describes the boiling points of the prediction set as a function of spectral moments of the bond matrix. Following the results obtained by us in the study of boiling points of alkanes with the present approach,[4] we improved the linear model introducing the square root

Table 2. Experimental and Calculated Boiling Points of Cycloalkanes of the Training Set

no.	cyclane	bp obsd	calcd	residual	no.	cyclane	bp obsd	calcd	residual
1	cyclopropane	−32.8	−36.99	4.19	41	methylcycloheptane	134	133.38	0.62
2	cyclobutane	12.51	1.77	10.74	42	1,1-dimethylcyclohexane	119.543	116.49	3.053
3	spiropentane	40.6	49.42	−8.82	43	*trans*-1,2-dimethylcyclohexane	123.419	123.9	−0.481
4	methylcyclobutane	36.3	33.49	2.81	44	*cis*-1,3-dimethylcyclohexane	120.088	121.28	−1.192
5	cyclopentane	49.262	52.5	−3.238	45	*trans*-1,3-dimethylcyclohexane	124.45	121.28	3.17
6	1,1-dimethylcyclopropane	20.63	23.95	−3.32	46	*cis*-1,4-dimethylcyclohexane	124.321	121.51	2.811
7	*cis*-1,2-dimethylcyclopropane	37.03	30.15	6.88	47	ethylcyclohexane	131.783	133.19	−1.407
8	ethylcyclopropane	36	37.46	−1.46	48	cyclooctane	151.14	145.25	5.89
9	bicyclo[3.1.0]hexane	79.2	85.82	−6.62	49	1,1,2-trimethylcyclopentane	113.729	112.39	1.339
10	1,1-dimethylcyclobutane	56	54.31	1.69	50	*cis,cis*-1,2,3-trimethylcyclopentane	123	117.00	6.00
11	*cis*-1,2-dimethylcyclobutane	68	62.41	5.59	51	*cis,trans*-1,2,3-trimethylcyclopentane	117.5	117.00	0.50
12	*trans*-1,2-dimethylcyclobutane	60	62.41	−2.41	52	*trans,cis*-1,2,3-trimethylcyclopentane	110.2	117.00	−6.8
13	*cis*-1,3-dimethylcyclobutane	60.5	59.56	0.94	53	1-ethyl-1-methylcyclopentane	121.522	121.05	0.472
14	*trans*-1,3-dimethylcyclobutane	57.5	59.56	−2.06	54	isopropylcyclopentane	126.419	127.4	−0.981
15	cyclohexane	80.738	84.36	−3.622	55	1,1,2-trimethyl-2-ethylcyclopropane	104	103.22	0.78
16	methylcyclopentane	71.812	75.98	−4.168	56	1-methyl-1,2-diethylcyclopropane	108.5	114.83	−6.83
17	1,1,2-trimethylcyclopropane	52.48	54.66	−2.18	57	7,7-bicycloylbicyclo[2.2.1]heptane	143.5	143.2	0.3
18	*cis,cis*-1,2,3-trimethylcyclopropane	71	61.37	9.63	58	2-ethylbicyclo[2.2.1]heptane	146.5	154.66	−8.16
19	*cis,trans*-1,2,3-trimethylcyclopropane	66	61.37	4.63	59	4-methylspiro[5.2]octane	149	151.49	−2.49
20	*cis*-1-ethyl-2-ethylcyclopropane	70	64.86	5.14	60	1,2-dimethylcycloheptane	153	150.71	2.29
21	propylcyclopropane	68.5	72.82	−4.32	61	1,1,2-trimethylcyclohexane	145.2	136.28	8.92
22	isopropylcyclopropane	58.34	63.18	−4.84	62	1,1,3-trimethylcyclohexane	136.626	130.74	5.886
23	bicyclo[3.2.0]heptane	109.3	112.2	−2.9	63	1,1,4-trimethylcyclohexane	135	131.32	3.68
24	bicyclo[4.1.0]heptane	111.5	111.69	−0.19	64	1-ethyl-1-methylcyclohexane	152.16	144.59	7.57
25	2-cyclopropylbutane	90.98	94.75	−3.77	65	propylcyclohexane	156.724	159.77	−3.046
26	propylcyclobutane	100.6	100.42	0.18	66	isopropylcyclohexane	154.763	150.6	4.163
27	isopropylcyclobutane	92.7	91.13	1.57	67	cyclononane	178.4	171.95	6.45
28	methylcyclohexane	100.934	104.36	−3.426	68	1,1,2,2-tetramethylcyclopentane	135	124.67	10.36
29	1,1-dimethylcyclopentane	87.846	90.62	−2.774	69	1,1,3,3-tetramethylcyclopentane	117.96	115.29	2.67
30	*trans*-1,2-dimethylcyclopentane	91.869	98.15	−6.281	70	*cis*-1,2-dimethyl-1-ethylcyclopentane	143	140.15	3.15
31	*cis*-1,3-dimethylcyclopentane	91.725	95.52	−3.795	71	*trans*-1,2-dimethyl-1-ethylcyclopentane	142	140.15	2.15
32	*trans*-1,3-dimethylcyclopentane	90.773	95.52	−4.747	72	1-methyl-1-propylcyclopentane	146	147.4	−1.4
33	1,1,2,2-tetramethylcyclopropane	75.6	74.28	1.32	73	1,1-diethylcyclopentane	151	148.92	2.08
34	1,1,2,3-tetramethylcyclopropane	78.5	84.01	−5.51	74	*trans*-1,3-diethylcyclopentane	150	150.87	−0.87
35	1-methyl-1-isopropylcyclopropane	82.1	84.83	−2.73	75	*cis*-1-methyl-3-isopropylcyclopentane	142	141.76	1.76
36	1,1-diethylcyclopropane	88.67	92.95	−4.28	76	*trans*-1-methyl-3-isopropylcyclopentane	143	141.76	2.76
37	2-methylbicyclo[2.2.1]heptane	125.8	130.33	−4.53	77	isobutylcyclopentane	147.95	151.47	−3.52
38	3,3-dimethylbicyclo[3.1.0]hexane	115.3	110.49	4.81	78	*sec*-butylcyclopentane	154.35	153.79	0.56
39	1,1,3,3-tetramethylcyclobutane	78.2	86.57	−8.37	79	2-cyclopropylhexane	142.95	150.35	−7.4
40	*trans*-1,2-diethylcyclobutane	115.5	122.24	−6.74	80	3-cyclobutylpentane	151.5	146.12	5.38

of the zeroth spectral moment. This equation is given as follows:

$$\text{bp (°C)} = 209.65(\mu_0)^{0.5} - 2.05\mu_2 - 1.713\mu_3 - $$
$$0.863\mu_4 + 0.418\mu_5 - 8.166 \times 10^{-3}\mu_7 - 373.52 \quad (1)$$

$$n = 80 \qquad r = 0.9937 \qquad s = 4.80 \qquad F = 960$$

From the statistical point of view this equation can be considered a very significant model considering that the regression coefficient is higher than 0.99 and the standard deviation represents less than the 5% of the variance in the experimental property. In Table 2 we give the values of experimental and calculated boiling points for the prediction set, and Figure 3 illustrates the linear relationships existing between them.

The quality of a QSPR model is mainly expressed by its predictive power, measured for a test set of compounds not included in the training set. In Table 3 we illustrate the experimetal and calculated boiling points for the test set of 26 compounds. The root of the mean square error for the prediction set is 4.62, which represents only 4% of the variance in the experimental boiling points of these

compounds. As can be appreciated, the model found to describe the boiling point of cycloalkanes has a very good predictive power. The linear relationship between the experimental and predicted boiling points for these compounds is given in Figure 4.

As we previously pointed out, the main advantage of the present approach to QSPR and QSAR studies is the possibility of expressing the studied property in terms of the structural fragments of the molecules. By using expressions given in Table 1 that relate spectral moments to structural fragments of graphs, we can obtain the contributions of these fragments to the boiling point. The procedure consists only of the substitution of the spectral moments present in eq 1 by their expressions in terms of fragments and then summation of the contributions of identical fragments. By this way we obtain the equation illustrated in Table 4.

This table permits us to calculate the boiling point of any cycloalkane by counting the number of fragments of different kinds in the structure of the corresponding molecule. The other important question that is related to this approach is that we can easily interpret the studied property in terms of the molecular structure. This interpretation not only permits us to obtain some knowledge about what structural features
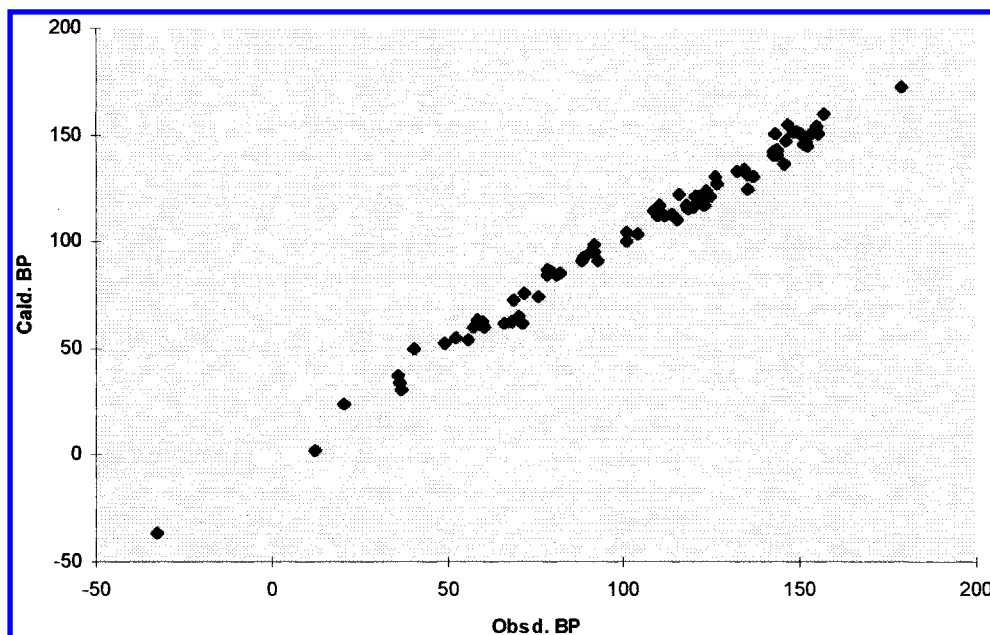
Figure 3. Correlation between experimental and calculated boiling points of cycloalkanes of the training set.
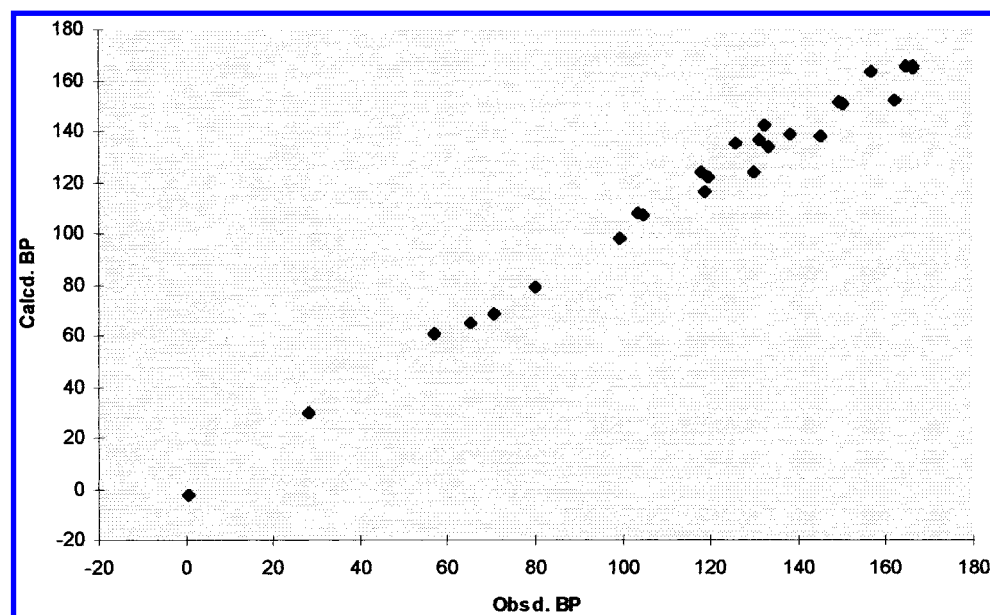

Figure 4. Correlation between experimental and calculated boiling points of cycloalkanes of the test set.

of the molecules influence the property and in what extension this influence is carried out by each substructure but also permit us to design new molecules having the desired property in a rational way.

The spectral moments of graph theoretical matrices appear to be a very promising structural invariant. The study of the spectral moments of the vertex adjacency matrix of molecular graphs has received great attention in the chemical literature.[12,13] The relationships between such moments and the energy in the Hückel theory was the first incentive for its study since the pioneering work of Hall[14] and Marcus.[15] Many other applications of this theory in quantum chemistry and physical chemistry have been reported up to now.[16-20] The other alternative of the use of spectral moments of graph theoretical matrices is what we are using in the present work: as structural descriptors to be used in QSPR and QSAR studies. Some reports of the use of spectral moments

of the vertex adjacency matrix of molecular graphs to the desrciption of physical properties of molecules have also been given in the literature. However, we think that the introduction of the present approach based on the bond adjacency matrix will contribute to the increase of the number of applications of spectral moments in computational and theoretical chemistry.

At present, when there exist several schemes of "rational" molecular design, we think that graph theoretical approaches need to be given an important step forward and that methods should be found that permit one to obtain significant quantitative models with "transparent" interpretation in terms of the structural features of molecules. The graph theoretical approach to chemistry has the necessary tools to carry out this labor efficiently. The scheme of the spectral moments of the edge adjacency matrix of molecular graphs represents a successful attempt in this way.

Spectral Moments of the Edge Adjacency Matrix

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Table 3. Experimental and Calculated Boiling Points of Cycloalkanes of the Test Set

		bp		
no.	cyclane	obsd	calcd	residual
1	methylcyclopropane	0.73	−2.34	3.07
2	*trans*-1,2-dimethylcyclopropane	28.21	30.15	−1.94
3	bicyclo[2.2.0]hexane	80.2	78.97	1.23
4	ethylcyclobutane	70.6	68.66	1.94
5	1-ethyl-1-methylcyclopropane	56.77	60.36	−3.59
6	*trans*-1,2-diethylcyclopropane	65	64.86	0.14
7	cycloheptane	118.79	116.11	2.68
8	*cis*-1,2-dimethylcyclopentane	99.532	98.15	1.382
9	ethylcyclopentane	103.466	107.67	−4.204
10	spiro[5.2]octane	125.5	135.02	−9.52
11	*cis*-1,2-dimethylcyclohexane	129.728	123.9	5.828
12	*trans*-1,4-dimethylcyclohexane	119.351	121.51	−2.159
13	1,1,2-trimethylcyclopentane	104.893	106.86	−1.967
14	propylcyclopentane	130.949	136.57	−5.621
15	2-cyclopropylpentane	117.74	123.66	−5.92
16	*cis*-bicyclo[4.3.0]nonane	166	164.59	1.41
17	1,1-dimethyl-2-ethylcyclopentane	138	138.33	−0.33
18	1,1-dimethyl-3-ethylcyclopentane	133	133.37	−0.37
19	*cis*-1,3-diethylcyclopentane	150	150.87	−0.87
20	butylcyclopentane	156.6	163.27	−6.67
21	*tert*-butylcyclopentane	144.85	138.18	6.67
22	dicyclobutylmethane	161.8	152.11	9.69
23	1,5-dimethylspiro[3.3]heptane	132.2	142.44	−10.24
24	4-methylspiro[5.2]octane	149	151.49	−2.49
25	2,6-dimethylbicyclo[3.2.1]octane	164.5	165.41	−0.91
26	3,7-dimethylbicyclo[3.3.0]octane	166	165.60	0.40

Table 4. Boiling Points of Cycloalkanes Expressed in Terms of Structural Fragments of Molecules

bp (°C) = $209.65|F_0|^{0.5} - 5.86|F_2| - 9.12|F_3| + 15.74|F_4| - 3.45|F_5| + 3.49|F_6| - 1.71|F_8| - 0.91|F_9| - 1.11|F_{10}| - 0.11|F_{11}| - 0.68|F_{12}| - 9.12|C_1| - 6.90|C_2| + 13.06|C_3| + 0.98|C_4| - 1.26|C_5| + 3.61|C_6| - 0.33|C_7| + 6.20|C_8| - 0.69|C_9| - 0.46|C_{10}| - 0.46|C_{11}| - 0.46|C_{12}| - 2.29|C_{13}| - 1.14|C_{14}| - 0.23|C_{15}| - 1.83|C_{17}| - 16.46|C_{18}| - 1.60|C_{19}| - 2.74|C_{20}| - 6.74|C_{21}| - 2.06|C_{22}| - 0.23|C_{23}| - 2.74|C_{24}| - 3.43|C_{25}| - 1.54|C_{26}| - 1.37|C_{27}| - 0.23|C_{28}| - 0.69|C_{29}| - 0.23|C_{30}| - 0.11|C_{31}| - 0.11|C_{32}| - 0.34|C_{33}| - 1.37|C_{34}| - 0.57|C_{35}| - 0.23|C_{36}| - 0.30|C_{37}| - 0.57|C_{38}| - 0.23|C_{39}| - 0.34|C_{40}| - 0.23|C_{41}| - 0.23|C_{42}| - 0.23|C_{43}| - 0.23|C_{44}| - 0.23|C_{45}| - 0.34|C_{46}| - 0.23|C_{47}| - 0.23|C_{48}| - 0.23|C_{49}| - 0.23|C_{50}| - 0.23|C_{51}| - 0.34|C_{52}| - 0.23|C_{53}| - 373.52$

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