

# Spectral Moments of the Edge Adjacency Matrix in Molecular Graphs. Benzenoid Hydrocarbons

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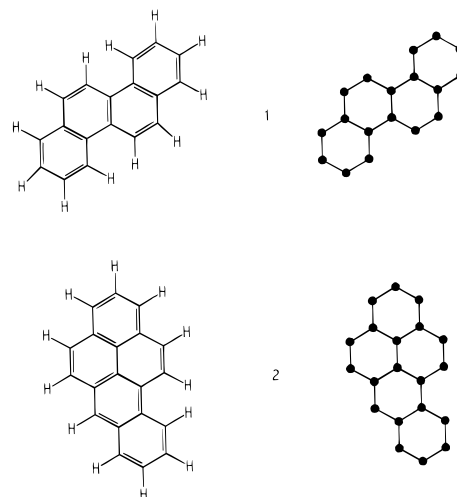
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The spectral moments of the edge adjacency matrix recently have been successfully employed in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) studies of alkanes, alkyl halides, benzyl alcohols, and cycloalkanes.<sup>1–3</sup> In this work we examined spectral moments of the edge adjacency matrix of benzenoid hydrocarbons. We designed combinatorial formulas for spectral moments up to the seventh order. Our expressions depend on counts of certain structural features that can easily be deduced from the molecular graph. The first few spectral moments of the edge adjacency matrix and of the vertex adjacency matrix depend on the very same structural parameters, implying that the two sets of moments are equivalent from the viewpoint of QSPR and QSAR studies. We demonstrate this for the total  $\pi$ -electron energy.

## 1. INTRODUCTION

In a series of recently published papers,<sup>1–3</sup> Estrada developed the theory of the spectral moments of the so-called edge adjacency matrix (which, in turn, is precisely the standard adjacency matrix of the line graph of the molecular graph<sup>4</sup>). Estrada's approach is the expansion of the spectral moments in terms of counts of certain fragments contained in the molecular graph. The same graph-theoretic technique was used earlier in the theory of the spectral moments of the standard adjacency matrix of the molecular graph.<sup>5–9</sup> (In line with Estrada's terminology, in what follows we refer to this "standard" adjacency matrix as the vertex adjacency matrix.) Estrada reported<sup>1–3</sup> a number of convincing quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) applications of the spectral moments of the edge adjacency matrix. These motivated us to examine the same moments for a special, but rather important, class of polycyclic molecules—the benzenoid hydrocarbons. As the main outcome of our research one should consider the (somewhat surprising) finding that the spectral moments of the edge adjacency matrix are determined by exactly the same structural features of the benzenoid molecules as are the spectral moments of the vertex adjacency matrix.

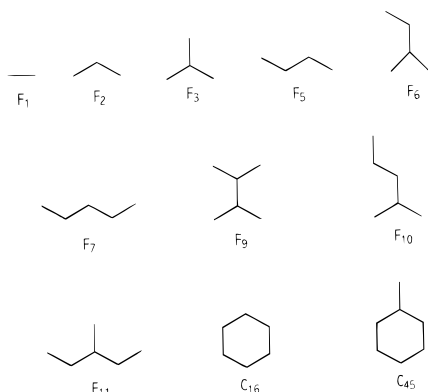
To describe the dependence of various physicochemical properties of organic substances on molecular structure, graph theory is often employed. Molecules are usually represented by so-called molecular graphs. The molecular graph of a conjugated hydrocarbon is the graph representation of the carbon-atom skeleton of the corresponding molecule. In this paper we are concerned with benzenoid hydrocarbons, i.e., with conjugated hydrocarbons composed entirely of condensed six-membered rings. In Figure 1 some examples of benzenoid hydrocarbons are presented, both by their structural formulas and corresponding molecular graphs.



**Figure 1.** Chrysene (1) and benzo[a]pyrene (2) presented by their structural formulas and molecular graphs.

Consider a molecular graph  $G$  with  $n$  vertices and  $m$  edges. It is commonly accepted to represent  $G$  by its vertex adjacency matrix  $\mathbf{A}$ . This is a square, symmetric matrix of order  $n$  whose  $(i,j)$ -entry is equal to unity if the vertices  $i$  and  $j$  are adjacent, and is equal to zero otherwise. The edge adjacency matrix  $\mathbf{E}$  is a square, symmetric matrix of order  $m$ , whose  $(i,j)$ -entry is equal to unity if the edges  $i$  and  $j$  are adjacent, and is equal to zero otherwise. In other words,  $\mathbf{A}$  reflects the adjacency of carbon atoms (existence of chemical bonds), whereas  $\mathbf{E}$  reflects the adjacency of these bonds. The edge adjacency matrix was mentioned in the chemical graph theory in refs 10 and 11. It was recently rediscovered<sup>12</sup> and found to be an important source of graph-theoretic invariants, suitable for generation of new molecular structure-descriptors.<sup>12–14</sup> Recall that the edge adjacency matrix of the molecular graph  $G$  is identical to the vertex adjacency matrix of the line graph of  $G$ .<sup>4</sup>

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**Figure 2.** Fragments of the molecular graph, contributing to the spectral moments (up to the seventh order) of the edge adjacency matrix of benzenoid hydrocarbons; their labeling is the same as that used by Estrada.<sup>3</sup>

The spectral moments of the vertex and edge adjacency matrices are defined as  $M_k = \text{tr} [A^k]$  and  $\mu_k = \text{tr} [E^k]$ , respectively, where  $\text{tr}$  stands for the trace (sum of diagonal entries) of the respective matrix.

The spectral moments of the **A** matrix have found noteworthy applications in the solid state physical chemistry.<sup>15–17</sup> When a continued fraction technique was used, the normalized moments were used to obtain the Hückel molecular orbital (HMO) density of states and other useful properties of solids. The applications of spectral moments of the same matrix in theoretical chemistry of conjugated molecules<sup>5–9,18–32</sup> are too numerous to be outlined here in due detail. In a series of papers moments were used for the estimation of HMO total  $\pi$ -electron energy and examination of its dependence on molecular structure.<sup>5–7,18–25</sup> A treatment based on the energy partitioning via spectral moments was proposed for dealing with aromaticity of conjugated systems.<sup>7,8</sup> Explicit expressions, in terms of counts of simple structural features, were designed for the first few spectral moments of various classes of molecular graphs. Particular attention was paid to benzenoid hydrocarbons,<sup>9,20,21,23,29</sup> acyclic polyenes,<sup>5</sup> and phenylenes.<sup>31</sup>

Investigations concerning spectral moments of the edge adjacency matrix began relatively recently.<sup>1–3</sup> These spectral moments were employed in QSPR and QSAR studies. For this purpose, the moments were expressed in terms of numbers of specific fragments contained in the molecular graph. Using the so-called moment-expansion technique, Estrada established the contributions of these molecular fragments to certain physicochemical properties of alkanes,<sup>1</sup> to the boiling points of alkyl halides,<sup>2</sup> to the antifungal activity of benzyl alcohols,<sup>2</sup> and to the boiling points of cycloalkanes.<sup>3</sup>

## 2. SPECTRAL MOMENTS OF THE EDGE ADJACENCY MATRIX OF BENZENOID HYDROCARBONS

Estrada's expressions for spectral moments of the **E**-matrix can be applied to any class of molecular graphs. If the spectral moments of nonweighted graphs are considered up to the seventh order, then not less than 12 acyclic and 53 cyclic fragments need to be taken into account.<sup>1–3</sup> In the special case of benzenoid hydrocarbons the number of relevant fragments is much smaller; these are depicted in Figure 2. Estrada's formulas for the first few spectral

moments of the **E**-matrix of benzenoid hydrocarbons read as follows:

$$\mu_0 = |F_1| \quad (1)$$

$$\mu_2 = 2|F_2| \quad (2)$$

$$\mu_3 = 6|F_3| \quad (3)$$

$$\mu_4 = 2|F_2| + 12|F_3| + 4|F_5| \quad (4)$$

$$\mu_5 = 30|F_3| + 10|F_6| \quad (5)$$

$$\mu_6 = 2|F_2| + 60|F_3| + 12|F_5| + 24|F_6| + 6|F_7| + 24|F_9| + 12|C_{16}| \quad (6)$$

$$\mu_7 = 126|F_3| + 84|F_6| + 112|F_9| + 14|F_{10}| + 14|F_{11}| + 14|C_{45}| \quad (7)$$

In these formulas the numbers of molecular fragments  $F_x$  and  $C_x$  are denoted by  $|F_x|$  and  $|C_x|$ , respectively. Thus, to apply eqs 1–7 one needs to count how many times each of these fragments is contained in the molecular graph. In the general case this is quite tedious and error prone. For instance, the simple tricyclic benzenoid systems anthracene and phenanthrene contain, respectively, 30 and 31 copies of the fragment  $F_5$ , values which are neither easy to compute nor to check. For benzenoids with more than, for example, six hexagons, the counting of the fragments depicted in Figure 2 becomes an almost prohibitively difficult task.

The structural features  $F_1$ ,  $F_2$ ,  $F_3$ , and  $C_{16}$  can be easily enumerated in any benzenoid molecule:  $|F_1| = m$ ,  $|F_2| = n_2 + 3n_3$ ,  $|F_3| = n_3$ ,  $|C_{16}| = h$ , where  $m$ ,  $n_2$ ,  $n_3$ , and  $h$  count the number of edges, vertices of degree 2, vertices of degree 3, and hexagons, respectively. The enumeration of the other fragments depicted in Figure 2 is a somewhat more perplexing combinatorial problem.

In the present paper we report alternative combinatorial formulas for spectral moments (up to  $\mu_7$ ) of the edge adjacency matrix of benzenoid hydrocarbons, eqs 8–14. Our expressions depend on invariants that can easily be deduced from the molecular graph.

Before presenting our main results, i.e., combinatorial formulas for  $\mu_k$ , we need to fix our notation. As much as possible we follow the notation and terminology suggested in refs 29 and 33, viz.:  $m$  is number of edges;  $n$  is number of vertices;  $h$  is number of hexagons ( $h = m - n + 1$ );  $B$  is number of bays;  $C$  is number of coves;  $F$  is number of fjords;  $b$  is number of bay regions ( $b = B + 2C + 3F$ );  $h_R$  is number of rings all of whose vertices are of degree 3 ( $h_R = h_{A3} + h_{A4} + h_{L4} + h_{L5} + h_{L6}$ ); and  $h_I$  is number of rings having exactly one vertex of degree 2 ( $h_I = h_{P3} + h_{P4}$ ).

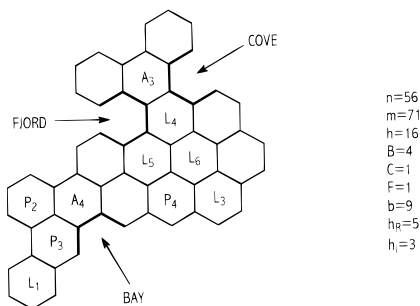
A self-explanatory example is depicted in Figure 3.

It is obvious that

$$\mu = m \quad (8)$$

and

$$\mu_1 = 0$$



**Figure 3.** Structural details of benzenoid hydrocarbons relevant for our expressions for the spectral moments, and their count in the given example.

In addition to this, we deduced the following formulas:

$$\mu_2 = 8m - 6n \quad (9)$$

$$\mu_3 = 12m - 12n \quad (10)$$

$$\mu_4 = 80m - 78n + 24 + [4b] \quad (11)$$

$$\mu_5 = 220m - 240n + 120 + [20b] \quad (12)$$

$$\mu_6 = 944m - 1026n + 612 + [96B + 198C + 300F + 12h_R + 6h_I] \quad (13)$$

$$\mu_7 = 3192m - 3640n + 2632 + [392B + 826C + 1260F + 56h_R + 28h_I] \quad (14)$$

Eqs 9–14 were designed by means of a reasoning similar to that used in ref 29. Namely, we may apply a theorem<sup>29</sup> stating that for any given value of  $k$ ,  $\mu_k$  increases with increasing size of the molecular graph at most as a linear function of  $n$ , and at most as a linear function of  $m$ . This implies that  $\mu_k$  should be presented in the following form

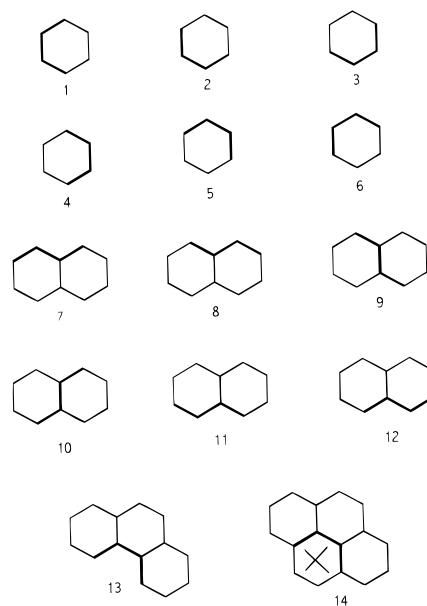
$$\mu_k = Am + Bn + C + r_k \quad (15)$$

Here,  $A$ ,  $B$ , and  $C$  are constants (dependent on  $k$ ), whereas  $r_k$  stands for the residual, embracing the effects of all other structural factors on the respective  $\mu_k$ . The parameters  $A$ ,  $B$ , and  $C$  in eq 15 were determined by means of a few selected examples of benzenoid hydrocarbons (linear polyacenes, parallelogram-type benzenoids). Then we tried to guess the form of  $r_k$  guided by our earlier experience gained by studying the moments  $M_k$  (cf. Section 4). The dependence of  $\mu_k$  on  $B$ ,  $C$ ,  $F$  (therefore on  $b$ ),  $h_R$ , and  $h_I$  is also linear. As expected,  $r_k$  happens to be numerically much smaller than the term  $Am + Bn + C$ , which greatly simplifies the finding of the respective expressions. In particular,  $r_k = 0$  for  $k = 0, 2$ , and  $3$ . In eqs 11–14 the residuals  $r_k$  are indicated by square brackets. It is an interesting fact that in all cases examined  $r_k$  is divisible by  $k$ .

Eqs 9–14 were checked on a large number of examples, including all possible types of benzenoid hydrocarbons. Exceptionally, the relations in eqs 13 and 14 do not apply to benzene. The final form of the combinatorial formulas for  $\mu_k$  could be proven in a rigorous mathematical manner.

### 3. EQUIVALENCE OF FORMULAS 1–7 AND 8–14

At the first glance, the expressions 1–7 are quite different from those in eqs 8–14. Nevertheless, they are mutually equivalent. To demonstrate this we first show that the right-



**Figure 4.** Possible arrangements of a fragment  $F_5$  in the molecular graph of a benzenoid hydrocarbon; for details, see text.

hand sides of eqs 3 and 10 coincide, and that the same is true for eqs 2 and 9 and for eqs 4 and 11.

As already noted,  $|F_3|$  is equal to the number  $n_3$  of vertices of degree 3. For benzenoid hydrocarbons<sup>33</sup>  $n_3 = 2(h - 1)$  and  $h = m - n + 1$ , implying

$$6|F_3| = 12(h - 1) = 12m - 12n$$

i.e., the right-hand sides of eqs 3 and 10 coincide.

Each vertex of degree 2 induces one fragment, and each vertex of degree 3 induces three fragments  $F_2$ . Therefore,  $|F_2| = n_2 + 3n_3 = n + 2n_3$ , because in benzenoid systems  $n_2 + n_3 = n$ . Then

$$2|F_2| = 2n + 4n_3 = 2n + 8(h - 1) = 2n + 8(m - n) = 8m - 6n$$

i.e., the right-hand sides of eqs 2 and 9 coincide.

Bearing in mind the above relations for  $|F_2|$  and  $|F_3|$ , by comparing eqs 4 and 11 we conclude that they will be equivalent if, and only if

$$|F_5| = 12m - 12n + 6 + b = 12(h - 1) + 6 + b = 6h + 6(h - 1) + b = 6h + 3n_3 + b \quad (16)$$

That relation 16 is indeed obeyed is seen from the following reasoning. In benzenoid systems there are three types of  $F_5$  fragments: type 1 –  $F_5$  is a subgraph of a single hexagon, type 2 –  $F_5$  is a subgraph of two (adjacent) hexagons, and type 3 –  $F_5$  spreads over three hexagons. Each hexagon contains six distinct  $F_5$  fragments of type 1 (cf. diagrams 1–6 in Figure 4). Therefore the number of such fragments is  $6h$ . Each pair of adjacent hexagons contains six distinct  $F_5$  fragments of type 2 (cf. diagrams 7–12 in Figure 4). On the other hand, each pair of adjacent hexagons implies the existence of a pair of vertices of degree 3. Therefore, the count of type 2 fragments  $F_5$  is equal to  $3n_3$ . Fragments  $F_5$  of type 3 must be of the form depicted in diagram 13 in Figure 4, i.e., they must correspond to a bay region. The hexagon marked by X (see diagram 14 in Figure

4) must not be present, because otherwise the respective  $F_5$  fragment would be of type 1 (with respect to X). Hence, the number of  $F_5$  fragments of type 3 is equal to the number  $b$  of bay regions.

By summing the numbers of  $F_5$  fragments of types 1, 2, and 3, namely  $6h$ ,  $3n_3$  and  $b$ , we arrive at the right-hand side of eq 16. Consequently, formulas 4 and 11 are equivalent.

The verification of the equivalence of the remaining pairs of expressions for the spectral moments of the edge adjacency matrix is significantly more cumbersome and will not be pursued in this paper.

#### 4. COMPARING SPECTRAL MOMENTS OF THE EDGE AND VERTEX ADJACENCY MATRICES OF BENZENOID HYDROCARBONS

Expressions for the first few (even) spectral moments of the vertex adjacency matrix of benzenoid hydrocarbons were determined previously.<sup>29,30</sup> They read as follows:

$$M_0 = n \quad (17)$$

$$M_2 = 2m \quad (18)$$

$$M_4 = 18m - 12n \quad (19)$$

$$M_6 = 158m - 144n + 48 + [6b] \quad (20)$$

$$M_8 = 1330m - 1364n + 704 + [80B + 168C + 256F + 16h_R + 8h_I] \quad (21)$$

Recall that for alternant hydrocarbons (and thus for benzenoids) all odd spectral moments are necessarily equal to zero.

Comparing eqs 8–14 with 17–21, we reach the remarkable and by no means expected conclusion that precisely the same structural invariants determine the first few spectral moments of both the vertex and edge adjacency matrix. In particular,  $\mu_3$ ,  $\mu_2$ , and  $M_2$  depend solely on  $m$  and  $n$ . The situation is analogous with  $\mu_5$ ,  $\mu_4$ , and  $M_6$ . They are all determined by  $m$ ,  $n$ , and  $b$ . Further,  $\mu_7$ ,  $\mu_6$ , and  $M_8$  are expressed in terms of  $m$ ,  $n$ ,  $B$ ,  $C$ ,  $F$ ,  $h_R$ , and  $h_I$ . All of the mentioned dependencies are linear, suggesting that the spectral moments of the two matrices might also be linearly dependent. This, in turn, implies that expressing some physicochemical property of benzenoid hydrocarbons as a linear combination of the lower  $M_k$  values or of the lower  $\mu_k$  values would yield identical or very similar results. In other words, there would be no advantage in using spectral moments of the edge adjacency matrix instead of the spectral moments of the vertex adjacency matrix. In the subsequent section we show this for the total  $\pi$ -electron energy of benzenoid hydrocarbons.

#### 5. AN APPLICATION OF SPECTRAL MOMENTS: TOTAL $\pi$ -ELECTRON ENERGY OF BENZENOID HYDROCARBONS

The total  $\pi$ -electron energy ( $E$ ) is an important theoretical characteristic of conjugated molecules and of benzenoid hydrocarbons in particular.<sup>34</sup> The possibility to express  $E$  as a linear function of the spectral moments has been considered by many authors.<sup>5,7,8,18,19,27,32</sup> Curiously, however, the simple

**Table 1.** Statistical Parameters Needed for the Comparison of the Quality of the Approximations 22 and 23; for Details See Text

$p$	correlation coefficient		average error (%)		sample dispersion $\cdot 10^4$	
	eq 22	eq 23	eq 22	eq 23	eq 22	eq 23
0	0.9993	0.9993	0.59	0.59	917.687	909.374
1	0.9998		0.31		218.176	
2		0.9998		0.31		218.176
3	0.99995		0.16		66.307	
4	0.99997	0.99995	0.13	0.16	44.633	66.307
5	0.999989		0.09		14.832	
6	0.999990	0.99997	0.08	0.13	13.673	44.633
7	0.999990	0.99997	0.08	0.13	13.447	43.873
8	0.999994	0.999989	0.06	0.08	8.215	14.184
9	0.999995	0.999989	0.05	0.08	6.733	14.149
10	0.999996	0.999992	0.05	0.07	5.706	10.611

**quantitative** approach described below does not seem to have been accomplished ever before.

In this section we report results of the investigation of the dependence of  $E$  of benzenoid hydrocarbons on both  $M_k$  and  $\mu_k$ . Our aim was to show that there is a certain advantage when using  $\mu_k$  instead of  $M_k$ . For that purpose  $E$  is approximated by means of the polynomials:

$$E \approx a_0 M_0 + a_1 M_2 + \dots + a_p M_{2p} + a_{p+1}; \quad p = 0, 1, 2, \dots, 10 \quad (22)$$

$$E \approx b_0 \mu_0 + b_2 \mu_2 + b_3 \mu_3 + \dots + b_p \mu_p + b_{p+1}; \quad p = 0, 2, 3, \dots, 10 \quad (23)$$

in which the multipliers  $a_k$  and  $b_k$ , where  $k = 0, 1, \dots, p+1$ , were determined by least-squares fitting. Such optimizations were done for all values of  $p$  indicated in eqs 22 and 23.

The calculations were performed on a set of 106 benzenoid hydrocarbons, taken from the book of Zahradnik and Pancir.<sup>35</sup> (This set is usually employed when approximate formulas for  $E$  of benzenoid molecules are studied.<sup>34</sup>) The correlation coefficients, average relative errors, and sample dispersions pertaining to eqs 22 and 23 are given in Table 1.

It is well known that  $M_4$  of benzenoid hydrocarbons is linearly dependent on  $M_0$  and  $M_2$ . The consequence of this is that the introduction of  $M_4$  into eq 22, i.e., the choice  $p = 2$ , results in statistical parameters identical to those for  $p = 1$ . For the same reason (namely because  $\mu_3$  and  $\mu_5$  are linearly dependent on the lower spectral moments), for eq 23 the choices  $p = 3$  and  $p = 5$  yield results identical to  $p = 2$  and  $p = 4$ , respectively. Accordingly, the respective results are omitted from Table 1.

The increase of  $p$  in eqs 22 and 23 necessarily increases the correlation coefficients and decreases the relative average errors and sample dispersions. For the first few values of  $p$  such improvements of the qualities of approximations are statistically significant. With increasing value of  $p$  these improvements decrease, and for  $p > 10$  the improvements become irrelevant.

One may observe that the sample dispersions for  $p = 1$ , 3, and 4 in eq 22 are identical to those for  $p = 2$ , 4, and 6 in eq 23, respectively. The sample dispersions for  $p = 0$  in eqs 22 and 23 are similar, although that for eq 23 is slightly smaller. This shows that  $M_2$  and  $\mu_2$  (or  $\mu_3$ ),  $M_6$  and  $\mu_4$  (or  $\mu_5$ ), as well as  $M_8$  and  $\mu_6$  are mutually linearly dependent. This also means that we can achieve the same quality of approximation of  $E$  of benzenoids by using either  $M_k$  or  $\mu_k$



in the moment expansion procedure. For instance, the approximations  $E \approx a_0 M_0 + a_1 M_2 + a_3 M_6 + a_4 M_8 + a_5$  and  $E \approx b_0 \mu_0 + b_2 \mu_2 + b_4 \mu_4 + b_6 \mu_6 + b_7$  have precisely the same accuracy.

## 6. CONCLUDING REMARKS

Although the edge and vertex adjacency matrices reflect quite different types of structural relations in the underlying molecules, there is a deep congruence between their lower spectral moments, at least for benzenoid hydrocarbons. The spectral moments of the two matrices are linearly dependent. Therefore, expressing a physicochemical property of benzenoid hydrocarbons in terms of the first few spectral moments of the vertex adjacency matrix, or of the edge adjacency matrix, yields either identical or very similar results. In general, in QSPR and QSAR studies of benzenoid hydrocarbons, on the basis of linear combination of spectral moments, it makes no difference whether one uses the vertex adjacency matrix or the edge adjacency matrix.

It seems that the above redundancy does not exist in structurally more diverse classes of molecules, but this still needs to be demonstrated.

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