

# Tenth Spectral Moment for Molecular Graphs of Phenylenes

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Our investigations are motivated by recent papers concerning the spectral moments of the edge-adjacency matrix, which were successfully employed in QSAR and QSPR studies of different classes of compounds [Estrada, E. *J. Chem. Inf. Comput. Sci.* **1996**, 36, 844–849; **1997**, 37, 320–328; **1998**, 38, 23–27]. In this work, the evaluation of the 10th spectral moment of the vertex-adjacency matrix for phenylenes is considered. This is achieved by using the method of Hall [Hall, G. G. *Theor. Chim. Acta* **1986**, 70, 323–332], which was originally applied to benzenoid systems and then adopted for molecular graphs of phenylenes [Marković, S.; Stajković, A. *Theor. Chem. Acc.* **1997**, 96, 256–260]. It is found that the 10th spectral moment can be expressed in terms of 6 mutually independent invariants that can be easily deduced from the molecular graph.

## 1. INTRODUCTION

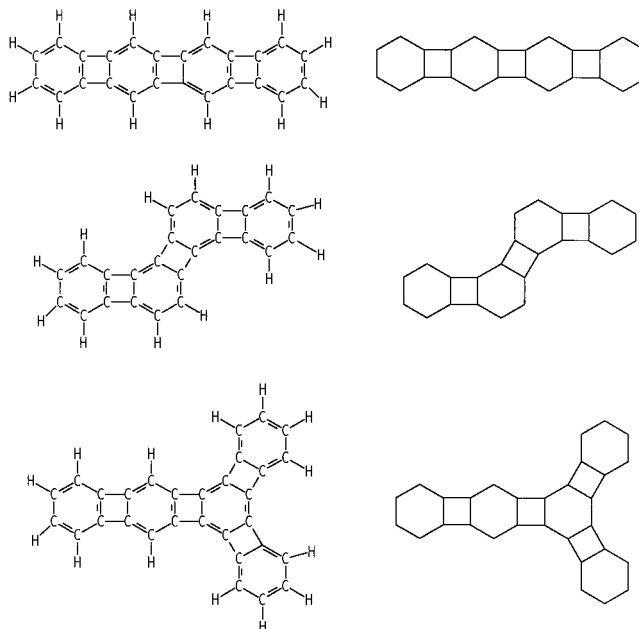
To explain the dependence of various physicochemical properties of compounds, molecular structure graph theory is often employed.<sup>1–3</sup> Concerning graph theory, the molecules are represented by their molecular graphs. Relevant information about the molecular structure is contained in the spectrum of the molecular graph and its spectral moments.

The molecular graph of a conjugated hydrocarbon is the graph representing the carbon-atom skeleton of the corresponding molecule. In this paper, we are concerned with a special class of conjugated hydrocarbons—phenylenes. These compounds are composed of six- and four-membered rings, where the six-membered rings (hexagons) are adjacent only to four-membered rings and every four-membered ring is adjacent to a pair of hexagons. In Figure 1, some examples of phenylenes are presented by their structural formulas and corresponding molecular graphs.

A phenylene containing  $h$  hexagons is called an  $[h]$ -phenylene. It is assumed that the number of four-membered rings of an  $[h]$ -phenylene amounts to  $h - 1$ , meaning that the structures in which alternating six- and four-membered rings are linked together in phenylenic super-rings are not considered in this paper.

The experimental chemistry of phenylenes is rapidly expanding, owing mainly to the work of Vollhardt's research group. Since the phenylenes combine strain with aromatic and antiaromatic rings and, as a consequence, exhibit unique physicochemical properties, they are especially interesting for theoreticians. More information on this matter can be found in the reviews<sup>4,5</sup> as well as in recent papers concerned with both experimental<sup>6–10</sup> and theoretical aspects<sup>11–19</sup> of phenylene chemistry.

Let  $G$  be a molecular graph with  $n$  vertexes and  $m$  edges. The vertex-adjacency matrix of  $G$ , denoted by  $\mathbf{A}$ , is a square, symmetric matrix of order  $n$  whose elements  $A(i, j)$  are equal to units and zeros, depending on whether the vertexes  $i$  and  $j$  are adjacent or not. Then the eigenvalues of  $\mathbf{A}$ ,  $x_1, x_2, \dots$ ,



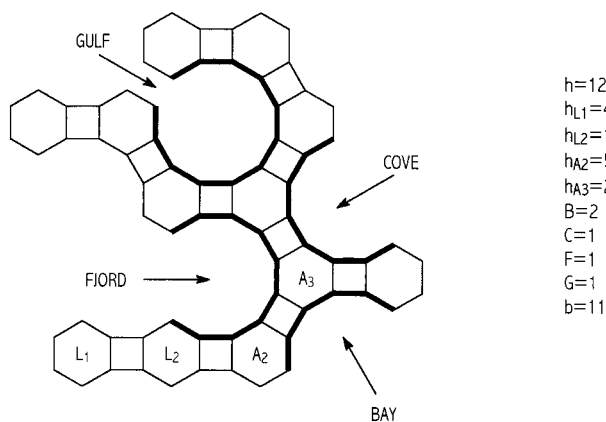
**Figure 1.** Some examples of phenylenes presented by their structural formulas and corresponding molecular graphs.

$x_n$ , form the spectrum of  $G$ . The  $k$ th spectral moment of  $G$  is given by

$$M_k = M_k(G) = \sum_{i=1}^n (x_i)^k \quad (1)$$

The spectral moments of the  $\mathbf{A}$  matrix have found noteworthy applications in solid-state physical chemistry.<sup>20–22</sup> Namely, using a continued fraction technique, the normalized moments were used to obtain the HMO density of states and other useful properties of the solids. The applications of the spectral moments of the same matrix in theoretical chemistry of conjugated molecules are too numerous to be outlined here in due detail.<sup>23–42</sup> In a series of papers, moments were used for the estimation of HMO total  $\pi$ -electron energy and the examination of its dependence on molecular struc-

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**Figure 2.** Types of hexagons; the bay regions of phenylenes: bay, cove, fjord, and gulf and their counts in the given example.

ture.<sup>23–33,35,39,40</sup> A treatment based on the energy partitioning via spectral moments was proposed for dealing with the aromaticity of conjugated systems.<sup>33,34</sup> In all applications of spectral moments, it is necessary to understand how they depend on the molecular structure. For this purpose, explicit expressions, in terms of counts of simple structural features, were designed for the first few spectral moments of various classes of molecular graphs. These formulas express the dependence of spectral moments on molecular topology and, thus, provide a connection between the molecular structure and some physicochemical properties of the compounds considered. In this field, particular attention has been paid to benzenoid hydrocarbons,<sup>26,27,30,37,38,40</sup> acyclic polyenes,<sup>25</sup> and phenylenes.<sup>42</sup> In the case of phenylenes, explicit topological formulas for the spectral moments, up to  $M_8$ , were derived.<sup>42</sup>

The investigations concerning the spectral moments of the edge-adjacency matrix (**E**) have recently commenced. **E** is a square, symmetric matrix of order  $m$  whose elements  $E(i,j)$  are equal to units and zeros, depending on whether the edges  $i$  and  $j$  of  $G$  are adjacent or not. Estrada employed the spectral moments of **E** in the quantitative structure–property (QSPR) and quantitative structure–activity (QSAR) relationship studies. For this purpose, the spectral moments of the **E** matrix were expressed in terms of the structural fragments of molecules, and then they were used to predict some physicochemical properties of alkanes,<sup>43</sup> the boiling points of alkyl halides,<sup>44</sup> the antifungal activity of benzyl alcohols,<sup>44</sup> and the boiling points of cycloalkanes.<sup>45</sup>

Estrada's research motivated us to take part in the exploration of the spectral moments of the **E** matrix<sup>46,47</sup> and to renew our investigations concerning the spectral moments of the **A** matrix. In the present paper, we consider the evaluation of the 10th spectral moment of the vertex-adjacency matrix for molecular graphs of phenylenes. In what follows, the spectral moments of the vertex-adjacency matrix will be simply called the spectral moments.

## 2. TOPOLOGICAL FORMULAS FOR THE SPECTRAL MOMENTS OF PHENYLENES

We first mention some topological invariants which will be needed in the text below. All symbols used in this paper refer to the graphs of phenylenes, although we follow the terminology suggested for benzenoid hydrocarbons.<sup>48</sup> Hence,  $h$  stands for the number of hexagons of phenylenes. There

are four types of hexagons in phenylenes that can be distinguished with respect to their mutual position:  $L_1$ ,  $L_2$ ,  $A_2$ , and  $A_3$ . Their definition is clear from a self-explanatory example given in Figure 2.  $h_{L1}$ ,  $h_{L2}$ ,  $h_{A2}$ , and  $h_{A3}$  represent the number of hexagons of types  $L_1$ ,  $L_2$ ,  $A_2$ , and  $A_3$ , respectively. In Figure 2, some structural details of the perimeter of phenylenes are also indicated: a bay, a cove, a fjord, and a gulf. The number of such fragments are denoted by  $B$ ,  $C$ ,  $F$ , and  $G$ , respectively. Then the number of bay regions ( $b$ ) is determined as  $b = B + 2C + 3F + 4G$ .

It is well-known that all odd spectral moments of bipartite graphs (and thus of phenylenes) are equal to zero. The expressions for the first few even spectral moments of the molecular graphs of phenylenes read as follows:

$$M_0 = 6h \quad (2)$$

$$M_2 = 16h - 4 \quad (3)$$

$$M_4 = 80h - 44 \quad (4)$$

$$M_6 = 484h - 352 + 6b \quad (5)$$

$$M_8 = 3136h - 2636 + 128b + 16h_{A_3} \quad (6)$$

$$M_{10} = 20\,976h - 19\,504 + 1680B + 3370C + 5060F + 6750G + 580h_{A_3} \quad (7)$$

The expressions (2)–(6) have been earlier communicated.<sup>42</sup> The topological formula for the 10th spectral moment of phenylenes (eq 7) is derived in the present paper. It is obvious that the actual form of  $M_k$  becomes more and more complicated with increasing  $k$ . One can expect that formulas for higher spectral moments would be hopelessly complicated, implying that investigations along the same lines would not be profitable.

Formula 7 expresses the dependence of  $M_{10}$  on molecular structure of phenylenes. The size of a molecule ( $h$ ) and number of bays, coves, fjords, gulfs, and  $A_3$ -type hexagons exert influence on the  $M_{10}$  of phenylenes. All the mentioned graphical invariants can be easily deduced from the molecular graphs of phenylenes. For instance, the calculation of  $M_{10}$  for the example given in Figure 2 reads

$$M_{10} = (20\,976 \times 12) - 19\,504 + (1680 \times 2) + 3370 + 5060 + 6750 + (580 \times 2) = 251\,908$$

## 3. METHOD FOR DERIVING THE $M_{10}$ OF PHENYLENES

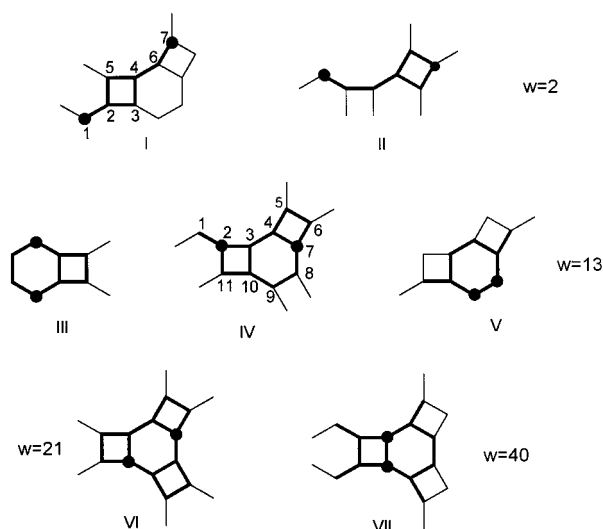
The derivation of eq 7 is achieved by using the method of Hall,<sup>30</sup> which was originally applied to benzenoid hydrocarbons<sup>30,38</sup> and then modified for phenylenes.<sup>42</sup>

It is well-known that  $M_k$  of an arbitrary molecular graph can be expressed as

$$M_k = \text{Tr}[\mathbf{A}^k] \quad (8)$$

where  $\text{Tr}$  denotes the trace of the respective matrix, and an element  $[\mathbf{A}^k]_{ij}$  is equal to the number of walks of length  $k$  between the vertexes  $i$  and  $j$ . In the case of bipartite graphs, eq 8 can be put into the form

$$M_{2k} = \text{Tr}[\mathbf{B}]^2 \quad (9)$$



**Figure 3.** Structural fragments of phenylenes enabling 2, 13, 21, and 40 walks of length 5. The vertexes where a certain walk starts and ends are marked by heavy dots.

where **B** denotes the symmetric matrix  $A^k$ . Recall that the trace of the square of a symmetric matrix is equal to the sum of the squares of all elements of that symmetric matrix. This fact provides a justification for presenting even spectral moments in the form

$$M_{2k} = \sum_{ij} (B_{ij})^2 \quad (10)$$

As a consequence of eq 10, the  $2k$ th spectral moment can be deduced from the matrix **B** (i.e.,  $A^k$ ) by squaring each element and adding them together. For such a calculation, we must know which numbers appear as the elements of the **B** matrix and how many times. Let  $b_w$  denote how many times a certain value  $w$  appears among the matrix elements of **B**. Then we have

$$M_{2k} = \sum_{w=1}^{\infty} b_w w^2 \quad (11)$$

Bearing in mind that an element  $B_{ij}$  is equal to the number of walks of length  $k$  between the vertexes  $i$  and  $j$ , we can conclude that  $b_w$  represents the number of structural fragments of alternant hydrocarbons considered, which enable  $w$  distinct walks of length  $k$ . In the case of the  $M_{10}$  of phenylenes,  $b_w$  represents the number of structural details of phenylenes enabling  $w$  distinct walks of length 5. Consequently, the problem of deriving the  $M_{10}$  of phenylenes is reduced to the recognition and enumeration of structural fragments of phenylenes that enable walks of length 5.

#### 4. RECOGNITION AND ENUMERATION OF STRUCTURAL FRAGMENTS ENABLING WALKS OF LENGTH 5

The first part of the problem (recognition) was resolved in the following manner: all possible fragments of phenylenes providing walks of length 5 were considered and classified according to their  $w$  values. A systematic examination shows that  $w$  can assume the values 1–5, 8–14, 16–19, 21–23, 34, and 37–40.

Now we have to determine the coefficients  $b_w$  (enumeration). This part of the task requires a very detailed combinatorial consideration. It turned out to be profitable to identify the vertexes from which  $w$  distinct walks of length 5 start and then to enumerate these vertexes. We observed that particular attention should be paid to various types of hexagons and structural fragments of phenylenes depicted in Figure 2. Our research shows that the coefficients  $b_w$  obey the following expressions:

$$b_1 = 12h - 20 - 2B - 2C - 2F - 2G + 8h_{A_3} \quad (12)$$

$$b_2 = 8B + 16C + 24F + 32G \quad (13)$$

$$b_3 = 8h - 8 \quad (14)$$

$$b_4 = 4h_{L_2} \quad (15)$$

$$b_5 = 2B + 4C + 6F + 8G \quad (16)$$

$$b_8 = 4h - 4 - 4B - 6C - 8F - 10G \quad (17)$$

$$b_9 = 4B + 4C + 4F + 4G \quad (18)$$

$$b_{10} = 4B + 10C + 16F + 22G + 8 - 8h_{A_3} \quad (19)$$

$$b_{11} = 8h - 12 - 6B - 12C - 18F - 24G + 10h_{A_3} \quad (20)$$

$$b_{12} = 4h_{L_1} \quad (21)$$

$$b_{13} = 4 + 6B + 12C + 18F + 24G - 4h_{A_3} \quad (22)$$

$$b_{14} = 4h_{A_3} + 8 \quad (23)$$

$$b_{16} = 2h_{L_2} \quad (24)$$

$$b_{17} = 8h - 8 - 12h_{A_3} \quad (25)$$

$$b_{18} = 2h_{A_2} + 4h_{L_2} \quad (26)$$

$$b_{19} = 4h_{A_2} + 12h_{A_3} \quad (27)$$

$$b_{21} = 6h_{A_3} \quad (28)$$

$$b_{22} = 4h_{L_1} + 4h_{A_2} \quad (29)$$

$$b_{23} = 8h_{L_2} \quad (30)$$

$$b_{34} = 2B + 4C + 6F + 8G \quad (31)$$

$$b_{37} = 4h - 4 - 4B - 6C - 8F - 10G \quad (32)$$

$$b_{38} = 4h - 4 + 6h_{A_3} - 4C - 8F - 12G \quad (33)$$

$$b_{39} = 4B + 10C + 16F + 22G - 12h_{A_3} \quad (34)$$

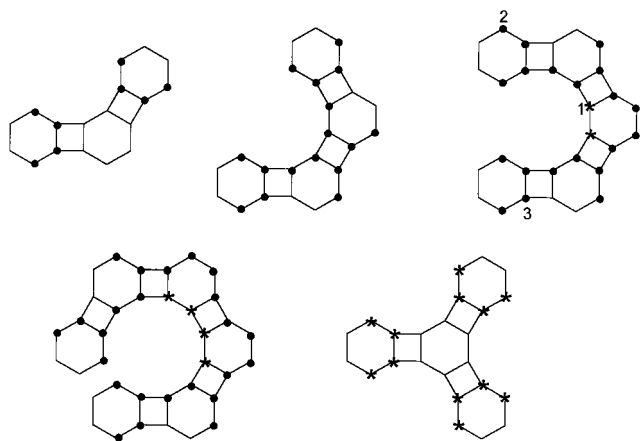
$$b_{40} = 6h_{A_3} \quad (35)$$

By substituting eqs 12–35 back into eq 11, we arrive at

$$M_{10} = 14\,872h - 12\,320 + 3756B + 7522C + 11\,288F + 15\,054G + 4048h_{A_3} + 2512h_{L_1} + 6104h_{L_2} + 4028h_{A_2}$$

which is easily transformed into eq 7.

Since the evaluation of  $b_w$  involves a very complex combinatorial consideration, we present here only the details



**Figure 4.** Arrangement of the vertexes which are the starting points for 1 (heavy dots) and 2 (asterisks) structural fragments of phenylenes enabling 2 walks of length 5.

concerning  $b_2$ ,  $b_{13}$ ,  $b_{21}$ , and  $b_{40}$ . Structural fragments of phenylenes enabling 2, 13, 21, and 40 walks of length 5 are depicted in Figure 3. As an illustration, we present the 2 walks of length 5 for fragment I and the 13 walks of length 5 for fragment IV.

$w = 2$ : 1-2-5-4-6-7, 1-2-3-4-6-7

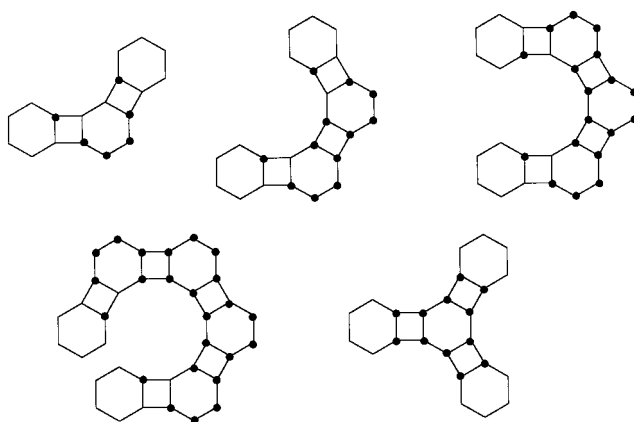
$w = 13$ : 2-1-2-3-4-7, 2-11-10-9-8-7,  
2-11-2-3-4-7, 2-11-10-3-4-7,

2-3-10-9-8-7, 2-3-4-5-6-7,  
2-3-4-7-4-7, 2-3-4-3-4-7, 2-3-4-7-8-7,

2-3-4-5-4-7, 2-3-4-7-6-7,  
2-3-2-3-4-7, 2-3-10-3-4-7

Let us pay attention to fragment I in Figure 3. There are 2 walks of length 5 between the vertexes marked by heavy dots, either starting at 1 and ending at 7 or starting at 7 and ending at 1. This means that fragment I provides 2 starting points for 2 walks of length 5. The situation is, certainly, analogous with all other structural details in Figure 3. It goes without saying that walks of both directions must be taken into account. For this reason, it is profitable to base the derivation of  $b_w$  on identification and enumeration of the vertexes which are the starting points for  $w$  distinct walks of length 5 (heavy dots in Figure 3). In the following text, the vertexes from which 2, 13, 21, and 40 walks of length 5 start will be called the  $W_2$ -,  $W_{13}$ -,  $W_{21}$ - and  $W_{40}$ -type vertexes.

Structural fragments of phenylenes enabling 2 walks of length 5 (fragments I and II in Figure 3) are located at different types of bay regions. Figure 4 shows the arrangement of the  $W_2$ -type vertexes that are spread over a bay, cove, fjord, and gulf, revealing that the bay and cove possess, respectively, 8 and 16  $W_2$ -type vertexes. In the cases of the fjord and gulf, some vertexes are designated by asterisks. These vertexes are also the starting points of the fragments providing 2 walks of length 5, but they are involved in 2 such fragments. For example, vertex 1 accomplishes 2 walks of length 5 with both vertexes 2 and 3. This means that the fjord and gulf provide, respectively, 24 and 32 starting points for 2 walks of length 5. On this basis, one can conclude that  $b_2$  can be expressed by eq 13.



**Figure 5.** Arrangement of the vertexes which are the starting points for structural fragments of phenylenes enabling 13 walks of length 5.

Now we have to check the validity of eq 13 for the case of branched molecules of phenylenes (which possess  $A_3$ -type hexagons). It is obvious that by the presence of an  $A_3$ -type hexagon, three bay regions are necessarily formed. Since the situation is analogous with all kinds of bay regions, we here consider only the case where all three bay regions are simple bays. As shown in Figure 4, there are 12 vertexes marked by asterisks which are spread over these bays, meaning that they represent 24 starting points for 2 walks of length 5. These points are arranged so that each bay includes eight of them, meaning that branched phenylenes formally satisfy eq 13 for  $b_2$ .

Thirteen walks of length 5 are accomplished at the  $L_1$ - and  $A_3$ -type hexagons and different kinds of bay regions (fragments III–V in Figure 3). It is obvious from Figure 3 that a terminal hexagon provides two  $W_{13}$ -type vertexes. Figure 5 reveals that a bay, cove, fjord, and gulf provide, respectively, 6, 12, 18, and 24  $W_{13}$ -type vertexes. It is also shown that a total of 12  $W_{13}$ -type vertexes are spread over the bays of an  $A_3$ -type hexagon (4 vertexes at each bay). (The situation is, of course, analogous to the cases where the bay regions of an  $A_3$ -type hexagon are the coves, fjords, and gulfs.) This can be understood so that each  $A_3$ -type hexagon decreases the number of  $W_{13}$ -type vertexes by 6. This consideration provides a justification to express  $b_{13}$  as

$$b_{13} = 2h_{L_1} + 6B + 12C + 18F + 24G - 6h_{A_3}$$

Since  $h_{L_1} = h_{A_3} + 2$ , the formula above is easily transformed into (22).

The dependences of  $b_{21}$  and  $b_{40}$  on the molecular structures of phenylenes are identical (eqs 28 and 35). Both  $W_{21}$ - and  $W_{40}$ -type vertexes are provided by the presence of the  $A_3$ -type hexagons in the molecules of phenylenes (fragments VI and VII in Figure 3). Twenty-one walks of length 5 can be accomplished between the opposite vertexes of an  $A_3$ -type hexagon ( $W_{21}$ -type vertexes), whereas 40 walks of length 5 are spread between the adjacent vertexes which belong both to the four-membered ring and to the  $A_3$ -type hexagon ( $W_{40}$ -type vertexes). An  $A_3$ -type hexagon provides six  $W_{21}$ -type and six  $W_{40}$ -type vertexes so that eqs 28 and 35 are straightforwardly obtained.

## 5. CONCLUDING REMARKS

Using the method of Hall,<sup>30</sup> a topological formula for the 10th spectral moments of the vertex-adjacency matrix of



phenylenes is deduced. The formula expresses the dependence of the 10th spectral moment on the molecular structure. The size of a molecule (number of hexagons) and number of bays, coves, fjords, gulfs, and  $A_3$ -type hexagons exert influence on the  $M_{10}$  of phenylenes. All six of the mentioned graphical invariants can be easily deduced from the molecular graph.

The formula for the  $M_{10}$  of phenylenes has already been used (together with those derived earlier) in a comparative study concerning the applicability of spectral moments of the vertex- and edge-adjacency matrix in QSPR and QSAR examinations of phenylenes.<sup>47</sup> It is worth noting that there is a deep congruence between the lower spectral moments of the vertex- and edge-adjacency matrixes of phenylenes. The spectral moments of the two matrixes are linearly dependent, implying that the two sets of moments are equivalent from the point of view of QSPR and QSAR studies.

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