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Effect of a Ring onto Values of Eigenvalue–Based Molecular Descriptors

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Abstract: The eigenvalues of the characteristic polynomial of a graph are sensitive to its symmetry-related characteristics. Within this study, we have examined three eigenvalue–based molecular descriptors. These topological molecular descriptors, among others, are gathering information on the symmetry of a molecular graph. Furthermore, they are being ordinarily employed for predicting physico–chemical properties and/or biological activities of molecules. It has been shown that these indices describe well molecular features that are depending on fine structural details. Therefore, revealing the impact of structural details on the values of the eigenvalue–based topological indices should give a hunch how physico–chemical properties depend on them as well. Here, an effect of a ring in a molecule on the values of the graph energy, Estrada index and the resolvent energy of a graph is examined.

Keywords: molecular descriptor; graph energy; Estrada index; resolvent energy; effect of a ring

MSC: 05C09; 05C92

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1. Introduction

Molecular descriptors are quantities that may be regarded as numerical representations of a molecule. They are carriers of information about some parts or the whole structure of a molecule and, therefore, implicitly about its physico–chemical properties. Because of their success in predicting the behavior of molecules, investigations of molecular descriptors have been intensive over the years. Such an activity resulted in introducing thousands of molecular descriptors [1]. Among them, a salient place is reserved for topological indices [2,3]. Reasons for this will not be detailed here, but, in a nutshell, the topological indices represent a good balance between the amount of information they are harvesting from a molecular structure and the computational complexity of their algorithms. The main applications of topological indices represent construction of mathematical predictive models (QSPR/QSAR) and in virtual screening [4]. In addition, some of them have proved to be useful in molecular design and in drug discovery [5]. They can be roughly classified into three major groups: degree–based [6], distance–based [7], and eigenvalue–based topological indices [8].

The eigenvalue–based topological molecular descriptors emerged in the seventies of the last century when a linkage between one of them and the total π-electron energy of conjugated molecules was established [9]. Nowadays, there are hundreds of these indices [10], but only a couple of them originate from the eigenvalues obtained from the adjacency matrix of a graph. These particular indices are mainly used in modeling the physico–chemical properties of molecules. In the rest of the text, we shall refer to them as the eigenvalue–based indices.

Probably the oldest eigenvalue–based topological index is the graph energy. Its roots can be traced to the Hückel molecular orbital theory, and in the majority of cases, it coincides with the total π-electron energy. The graph energy is defined as follows [9]:

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \tag{1}$$

where λ_i is the ith eigenvalue obtained from the adjacency matrix.

Hundreds of papers are written about graph energy and several books. Such a vivid interest in this descriptor is not waning even today (e.g., see [10–15] and the references cited therein).

The second representative of this class of topological molecular descriptors that attracted much attention is the Estrada index. It was introduced at the beginning of the XXI century, aiming to model the folding of polypeptide chains. The Estrada index is defined as follows [16]:

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}. \tag{2}$$

The λ_i is the ith eigenvalue obtained from the adjacency matrix.

This index gained considerable popularity, resulting in numerous papers [15,17–19]. Such success of Estrada index may be attributed to the fact that this index found applications beyond chemistry. Namely, the authors of [20] have applied this graph invariant as a measure of subgraph centrality to study some real–world networks. In addition, the Estrada index was applied to quantify robustness of weighted networks [21].

The last member of the eigenvalue–based topological indices that will be treated here is the resolvent energy of a graph ($ER(G)$). The resolvent energy,

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n - \lambda_i} \tag{3}$$

was introduced recently [22]. Despite its juvenility, this index has attracted the attention of scientists thanks to its specific features and a noticeable predictive potential [13,17,23–29]. For example, it has been shown that discriminating power of resolvent energy outperforms such feature of graph energy and Estrada index [30]. This makes resolvent energy a proper candidate for isomers-distinguishing calculations. In addition, this topological descriptor exhibited good performance in modeling physico–chemical properties, such as boiling point, heat of formation, and log$P$ of hydrocarbons [24].

Lately, several articles have appeared in which the comparative analysis of the above–mentioned topological indices has been exhibited [13,17,23–25]. A similar type of analysis is performed here, aiming to investigate the influence of a ring in a molecule on the values of the eigenvalue–based topological indices.

Molecules containing rings are of a great importance in chemistry and biology. The presence of a ring significantly influences many molecular properties. For instance, cyclic structures in saturated hydrocarbons are related with an additional instability, also known as ring strain. On the other hand, in the case of conjugated polycyclic molecules, the size of the rings determines whether cyclic electron delocalization will cause either stabilization (in aromatic compounds) or destabilization effects (in antiaromatic compounds). A method for assessing the effect of a ring on the value of the graph energy has been introduced already in 1977 [31]. In the present work, it will be shown how this methodology can be generalized so to be applicable to other eigenvalue–based topological descriptors.

2. Preparations

The method for measuring the effect of a ring on the value of the graph energy is long-time known [31–34]. It is based on the relation between the values of coefficients of the characteristic polynomial $\phi(G, \lambda)$ of a molecular graph and some of its structural details.

This relation was established by H. Sachs (e.g., [35], pp. 35–38), showing that the bonds, rings, and their specific combinations determine the values of the coefficients of the $\phi(G, \lambda)$. The effect of a cycle on the graph energy has been widely applied to study energetic aspects of cyclic electron delocalization in polycyclic conjugated molecules (see [33] and references cited therein).

In [31], the authors derived a polynomial similar to the $\phi(G, \lambda)$, but in which the effects of a ring R were excluded. This polynomial has the following form

$$\phi(G \setminus R, x) = \phi(G, x) + 2 \cdot \phi(R, x), \tag{4}$$

where $\phi(G, x)$ and $\phi(R, x)$ are the characteristic polynomials of a graph G and a ring R, respectively.

Then the energy effect of a ring R could be seen as

$$ef_E(R) = E[\phi(G, x)] - E[\phi(G \setminus R, x)] \tag{5}$$

where $E[\phi(G, x)]$ and $E[\phi(G \setminus R, x)]$ are the energies obtained by summing the absolute values of the roots of polynomials $\phi(G, x)$ and $\phi(G \setminus R, x)$, respectively [33,36,37].

Due to the *complex conjugate root theorem (CCR)* [38] the $E[\phi(G \setminus R, x)]$ is always the real number, despite complex roots that may occur in the polynomial $\phi(G \setminus R, x)$. Thence, the energy effect is also a real quantity.

This elegant approach for assessing the effect of a ring on the value of the graph energy can be applied also to some other eigenvalue–based descriptors. The only requirement is that the mathematical function used in the definition of the descriptor TI has the property $f : \mathbb{C} \to \mathbb{R}$. This provides that the value of the effect of a ring is in the realm of real numbers. Then, by generalizing the Equation (5) we get

$$ef_{TI}(R) = TI[\phi(G, x)] - TI[\phi(G \setminus R, x)] \tag{6}$$

where $TI[\phi(G, x)]$ and $TI[\phi(G \setminus R, x)]$ are topological indices that are obtained from the roots of $\phi(G, x)$ and $\phi(G \setminus R, x)$, respectively.

The Estrada index and the resolvent energy of a graph are molecular topological descriptors for which the effect of a ring, using Equation (6), can be calculated.

The CCR enables us (by using simple algebraic manipulations) to extend the domain of the Formula (2) onto complex numbers:

$$EE(G) = \sum_{k=1}^{n} \cos b_k \cdot e^{a_k} \tag{7}$$

where a_k and b_k are the real and complex part of the complex eigenvalue (root) $z_k = a_k + b_k \cdot i$.

The effect of ring on the value of the Estrada index is being calculated by applying the Equation (7) in the Equation (6):

$$ef_{EE}(R) = EE[\phi(G, x)] - EE[\phi(G \setminus R, x)]. \tag{8}$$

The effect of a ring on the value of the resolvent energy of a graph can be calculated in a more direct way. Using the result given in [22], [Theorem 8], we get

$$ef_{ER}(R) = \frac{\phi'(G, n)}{\phi(G, n)} - \frac{\phi'(G \setminus R, n)}{\phi(G \setminus R, n)} \tag{9}$$

where n is total number of vertices in a molecular graph G.

3. Results and Discussion

Previous investigations of the energy effect of a ring detected an influence of the size of a ring, the size of a molecule, and the ring annelation on its value. Hence, three in-silico experiments were designed, aiming to investigate an impact of these features on the values of $ef_{EE}(R)$ and $ef_{ER}(R)$. Obtained results were compared with those calculated for $ef_E(R)$.

The first experiment is directed toward assessing the influence of the size of a ring on the ring-effects $ef_{EE}(R)$, $ef_{ER}(R)$, and $ef_E(R)$. To examine this factor, but at the same time to eliminate the influence of the size of a molecule, the 20-sized ring has been used as a starting point. Then, the edge, always starting from the same vertex, but changing the end-vertex in each new iteration, is inserted (see Figure 1). That is how we get the rings whose size varies from 3 up to 20 vertices.

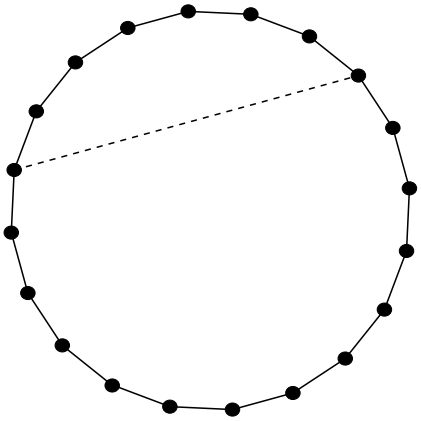

Figure 1. Reducing the ring size by inserting dashed line as an edge.

The Python script (as a Jupyter notebook) was coded for the calculation of the ring-effects. The NumPy [39] module was used for easier handling of the polynomials, the NetworkX [40] for the manipulation of molecular graphs, and the mpmath [41] module for enhancing the precision of the calculation. The results are given in Table 1.

Table 1. The values of the effects of a ring on the values of the resolvent energy, Estrada index, and the energy of a graph for rings of size varying from 3 up to 20 vertices.

n	ef_{ER}	ef_{EE}	ef_E
3	3.83×10^{-5}	1.51049	0.19701
4	2.56×10^{-6}	0.44700	−0.41860
5	1.60×10^{-7}	0.10483	0.12766
6	9.63×10^{-9}	0.02012	0.26441
7	5.63×10^{-10}	0.00326	0.09584
8	3.22×10^{-11}	0.00046	−0.17942
9	1.82×10^{-12}	5.60×10^{-5}	0.07505
10	1.01×10^{-13}	6.14×10^{-6}	0.19042
11	5.33×10^{-15}	6.08×10^{-7}	0.05920
12	6.66×10^{-16}	5.48×10^{-8}	−0.11716
13	0.0	4.53×10^{-9}	0.04593
14	0.0	3.47×10^{-10}	0.16718
15	0.0	2.48×10^{-11}	0.03404
16	0.0	1.48×10^{-12}	−0.09000
17	0.0	1.56×10^{-13}	0.02277
18	0.0	-9.95×10^{-14}	0.16534
19	0.0	-4.26×10^{-14}	−0.10270
20	0.0	-1.42×10^{-14}	−0.23598

Presented results clearly indicate a trend of the exponential decreasing of the values of $ef_{ER}(R)$ and $ef_{EE}(R)$ with an increase in the size of the ring. The pictorial representations are given in Figures 2 and 3.

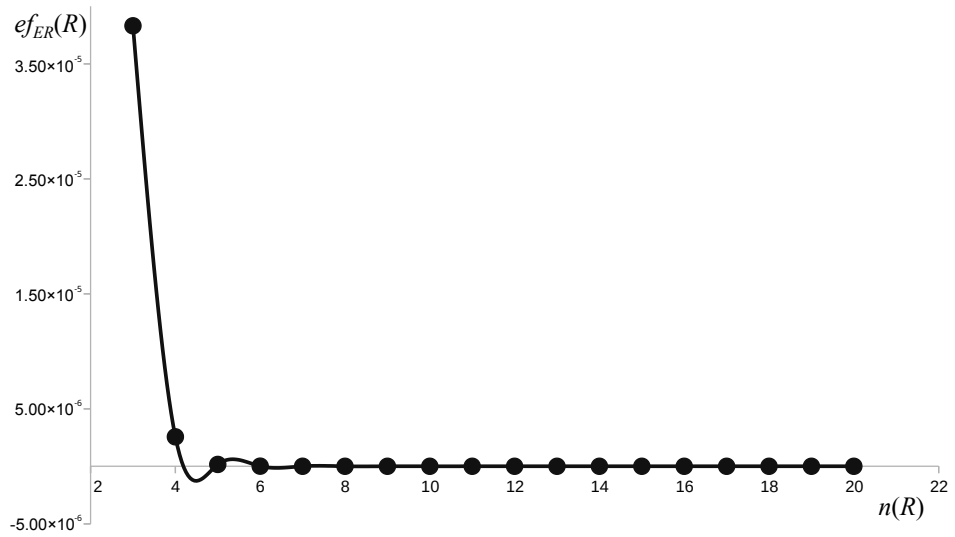

Figure 2. Impact of the size of a ring on the values of the ring-effect of the resolvent energy of a graph.

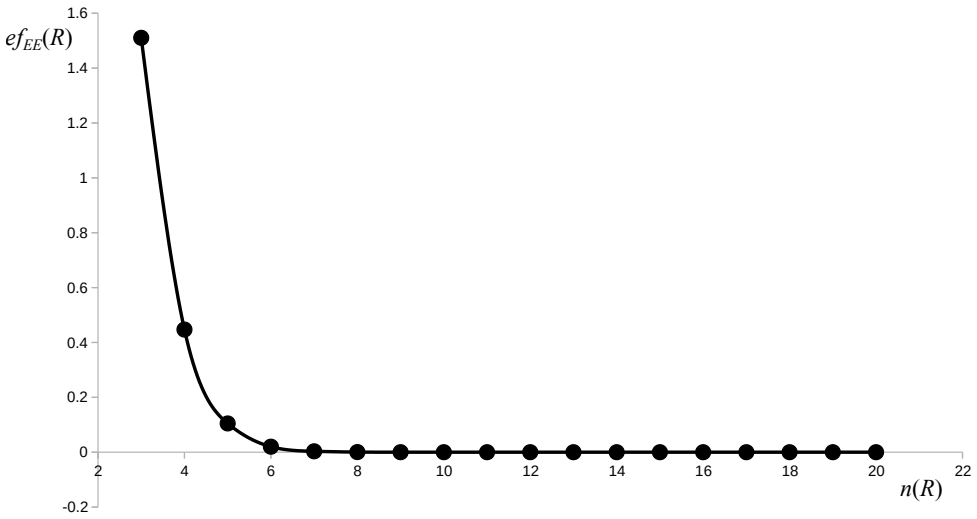

Figure 3. Impact of the size of a ring on the values of the ring-effect of the Estrada index.

From the data given in Table 1, it can be deduced that the ring-effects of the resolvent energy of a graph and the Estrada index are negligible for rings with a size greater than 6 vertices. Moreover, it is interesting that the ring-effect of the resolvent energy of a graph does not exist when the size of a ring is greater than or equal to 13 vertices. This finding was double-checked by increasing the precision of the calculations up to 50 decimals.

The effect of a ring on the value of the energy (a.k.a., energy effect) shows a rather different relationship to the size of a ring (see Figure 4).

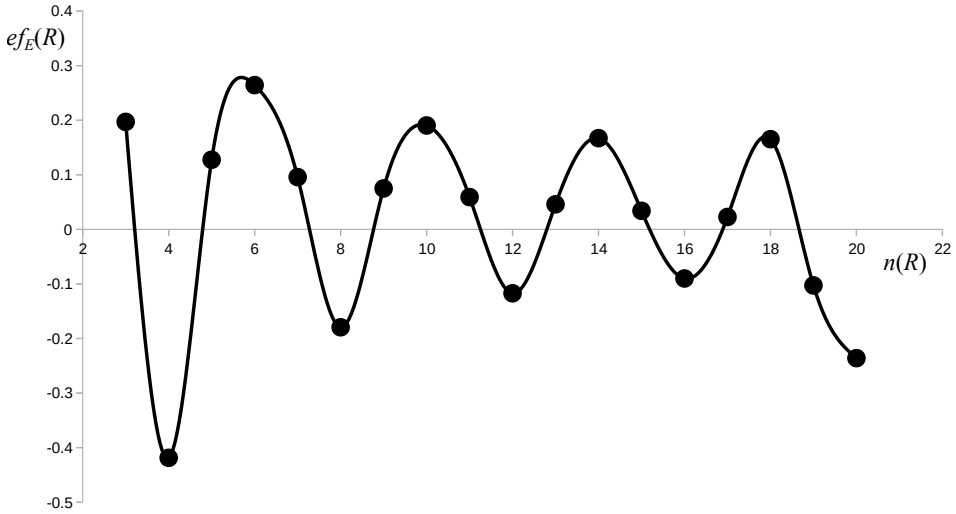

Figure 4. Impact of the size of a ring on the values of the energy effect.

Its values are negative for all $4k$-rings and positive for all $4k + 2$-rings. This follows the extended Hückel rule of ring influence on the stability of a molecule. At this point, it should be noted that there is a detailed mathematical analysis showing that the ef_E–values generally follow the extended $(4n + 2)$ rule [33]. Such a physico-chemical meaning of varying the values of $ef_{ER}(R)$ and $ef_{EE}(R)$ cannot be noticed.

The second experiment is checking the influence of the size of a molecule on the values of $ef_{ER}(R)$, $ef_{EE}(R)$, and $ef_E(R)$. In this experiment, the size of a ring was kept constant, while the molecule was being enlarged in each iteration. To check the influence of this factor, the homologous series of acenes starting with benzene and ending with dodecacene were used (see Figure 5). The values of $ef_{ER}(R)$, $ef_{EE}(R)$, and $ef_E(R)$ of a terminal benzene ring were being tracked and recorded.

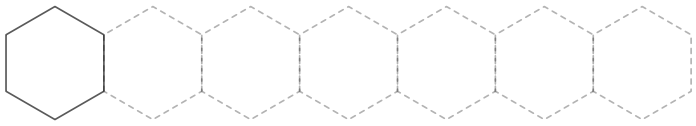

Figure 5. An acene.

The results are obtained by the Python script, coded in the form of the Jupyter notebook, and gathered in Table 2.

Table 2. The effect of the terminal benzene-ring on the values of the resolvent energy, the Estrada index, and the energy of a graph in the class of acenes up to 50 carbon atoms.

n	ef_{ER}	ef_{EE}	ef_E
6	5.41×10^{-5}	0.01920	0.27259
10	1.34×10^{-6}	0.02012	0.12111
14	1.21×10^{-7}	0.02012	0.09511
18	2.03×10^{-8}	0.02012	0.09004
22	4.92×10^{-9}	0.02012	0.08955
26	1.52×10^{-9}	0.02012	0.08995
30	5.55×10^{-10}	0.02012	0.09037
34	2.31×10^{-10}	0.02012	0.09068
38	1.06×10^{-10}	0.02012	0.09089
42	5.24×10^{-11}	0.02012	0.09101
46	2.77×10^{-11}	0.02012	0.09110
50	1.54×10^{-11}	0.02012	0.09115

The records show that the effect of a ring on the value of the Estrada index is almost insensitive to the size of a molecule. The Estrada ring effect rises with increasing the size of a molecule from 6 to 10 carbon atoms. Further enlarging of a molecule does not affect the value of the $ef_{EE}(R)$, as is evident from Table 2. The ring effects on the value of the energy and the resolvent energy, in contrast to the Estrada ring effect, are exponentially decreasing with the number of atoms in the acene. The value of the $ef_{ER}(R)$ is decreasing in each iteration, while the $ef_E(R)$ is reaching the minimum for acene having 22 carbon atoms, and it slightly increases afterward. Figures 6–8 illustrate the way of changing the $ef_{ER}(R)$, $ef_{EE}(R)$, and $ef_E(R)$ with the increasing size of a molecule.

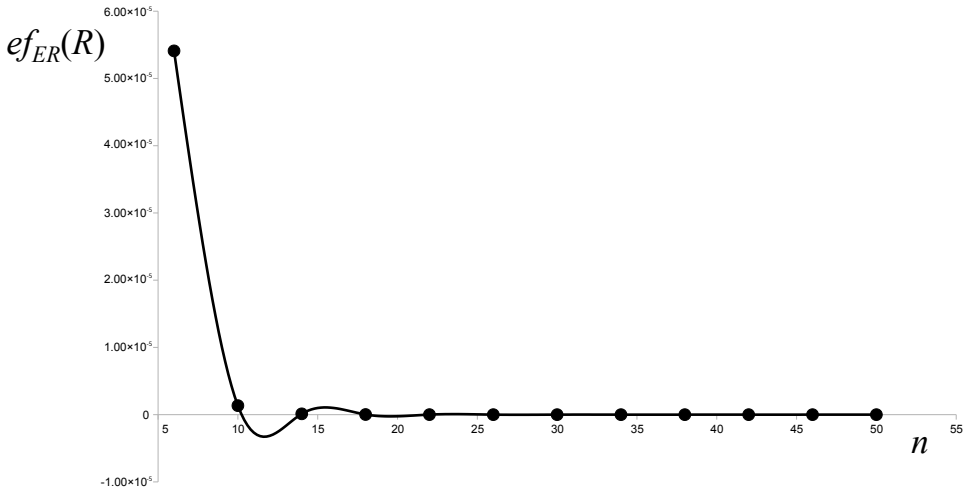

Figure 6. Distribution of the resolvent energy ring-effects with the size of a molecule.

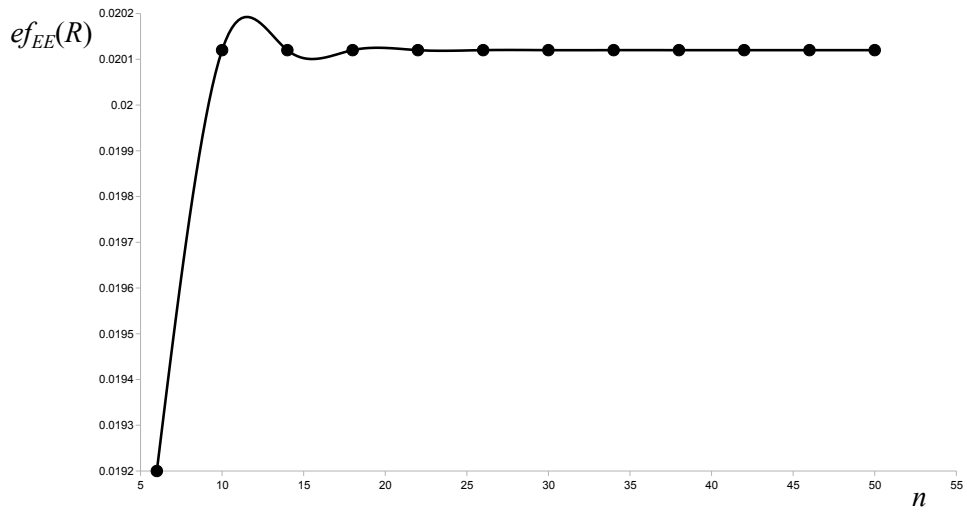

Figure 7. Distribution of the Estrada ring-effects with the size of a molecule.

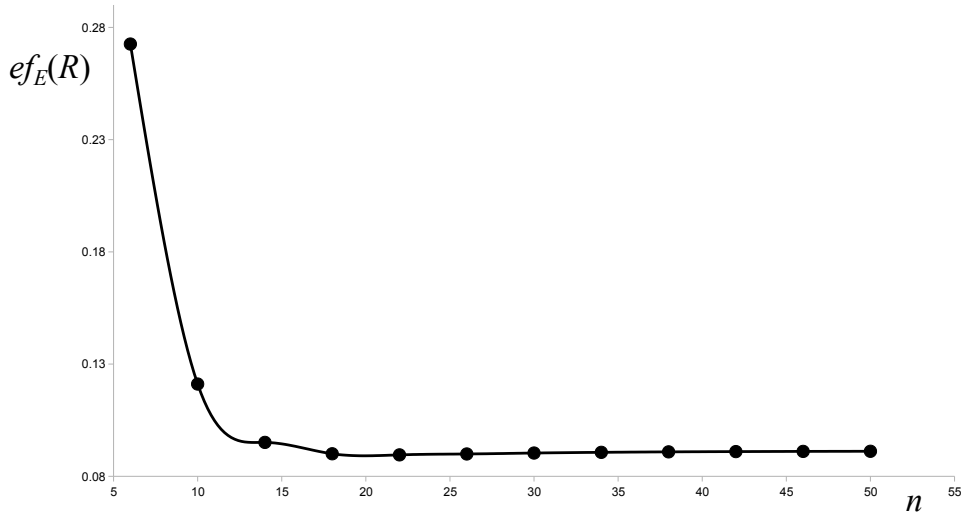

Figure 8. Distribution of the energy ring-effects with the size of a molecule.

The third in-silico experiment is designed to evaluate the influence of the annelation of a ring on the values of $ef_{ER}(R)$, $ef_{EE}(R)$, and $ef_E(R)$, but in the same time to keep the size of a ring and of a molecule constant. The energy effects of a benzene ring were calculated. There are 12 types of benzene annelations in a polycylic aromatic compounds, that are depicted in the Figure 9.

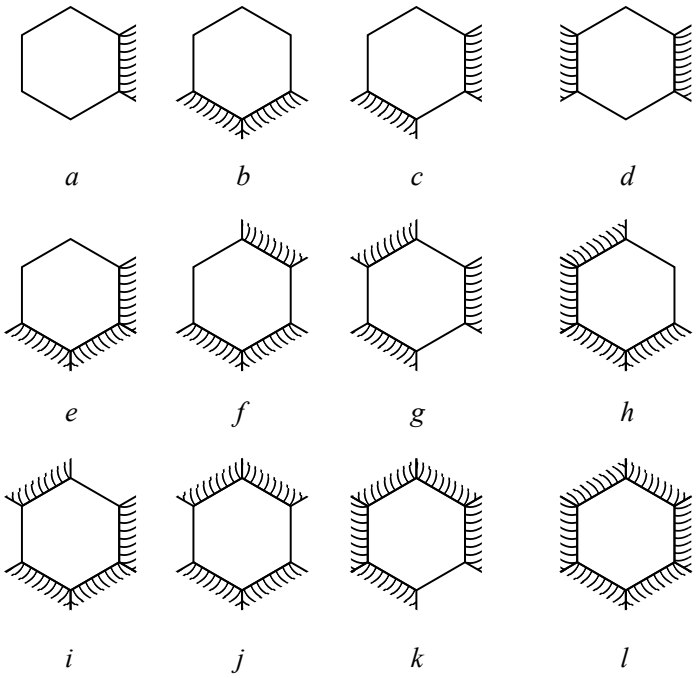

Figure 9. Benzene annelations.

The idea was to use a benzenoid molecule that has all types of benzene annelations, shown in Figure 9, for assessing the influence of this factor on the values of $ef_{ER}(R)$, $ef_{EE}(R)$, and $ef_E(R)$. In the Figure 10, the benzenoid hydrocarbon is depicted that is used for the evaluation of the influence of benzene annelation on the above-mentioned ring-effects. The rings on which the calculation was performed are denoted by letters that correspond to the notification given in Figure 9. Results are summarized in Table 3.

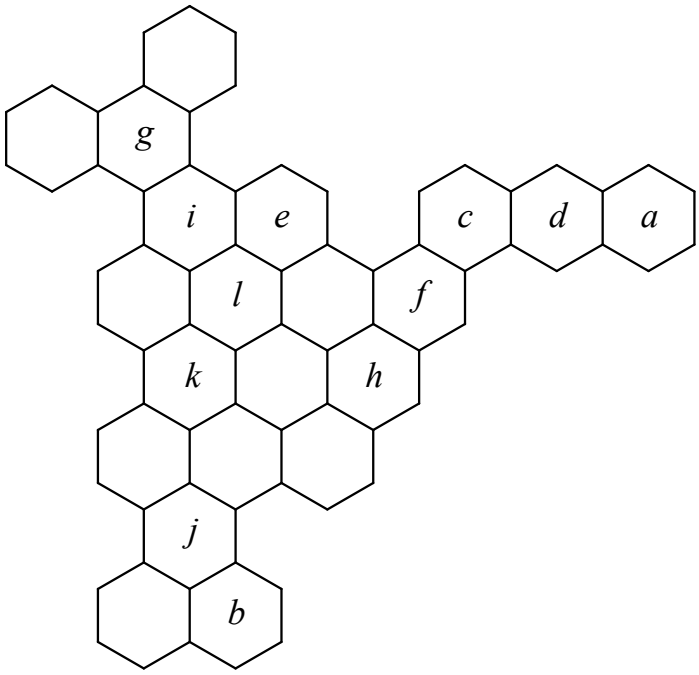

Figure 10. Benzenoid hydrocarbon having benzene rings with all types of annelations.

Table 3. Values of $ef_{ER}(R)$, $ef_{EE}(R)$, and $ef_E(R)$ for all types of benzene annelations. Values of the $ef_{ER}(R)$ are multiplied by 10^{12}.

Annelation	$ef_{ER} \cdot 10^{12}$	ef_{EE}	ef_E
a	1.199	0.020	0.107
b	1.199	0.020	0.103
c	1.201	0.021	0.043
d	1.201	0.021	0.080
e	1.201	0.021	0.091
f	1.201	0.022	0.067
g	1.201	0.022	0.034
h	1.201	0.022	0.044
i	1.201	0.022	0.043
j	1.201	0.022	0.028
k	1.201	0.022	0.032
l	1.201	0.022	0.032

The results show that the effect of a ring on the values of the resolvent energy and the Estrada index does not experience any impact from the ring annelation. On the other hand, the energy effect significantly varies with the type of benzene annelation. These variations of $ef_E(R)$ may be explained by the Clar structures of the investigated benzenoid hydrocarbon. Namely, Clar aromatic sextet theory [42] describes distribution of π-electrons in benzenoid hydrocarbons. Within this approach hexagons containing aromatic sextet are described as "full", while other hexagons are marked as "empty". In most cases, the agreement between Clar structures and the energy effect values are excellent. Roughly speaking, benzene annelations that contain more π-electron sextets in the Clar structures should have the greater value of the energy effect and vice versa.

4. Conclusions

The comparative analysis of the effects of a ring on the values of the resolvent energy, Estrada index, and the energy of a graph is performed here. Three in-silico experiments that assess the impact of ring size, molecule size, and ring annelations were performed and the following conclusions have been derived:

- Enlarging the size of a ring decreases the values of the $ef_{ER}(R)$ and $ef_{EE}(R)$. Rings with a size exceeding 12 non-hydrogen atoms do not have $ef_{ER}(R)$. The energy effect varies with the ring size in accordance with the extending Hückel rule.
- The size of acene does not affect the ef_{EE}. Interestingly, the effect of a ring on the value of the Estrada index is rising from benzene to the first member in acene series (naphthalene). The values of $ef_{ER}(R)$ are exponentially decreasing with the size of an acene. The $ef_{E}(R)$ is decreasing for acenes up to 22 carbon atoms, and the negligible rise in its value is detected afterward.
- The third experiment shows that the benzene annelation does not influence the values of $ef_{ER}(R)$ and $ef_{EE}(R)$. The results indicate a considerable impact of the benzene annelation on the values of the energy effect.

The $ef_{ER}(R)$ and $ef_{EE}(R)$, juxtaposed to the $ef_{E}(R)$, are showing significantly different behavior. This implies that in comparison with the energy of a graph, the resolvent energy, and the Estrada index are gathering completely different structural details. Although the previous investigations detected similar behavior of the resolvent energy and the Estrada index [17,23–25,30], the effect of a ring detected differences that certainly contribute to the observed fine variations in the predictive potential of the Estrada index and the resolvent energy of a graph.

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