Research Article

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Theoretical study of energy, inertia and nullity of phenylene and anthracene

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Abstract: Energy of a molecule plays an important role in physics, chemistry and biology. In mathematics, the concept of energy is used in graph theory to help other subjects such as chemistry and physics. In graph theory, nullity is the number of zeros extracted from the characteristic polynomials obtained from the adjacency matrix, and inertia represents the positive and negative eigenvalues of the adjacency matrix. Energy is the sum of the absolute eigenvalues of its adjacency matrix. In this study, the inertia, nullity and signature of the aforementioned structures have been discussed.

Keywords: topological indices, energy, inertia, nullity

1 Introduction

A *molecular graph* is a mathematical object defined as $G = (V, E)$, where V is the set of vertices also called atoms and E is the set of edges also called bonds. Usually in molecular graphs, hydrogen atoms are not considered. The graph in this study is finite, undirected and simple. The degree of the vertex v is the number of vertices adjacent

to that vertex v . Adjacent vertices are those which have edges in between them. Adjacent edges are those that have common vertex in between them. Let $A = [a_{ij}]$, $i, j \in \{1, 2, 3, \dots, q\}$ be the adjacency matrix of the graph G , and A is the square matrix of order n . The eigenvalues $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_{q-1}, \lambda_q$ of A are called the eigenvalues of the graph G . A is a symmetric matrix with the properties that its trace is zero, all of its eigenvalues are real and sum of all these eigenvalues is zero. The absolute sum of all the eigenvalues is called an energy of the graph G . Mathematically, it is denoted as $E = \sum_{i=1}^q |\lambda_i|$. The set of all eigenvalues is also called the spectrum of the graph G .

The eigenvalues play an important role in the field of mathematics, but these values are also very important in other fields such as chemistry, economics and many more. As far as our study concerns about eigenvalues, these values interpret in chemistry not only as the form of energy but also as different physicochemical properties of a chemical compound. We need to understand the relationship between mathematics and chemistry. The positive eigenvalues are linked with antibonding level, negative eigenvalues are linked with bonding levels and zero eigenvalues are linked with nonbonding level [1–3]. The number of positive eigenvalues $p(G)$ represents the positive inertia index, while the number of negative eigenvalues $n(G)$ represents negative inertia index; and nullity $\eta(G)$ is the number of zeros that appear in the roots of characteristics polynomial. All the eigenvalues form a set called spectrum of G . The signature $s(G)$ of the graph G is just a number that is generated by the difference in the number of positive and negative eigenvalues. Because nullity plays a vital role in the stability of molecules and if nullity is zero, this shows that the molecule is predicted to have a stable, closed-shell, electron configuration. If nullity is greater than zero, then the molecule is unstable, highly reactive, nonexistent and open shell. So it is observed that phenylene and anthracene are stable, closed-shell molecules because they are represented by their nullity which is equal to zero.

Phenylene belongs to the special class of conjugated hydrocarbons which plays an important role in the field

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Figure 2: Anthracene.

of chemistry. The geometrical construction of *phenylene* is as follow: its shape is based on two mathematical objects, namely, hexagon and square. These objects are connected in such a way that a square is connected with two hexagons, which show that every two hexagons are totally separated (see Figure 1).

The molecular graph of *anthracene* consists of three fused benzene rings (see Figure 2). Actually, it is a part of coal tar which is a very useful component in daily life. Coal tar, which contains around 1.5% anthracene, remains a major source of this material. Its chemical formula is $C_{14}H_{10}$. It is used in the production of the different dyes.

Quantitative structure activity relationship (QSAR) is a regression and classification model is used in chemical and biological sciences and for many other purposes, but the most important one is to characterize the chemical structures of different compounds in terms of a single real number. This number represents the correlation between chemical structures of different compounds and the related chemical and biological activities or properties [4,5]. There are a lot of categorical QSAR models (categorical

models are not correlation driven) but the topological index is the popular one because of its effectiveness [1,6].

For further study of energy, see refs. [7–9]. A graph spectrum-based invariant, put forward by Estrada, is defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i}$. Although invented in the year 2000, the Estrada index has already found a remarkable variety of applications in refs. [10–16]. Initially it was used to quantify the degree of folding of long-chain molecules, especially protein. Malik and Farooq have found the energy and Estrada index of $TUC_4C_8[m, n]$ nanotubes and also found some conjuncture on energy and Estrada index [17,18]. For more results on Estrada index, see ref. [19]. Ma et al. discussed the positive and negative inertia index of trees, unicyclic graphs and bicyclic graphs [20]. In ref. [21], Omid studied the nullity of bipartite graphs.

In this study, we have observed the following inequalities: $E_x(P) > E_s(P)$, $EE_x(P) < EE_s(P)$, $E_x(A) > E_s(A)$ and $EE_x(A) > EE_s(A)$, where $E_x(P)$, $E_s(P)$, $E_x(A)$ and $E_s(A)$ are the exact and estimated values of energy of phenylene and anthracene, respectively, and $EE_x(P)$, $EE_s(P)$, $EE_x(A)$ and $EE_s(A)$ are the exact and estimated values of Estrada index of phenylene and anthracene, respectively. In addition, we have also calculated the inertia, nullity and signature of phenylene and anthracene. The exact values are those values that we calculate from the graph by using softwares, and estimated values are those that we extract from the (polynomial) curves.

2 Method

In this section, we discuss the process of finding the energy and Estrada index of the phenylene and anthracene by using the computational methods. In the first

Figure 1: Phenylene.

Table 1: The quadratic curves for the energy and Estrada index of phenylene

(m, n)	Energy ($E(P)$)	Estrada index ($EE(P)$)
$(1, n)$	$-0.0009n^2 + 8.4872n - 0.4467$	$-9 \times 10^{-9}n^2 + 18.089n - 4.3925$
$(2, n)$	$0.0027n^2 + 17.354n - 1.0234$	$6 \times 10^{-8}n^2 + 35.724n - 3.9426$
$(3, n)$	$-0.0001n^2 + 26.226n - 1.4013$	$1 \times 10^{-9}n^2 + 55.789n - 5.9133$
$(4, n)$	$-0.0011n^2 + 35.143n - 1.9339$	$3 \times 10^{-8}n^2 + 74.234n - 6.2703$
$(5, n)$	$-0.0004n^2 + 44.12n - 2.6087$	$3 \times 10^{-8}n^2 + 93.085n - 7.0307$
$(6, n)$	$-0.0008n^2 + 52.982n - 3.0532$	$4 \times 10^{-8}n^2 + 111.93n - 7.7911$
$(7, n)$	$-0.0011n^2 + 61.888n - 3.5766$	$4 \times 10^{-8}n^2 + 130.78n - 8.5516$
$(8, n)$	$-0.0014n^2 + 70.793n - 4.1001$	$5 \times 10^{-8}n^2 + 149.63n - 9.312$
$(9, n)$	$-0.0016n^2 + 79.698n - 4.6236$	$5 \times 10^{-8}n^2 + 168.48n - 10.072$
$(10, n)$	$-0.0019n^2 + 88.604n - 5.147$	$6 \times 10^{-8}n^2 + 187.34n - 10.833$

Table 2: The quadratic curves extracted from the coefficient of the equations given in Table 1

	Energy ($E(P)$)	Estrada index ($EE(P)$)
n^2	$-6 \times 10^{-6}m^2 - 0.0002m + 0.0007$	$-6 \times 10^{-11}m^2 + 6 \times 10^{-9}m + 6 \times 10^{-9}$
n	$0.0005m^2 + 8.8999m - 0.4393$	$0.0017m^2 + 18.831m - 1.1281$
1	$-0.0007m^2 - 0.5161m + 0.0729$	$-0.0015m^2 - 0.7436m - 3.2623$

step, we use HyperChem to draw the molecule of our chemical structures [22]. In the second step, we construct an adjacency matrix of the graph by using TopoCluj [23]. In the third step, we find the energy with the help of MATLAB which is represented in Table 1. In the fourth step, we find the suitable curve (polynomial) of degree two with the help of “cftoolbox” of MATLAB [24,25]. The results obtained from this data are displayed in Table 2. In Tables 3 and 4, we found the errors between the exact and the estimated values extracted from the curve for energy and Estrada index of phenylene. We also calculated the inertia index, nullity and signature of the phenylene

Table 4: The exact values $EE_x(P)$ and estimated values $EE_s(P)$ of the Estrada index of the phenylene

(m, n)	$EE_x(P)$	$EE_s(P)$	Error
$(10, 1)$	176.5041	176.5141	0.0099
$(10, 2)$	363.8355	363.8555	0.0200
$(10, 3)$	551.1702	551.2074	0.0372
$(10, 4)$	738.5094	738.5593	0.0499
$(10, 5)$	925.8424	925.9112	0.0687
$(10, 6)$	1113.1775	1113.2631	0.0851
$(10, 7)$	1300.5126	1300.6150	0.1023
$(10, 8)$	1484.8476	1487.9669	0.1189
$(10, 9)$	1675.1827	1675.3188	0.1358
$(10, 10)$	1862.5178	1862.6707	0.1527

Table 3: The exact values $E_x(P)$ and estimated values $E_s(P)$ of the energies of the Phenylene

(m, n)	$E_x(P)$	$E_s(P)$	Error
$(10, 1)$	84.51	84.21	0.30
$(10, 2)$	172.99	172.69	0.30
$(10, 3)$	261.40	261.17	0.23
$(10, 4)$	349.96	349.66	0.30
$(10, 5)$	438.61	438.15	0.46
$(10, 6)$	527.16	526.66	0.50
$(10, 7)$	615.43	615.17	0.26
$(10, 8)$	704.11	703.69	0.42
$(10, 9)$	792.63	792.22	0.41
$(10, 10)$	881.11	880.74	0.37

and are displayed in Table 5. Similar process has been used for anthracene. In Tables 6 and 7, we found the polynomials by using the abovementioned techniques, and then in Tables 8 and 9, we calculated the errors of the exact and estimated values of the energy and Estrada index of anthracene. Finally, in Table 10, we displayed the inertia index, nullity and signature of anthracene.

2.1 Results of phenylene

In this section, we will study the energy, Estrada index, nullity, inertia and signature of phenylene. We will also

Table 5: The inertia, nullity and signature of phenylene

$P = \text{Phenylene}$	$p(P)$	$n(P)$	$\eta(P)$	$s(P)$
(8, 1)	24	24	0	0
(8, 2)	48	48	0	0
(8, 3)	72	72	0	0
(8, 4)	96	96	0	0
(8, 5)	120	120	0	0
(8, 6)	144	144	0	0
(8, 7)	168	168	0	0
(8, 8)	192	192	0	0
(8, 9)	216	216	0	0
(8, 10)	240	240	0	0
(8, 11)	264	264	0	0
(8, 12)	288	288	0	0

Table 8: The exact values $E_x(A)$ and estimated values $E_s(A)$ of the energy of the anthracene

(m, n)	$E_x(A)$	$E_s(A)$	Error
(10, 1)	218.7247	218.6827	0.0420
(10, 2)	453.8533	453.7937	0.0596
(10, 3)	688.9118	688.9047	0.0071
(10, 4)	924.0977	924.0157	0.0820
(10, 5)	1159.1496	1159.1268	0.0229
(10, 6)	1394.2470	1394.2377	0.0093
(10, 7)	1629.3590	1629.3487	0.0103
(10, 8)	1864.4720	1864.4597	0.0123
(10, 9)	2099.5850	2099.5707	0.0143
(10, 10)	2334.6970	2334.6818	0.0152

show the comparison between exact and estimated values of energy and Estrada index of phenylene.

Proposition 2.1. Let P be the graph of (m, n) -phenylene, then the energy and Estrada index of P are given by

$$E(P) = -6 \times 10^{-6}m^2n^2 - 0.0002n^2m + 0.0007n^2 + 0.0005nm^2 + 8.8999nm - 0.4393n - 0.0007m^2 - 0.5161m + 0.0729 \quad (1)$$

$$EE(P) = -6 \times 10^{-11}m^2n^2 + 6 \times 10^{-9}n^2m + 6 \times 10^{-9}n^2 + 0.0017nm^2 + 18.831nm - 1.1281n - 0.0015m^2 - 0.7436m - 3.2623 \quad (2)$$

The two curves that are representing the energy and Estrada index of the graph are given by equations (1) and (2), respectively. We observed that the exact value of the energy of phenylene is always greater than the estimated values of the energy of phenylene, i.e., $E_x(P) > E_s(P)$, where E_x represents the exact value of energy of phenylene

Table 6: The quadratic curves suitable for the Energy and Estrada index of anthracene

(m, n)	Energy ($E(A)$)	Estrada index ($EE(A)$)
($m, 1$)	$7 \times 10^{-6}n^2 + 42.356n - 3.2224$	$3 \times 10^{-14}n^2 + 135.29n + 8.3861$
($m, 2$)	$3 \times 10^{-6}n^2 + 63.382n - 4.1488$	$-1 \times 10^{-13}n^2 + 229.68n - 32.84$
($m, 3$)	$9 \times 10^{-6}n^2 + 85.212n - 6.1953$	$-1 \times 10^{-13}n^2 + 324.07n - 74.066$
($m, 4$)	$3 \times 10^{-6}n^2 + 106.53n - 7.5104$	$-3 \times 10^{-13}n^2 + 418.46n - 115.29$
($m, 5$)	$4 \times 10^{-6}n^2 + 127.94n - 8.9824$	$-2 \times 10^{-13}n^2 + 512.85n - 156.52$
($m, 6$)	$4 \times 10^{-6}n^2 + 149.38n - 10.476$	$1 \times 10^{-13}n^2 + 607.23n - 197.74$
($m, 7$)	$3 \times 10^{-6}n^2 + 170.82n - 11.965$	$6 \times 10^{-14}n^2 + 701.62n - 238.97$
($m, 8$)	$3 \times 10^{-6}n^2 + 192.25n - 13.453$	$-5 \times 10^{-13}n^2 + 796.01n - 280.2$
($m, 9$)	$2 \times 10^{-6}n^2 + 213.68n - 14.941$	$2 \times 10^{-13}n^2 + 890.4n - 321.42$
($m, 10$)	$2 \times 10^{-6}n^2 + 235.11n - 16.429$	$-5 \times 10^{-13}n^2 + 984.79n - 362.65$

Table 7: The quadratic curves extracted from the coefficient of the equations in Table 6

	Energy ($E(A)$)	Estrada index ($EE(A)$)
n^2	$-2 \times 10^{-8}m^2 - 2 \times 10^{-7}m + 5 \times 10^{-6}$	$-3 \times 10^{-15}m^2 + 2 \times 10^{-14}m - 1 \times 10^{-13}$
n	$2 \times 10^{-5}m^2 + 21.432m + 20.789$	$3 \times 10^{-14}m^2 + 94.388m + 40.903$
1	$-4 \times 10^{-5}m^2 - 1.4874m - 1.5503$	$-7 \times 10^{-5}m^2 - 41.225m + 49.611$

Table 9: The exact values $EE_x(A)$ and estimated values $EE_s(A)$ of the Estrada index of the anthracene

(m, n)	$EE_x(A)$	$EE_s(A)$	Error
(10, 1)	622.1380	622.1370	0.0010
(10, 2)	1606.9220	1606.9200	0.0020
(10, 3)	2591.7070	2591.7030	0.0040
(10, 4)	3576.4930	3576.4860	0.0070
(10, 5)	4561.2790	4561.2690	0.0100
(10, 6)	5546.0650	5546.0520	0.0130
(10, 7)	6530.8500	6530.8350	0.0150
(10, 8)	7515.6360	7515.6180	0.0180
(10, 9)	8500.4220	8500.4010	0.0210
(10, 10)	9485.2070	9485.1840	0.0230

Table 10: The inertia, nullity and signature of anthracene

$G = \text{Anthracene}$	$p(G)$	$n(G)$	$\eta(G)$	$s(G)$
(8, 1)	35	35	0	0
(8, 2)	70	70	0	0
(8, 3)	105	105	0	0
(8, 4)	140	140	0	0
(8, 5)	175	175	0	0
(8, 6)	210	210	0	0
(8, 7)	280	280	0	0
(8, 8)	315	315	0	0
(8, 9)	350	350	0	0
(8, 10)	385	385	0	0
(8, 11)	420	420	0	0
(8, 12)	455	455	0	0

and E_s represents the estimated value of energy of phenylene. Also error is always positive between the exact and estimated values of energy of phenylene, i.e., $\text{Error} > 0$.

Similarly, we have observed that the exact value of Estrada index of phenylene is always less than the estimated values of Estrada index of phenylene, i.e., $EE_x(P) < EE_s(P)$, where EE_x represents the exact value of Estrada index and EE_s represents the estimated value of Estrada index. As shown in Table 1, for every curve, the value of m and n ranges from 1 to 10.

Also the errors between the exact values and the estimated values of energy and Estrada index are summarized in Tables 3 and 4.

2.2 Results of anthracene

In this section, we will study the energy, Estrada index, nullity, inertia and signature of anthracene. We will also

Figure 3: Energy of phenylene. **Figure 4:** Energy of anthracene.

show the comparison between the exact and estimated values of energy and Estrada index of anthracene.

Proposition 2.2. Let A be the graph of (m, n) -anthracene, then the energy and Estrada index of A are given by

$$E(A) = -2 \times 10^{-8}m^2n^2 - 2 \times 10^{-7}n^2m + 5 \times 10^{-6}n^2 + 2 \times 10^{-5}nm^2 + 21.432nm + 20.789n - 4 \times 10^{-5}m^2 - 1.4874m - 1.5503 \quad (3)$$

$$EE(A) = -3 \times 10^{-15}m^2n^2 + 2 \times 10^{-14}n^2m - 1 \times 10^{-13}n^2 + 3 \times 10^{-14}nm^2 + 94.388nm + 40.903n - 7 \times 10^{-15}m^2 - 41.225m + 49.611. \quad (4)$$

Figure 5: Estrada index of phenylene.

Figure 6: Estrada index of anthracene.

The errors of energy and Estrada index are as given in Tables 8 and 9.

We observed that exact value of the energy of anthracene is always greater than the estimated values of the energy of anthracene, i.e., $E_x(A) > E_s(A)$. Error is always positive between the exact and estimated values of the energy of anthracene, i.e., $\text{Error} > 0$. Similarly, we have observed that the exact value of Estrada index of anthracene is always greater than the estimated values of Estrada index of anthracene, i.e., $EE_x(A) > EE_s(A)$.

3 Conclusion

We studied Estrada index, energy, inertia, nullity and signature of phenylene and anthracene. The following inequalities $E_x(P) > E_s(P)$, $EE_x(P) > EE_s(P)$, $E_x(A) > E_s(A)$

and $EE_x(A) > EE_s(A)$ have been observed between the exact and estimated values of the energy of phenylene and anthracene.

Also, since the nullity of phenylene and anthracene is zero, the molecule of these structures are stable and closed shell. At the end, we give a graphical representation of these parameters (Figures 3–6).

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