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Retraction

Retracted: Computing the Energy and Estrada Index of Different Molecular Structures

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

(1) Discrepancies in scope
(2) Discrepancies in the description of the research reported
(3) Discrepancies between the availability of data and the research described
(4) Inappropriate citations
(5) Incoherent, meaningless and/or irrelevant content included in the article
(6) Peer-review manipulation

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

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[1] Z. S. Mufti, R. Anjum, Q. Xin, F. Tchier, I. Anwar-ul-Haq, and Y. U. Gaba, "Computing the Energy and Estrada Index of Different Molecular Structures," *Journal of Chemistry*, vol. 2022, Article ID 6227093, 7 pages, 2022.

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Research Article

Computing the Energy and Estrada Index of Different Molecular Structures

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Graph energy is an invariant that is derived from the spectrum of the adjacency matrix of a graph. Graph energy is actually the absolute sum of all the eigenvalues of the adjacency matrix of a graph i.e. $E = \sum_{i=1}^{n} |\lambda_i|$, and the Estrada index of a graph G is elaborated as $\mathrm{EE}(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where, $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of a graph. In this paper, energy $E(G)$ and Estrada index $\mathrm{EE}(G)$ of different molecular structures are obtained and also established inequalities among the exact and estimated values of energies and Estrada index of TUC_4C_8 nanosheet and naphthalene.

1. Introduction

Chemical graph theory is a branch of mathematical chemistry and mathematical chemistry gives a natural way to understand the mathematical structures which actually act behind the existing chemical concepts to inaugurate the novel mathematical ideas and mathematical techniques in chemistry. The chemical graph theory is the intersection of graph theory and chemistry. In chemical graph theory, one can pick the molecular structure of different compounds and transform them into a molecular graph and then apply different graph invariants such as the energy of a graph. This graph invariant is much more popular in both mathematicians and chemists and was invented in 1978 by Ivan Gutman [1].

When graph energy was introduced in 1978, no one was attracted to this invariant. Even its chemical roots belong to 1940. Mathematicians were not interested initially but when the 20th century was started, a dramatic change occurred and graph energy got great respect from the whole world when the number of countries such as Pakistan, Australia, Austria, Brazil, Canada, and many more produced numbers of papers in graph energy. The definition of graph energy is motivated by already existing results for the Huckel molecular orbital total π-electron energy [2, 3]. The energy of a graph defined here totally coincides with the total π-electron energy computed using Huckel molecular orbital theory. The energy of a graph will be zero if the graph is totally disconnected.

About 20 years ago Estrada introduced a new index called the Estrada index. The Estrada index is denoted by EE(G) and is defined as $\mathrm{EE}(G) = \sum_{i=1}^{n} e^{\lambda_i}$ [4]. The application of the Estrada index is to measure the folding degree of long-chain proteins [5–8]. To measure the degree of long-chained molecules such as proteins, weighted graphs were used. This index is also used in complex networks to measure the centrality measures of these structures such as social, communication, and metabolic [9–11]. For detailed surveys on the Estrada index, readers can check [4, 12–22].

The motivation of the paper was to find the energy and Estrada index of nanostructures. Matrices are used nowadays for dealing with different types of problems in daily life. We are dealing with square matrices which are very useful in different applications such as in the solving system of equations, by using its determinant to find the area and orthogonal vectors. In this paper, we find the energy of a graph by finding the eigenvalues of its adjacency matrix. Let G be a simple undirected graph in which V denotes the vertex set containing $v_1, v_2, \ldots, v_n$ as atoms and E denotes the edge set $e_1, e_2, \ldots, e_n$ as bonds. The adjacency matrix $A(G)$ of a graph G is a square matrix that can be obtained by the adjacent and nonadjacent vertices in such a way if (i, j)-entry of a matrix is 1 whenever the vertices v_i and v_j are adjacent, otherwise 0. The eigenvalues of the adjacency matrix of order n are $\lambda_1, \lambda_2, \ldots, \lambda_n$ and the set of these eigenvalues is called a spectrum of the graph and since the adjacency matrix is symmetric so all the eigenvalues are real.

2. Methodology

We follow the following steps to compute the energy and Estrada index of the TUC_4C_8 nanosheet and naphthalene:

(1) We draw a chemical structure in HyperChem [23]. HyperChem is a molecular editor, which offers a wide range of molecular and quantum mechanics calculations.

(2) The Adjacency matrix is found using TOPOCLUJ [24].

(3) By using MATLAB, the eigenvalues of the adjacency matrix are found [25].

(4) A polynomial of your desired order is constructed which best fits the data using the cf toolbox [26].

3. Energy and Estrada Index of TUC_4C_8 Nanosheet

Carbon nanosheets(CNTS) belong to a special class of nanomaterials that consist of a two-dimensional hexagonal lattice of carbon atoms. It plays an important role in basic sciences, engineering, and nanotechnology. Carbon nanosheets are not just used in chemistry it is also used in different field of science it is also used in conducting molecules like in semiconducting or electronic properties of metallic. Carbon nanosheets were discovered in 1991 by S. Iijima. Due to the unique chemical and physical properties of carbon nanosheets(CNTS), there is a hopeful continuous growth of telecommunication. The length range of CNTS is less than 100 nm to 0.5 m. Carbon nanosheets(CNTS) classify into two types: single-walled carbon nanosheets and multiwalled carbon nanosheets.

(1) Single-walled carbon nanosheets(SWCTs): Single-walled carbon nanosheets consist of single graphene. It does not have any complex structure because of impurity. It bends easily [27].

(2) Multiwalled carbon nanosheets(MWCTs): Multi-walled carbon nanosheets consist of multigraphene. It has a complex structure due to its high purity. It cannot be bent easily [28, 29].

Now, we construct the quadratic polynomial which best fits the curve. We will also find the difference between $E_{\text{exact}}(T)$, $E_{\text{estimated}}(T)$, and $\mathrm{EE}_{\text{exact}}(T)$, $\mathrm{EE}_{\text{estimated}}(T)$ of TUC_4C_8 nanosheet 1 as shown in Figure 1.

Proposition 1. *Let T be the graph of TUC_4C_8 nanosheet, then the energy $E(T)$ and the Estrada index $EE(T)$ of T are given below:*

$$\begin{aligned} E(N) = {} & -1.8\times 10^{-3}m^4n^2 + 1.91\times 10^{-2}m^3n^2 - 6.96\times 10^{-2}m^2n^2 + 1.02\times 10^{-1}m^1n^2 - 5.07\times 10^{-2}n^2 \\ & + 2.64\times 10^{-2}nm^4 - 2.985\times 10^{-1}nm^3 + 1.1526nm^2 \\ & + 4.1125nm + 2.748n - 213\times 10^{-2}m^4 + 2.228\times 10^{-1}m^3 - 7.712\times 10^{-1}m^2 + 2.8762m - 3.89\times 10^{-1}, \end{aligned} \tag{1}$$

$$\begin{aligned} \mathrm{EE}(N) = {} & -3\times 10^{-4}m^4n^2 + 3.6\times 10^{-3}m^3n^2 - 1.6\times 10^{-2}m^2n^2 + 2.86\times 10^{-2}mn^2 - 1.6\times 10^{-2}n^2 + 1.6\times 10^{-3}m^4n \\ & - 2.01\times 10^{-2}m^3n + 8.74\times 10^{-2}m^2n \\ & + 13.379mn + 3.127n - 2\times 10^{-3}m^4 + 2.5\times 10^{-2}m^3 - 1.081\times 10^{-1}m^2 + 3.2289m - 1.02\times 10^{-1}. \end{aligned} \tag{2}$$

The equations (1) and (2) characterize the energy $E(N)$ and Estrada index $\mathrm{EE}(N)$, respectively. We have established the inequality $E_{\text{exact}}(N) > E_{\text{estimated}}(N)$, where E_{exact} and $E_{\text{estimated}}$ show the exact and estimated value of energy. This inequality poses that the exact value E_{exact} is always greater than $E_{\text{estimated}}$. So, the error among E_{exact} and $E_{\text{estimated}}$ is always positive.

But on the other hand, the exact value $\mathrm{EE}_{\text{exact}}(N)$ is always smaller than $\mathrm{EE}_{\text{estimated}}(N)$ which describes the error between $\mathrm{EE}_{\text{exact}}$ and $\mathrm{EE}_{\text{estimated}}$ is negative.

In Table 1, m is an integer from 1 to 10 while n is fixed, and in Tables 2 and 3 quadratic equations are constructed.

Error among the E_{exact} and $E_{\text{estimated}}$ are shown in Table 4 and (Table 5).

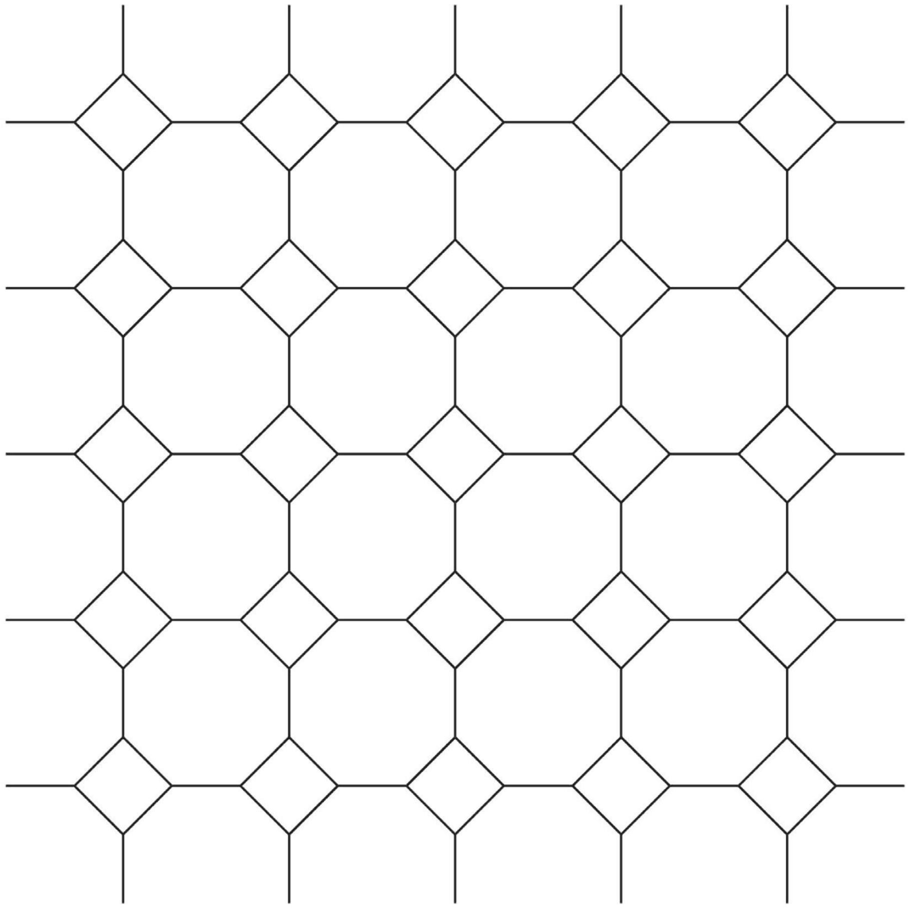

Figure 1: TUC_4C_8 nanosheet.

Table 1: The quadratic equation for the $E(N)$ and $EE(G)$ of TUC_4C_8 nanosheet.

(m, n)	Energy (E(N))	Estrada index (EE(N))
$(1, n)$	$-0.001n^2 + 7.741n + 1.9175$	$-0.0001n^2 + 16.5749n + 3.0418$
$(2, n)$	$-0.0011n^2 + 13.6178n + 3.7202$	$0.0012n^2 + 30.0994n + 6.00914$
$(3, n)$	$-0.0012n^2 + 19.5378n + 5.5891$	$-0.0013n^2 + 43.6375n + 9.1248$
$(4, n)$	$0.0053n^2 + 25.294n + 7.583$	$-0.004n^2 + 57.1646n + 12.172$
$(5, n)$	$-0.0182n^2 + 31.313n + 9.2495$	$-0.0105n^2 + 70.6945n + 15.215$
$(6, n)$	$-0.1515n^2 + 38.655n + 9.625$	$-0.0316n^2 + 84.2794n + 18.1878$
$(7, n)$	$-0.5176n^2 + 49.0138n + 7.2347$	$-0.0853n^2 + 98.0099n + 20.9764$
$(8, n)$	$-1.2827n^2 + 64.7168n + 0.0926$	$-0.1968n^2 + 112.015n + 23.4188$
$(9, n)$	$-2.6562n^2 + 88.725n - 14.2985$	$-0.3985n^2 + 126.4621n + 25.305$
$(10, n)$	$-4.8907n^2 + 124.633n - 38.947$	$-0.73n^2 + 141.557n + 26.377$

Table 2: All aforementioned are derived from the coefficient of the curves given in Table 1.

(n)	Energy (E(N))
n^2	$-18 \times 10^{-3}m^4 + 191 \times 10^{-2}m^3 - 696 \times 10^{-2}m^2 + 102 \times 10^{-1}m - 507 \times 10^{-2}$
n	$264 \times 10^{-2}m^4 - 2985 \times 10^{-1}m^3 + 1.1526m^2 4.1125m + 2.748$
1	$-213 \times 10^{-2}m^4 + 2228 \times 10^{-1}m^3 - 7712 \times 10^{-1}m^2 + 2.8762m - 389 \times 10^{-1}$

Table 3: All aforementioned equations are derived from the coefficient of the curves given in Table 1.

(n)	Estrada index EE(N)
n^2	$-3 \times 10^{-4}m^4 + 3.6 \times 10^{-3}m^3 - 1.6 \times 10^{-2}m^2 + 2.86 \times 10^{-2}m - 1.6 \times 10^{-2}$
n	$1.6 \times 10^{-3}m^4 - 2.01 \times 10^{-2}m^3 + 8.74 \times 10^{-2}m^2 + 13.379m + 3.127$
1	$-2 \times 10^{-3}m^4 + 2.5 \times 10^{-2}m^3 - 1.081 \times 10^{-1}m^2 + 3.2289m - 1.02 \times 10^{-1}$

Table 4: The $E_{\text{exact}}(T)$ and $E_{\text{estimated}}(T)$ of TUC_4C_8 nanosheet.

(m, n)	$E_{\text{exact}}(T)$	$E_{\text{estimated}}(T)$	Error
(5, 1)	40.6012	40.5443	0.0569
(5, 2)	71.8027	71.7646	0.0381
(5, 3)	103.5458	103.3415	0.2043
(5, 4)	134.4458	134.2103	0.2355
(5, 5)	165.8416	165.3595	0.4821

Table 5: The $EE_{\text{exact}}(T)$ and $EE_{\text{estimated}}(T)$ of the TUC_4C_8 nanosheet.

(m, n)	$EE_{\text{exact}}(T)$ (N)	$EE_{\text{estimated}}(T)$	Error
(4, 1)	69.3326	69.3403	−0.0077
(4, 2)	126.4852	126.516	−0.0308
(4, 3)	183.6298	183.689	−0.0592
(4, 4)	240.7664	240.861	−0.0946
(4, 5)	298.895	298.04	−1

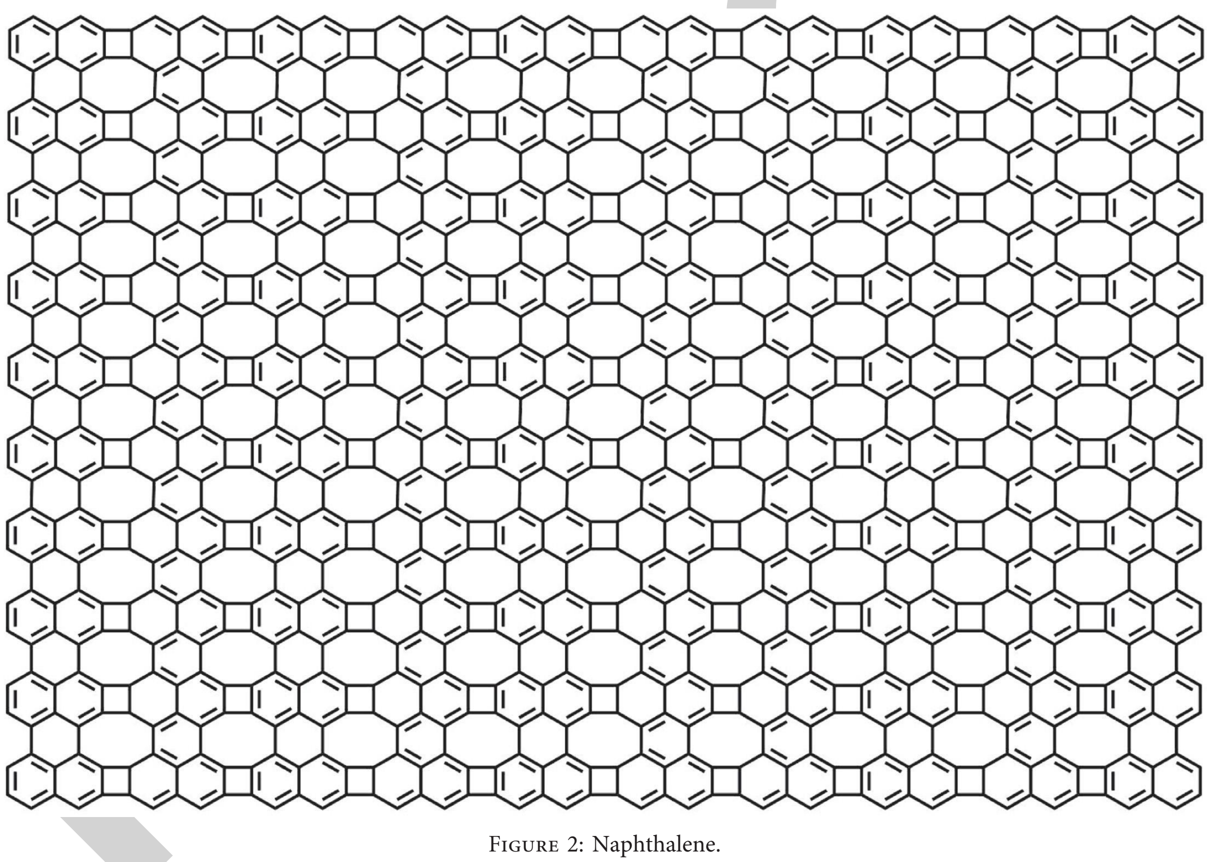

Figure 2: Naphthalene.

Table 6: The polynomial of order 2 for the $E(G)$ and $EE(N)$ of naphthalene.

(m, n)	Energy (E(N))	Estrada index (EE(N))
$(1, n)$	$0.0019n^2 + 14.5781n - 0.9285$	$-0.0117n^2 + 28.7981n - 3.5494$
$(2, n)$	$0.0023n^2 + 29.7505n - 1.8301$	$-0.0413n^2 + 62.09\text{n} - 2.8202$
$(3, n)$	$0.0031n^2 + 44.9205n - 2.7308$	$0.085n^2 + 94.4701n - 10.3612$
$(4, n)$	$0.0043n^2 + 60.0881n - 3.6279$	$0.03015n^2 + 127.04n - 15.7054$
$(5, n)$	$0.0059n^2 + 75.2533n - 4.5214$	$0.06667n^2 + 160.8653n - 19.433$
$(6, n)$	$0.0079n^2 + 90.4161n - 5.4113$	$1.6043nn^2 + 196.5316n - 24.9634$
$(7, n)$	$0.0103n^2 + 105.5765n - 6.2976$	$4.0707n^2 + 234.1325n - 34.0192$
$(8, n)$	$0.0131n^2 + 120.7345n - 7.1803$	$9.6511n^2 + 273.6896n - 45.7622$
$(9, n)$	$0.0163n^2 + 135.8901n - 8.0594$	$20.5835n^2 + 316.0045n - 59.6014$
$(10, n)$	$0.0199n^2 + 151.0433n - 8.9349$	$39.7109n^2 + 363.9428n - 81.673$

Table 7: The polynomial of order 2 derived from the coefficient of the curves given in Table 6.

n	Energy (E(N))
n^2	$2\times 10^{-4}m^2 - 2\times 10^{-4}m + 1.9\times 10^{-3}$
n	$-1.2\times 10^{-3}m^2 + 15.176m - 5.967\times 10^{-1}$
1	$1.8\times 10^{-3}m^2 - 9.097\times 10^{-1}m - 1.79\times 10^{-2}$

Table 8: The polynomial of order 2 derived from the coefficient of the curves given in Table 6.

n	Estrada index EE(N)
n^2	$-0.0001m^6 + 0.0041m^5 - 0.0423m^4 + 0.1805m^3 - 0.2864m^2 + 0.0798m + 0.0529$
n	$0.0006m^6 - 0.0163m^5 + 0.159m^4 - 0.5569m^3 + 0.1969m^2 + 34.682m - 5.6672$
1	$-0.0051m^6 + 0.1755m^5 - 2.3788m^4 + 15.91\,m^3 - 54.385m^2 + 83.077m - 45.943$

Table 9: The $E_{\text{exact}}(N)$ and $E_{\text{estimated}}(N)$ values of the naphthalene.

(m,n)	$E_{\text{exact}}(N)$	$E_{\text{estimated}}(N)$	Error
(2, 1)	27.9798	27.9227	0.0571
(2, 2)	57.6801	57.6322	0.0479
(2, 3)	87.4421	87.3202	0.1219
(2, 4)	117.2087	117.12	0.0887
(2, 5)	146.9799	146.9514	0.0285
(2, 6)	176.7557	176.739	0.0167
(2, 7)	206.5361	206.248	0.0345
(2, 8)	236.3211	236.248	0.0731
(2, 9)	266.1107	266.0206	0.0901
(2, 10)	295.9049	295.8252	0.0797

Table 10: The $\text{EE}_{\text{exact}}(N)$ and $\text{EE}_{\text{estimated}}(N)$ values of the Estrada indices of the naphthalene.

(m,n)	$\text{EE}_{\text{exact}}(N)$	$\text{EE}_{\text{estimated}}(N)$	Error
(3, 1)	83.11256	91.6297	−8.51714
(3, 2)	177.7729	186.3548	−8.5819
(3, 3)	272.012	281.2499	−9.2379
(3, 4)	366.2511	376.315	−10.0639
(3, 5)	460.4902	471.5501	−11.0599
(3, 6)	554.7293	566.9552	−12.2259
(3, 7)	648.9684	662.5303	−13.5619
(3, 8)	743.2075	758.2754	−15.0679
(3, 9)	837.4466	854.2309	−16.7843
(3, 10)	932.1173	950.2756	−18.1583

4. Energy and Estrada Index of Naphthalene

Naphthalene is a very important polycyclic aromatic hydrocarbon and it is useful in indoor and outdoor environments. It is actually a part of crude oil. The construction of naphthalene is based on two fused benzene rings that are connected with each other. Naphthalene is also used in mothballs which are widely used throughout the world. It is also used as an insect repellent product. Naphthalene is vibrantly volatile and insoluble in water, also the part of coal tar. In this section, we find the energy and Estrada index of naphthalene 2 which is given in Figure 2.

Proposition 2. *Let N be the chemical graph of naphthalene. Then, the energy $E(N)$ and Estrada index $EE(N)$ of the chemical graph of naphthalene are given below.*

$$\begin{aligned} E(N) = {} & 2\times 10^{-4}m^2n^2 - 2\times 10^{-4}mn^2 + 1.9\times 10^{-3}n^2 - 1.2\times 10^{-3}nm^2 + 15.176nm - 5.967\times 10^{-1}n \\ & + 1.8\times 10^{-3}m^2 - 9.097\times 10^{-1}m - 1.79\times 10^{-2}, \end{aligned} \tag{3}$$

$$\begin{aligned} \text{EE}(N) = {} & -1\times 10^{-4}m^6n^2 + 4.1\times 10^{-3}m^5n^2 - 4.23\times 10^{-2}m^4n^2 + 1.805\times 10^{-1}m^3n^2 - 2.864 \\ & \times 10^{-1}m^2n^2 + 7.98\times 10^{-2}mn^2 + 5.27\times 10^{-2}n^2 + 6\times 10^{-4}m^6n \\ & - 1.63\times 10^{-2}m^5n + 1.59\times 10^{-1}m^4n - 5.569\times 10^{-1}m^3n + 1.969\times 10^{-1}m^2n + 34.682mn - 5.6672n \\ & - 5.1\times 10^{-3}m^6 + 1.755\times 10^{-1}m^5 \\ & - 2.3788\,m^4 + 15.91m^3 - 54.385m^2 + 83.077m - 45.943. \end{aligned} \tag{4}$$

Equation (3) represents the energy and (4) represents the Estrada index, respectively. E(N) shows the energy of naphthalene and EE(N) shows the Estrada index of naphthalene. In the case of naphthalene, we observed this inequality $E_{\text{exact}}(N) > E_{\text{estimated}}(N)$, where $E_{\text{exact}}(N)$ and $E_{\text{estimated}}$ shows the exact and estimated value of energy, respectively.

In the case of the Estrada index, we observed this inequality $\text{EE}_{\text{exact}}(N) < \text{EE}_{\text{estimated}}(N)$, where $\text{EE}_{\text{exact}}(N)$ and $\text{EE}_{\text{estimated}}$ reflects the exact and the estimated value of the

Estrada index. The detailed analysis has been discussed critically.

In Table 6, m is an integer from 1 to 10 and n is fixed, and in Tables 7 and 8 quadratic equations are constructed.

Also, the error between the $E_{\text{exact}}(N)$, $E_{\text{estimated}}(N)$, and $EE_{\text{exact}}(N)$, $EE_{\text{estimated}}(N)$ are shown in Tables 9 and 10.

5. Conclusion

In this paper, we compute the energy ($E_{\text{exact}}(N)$) and Estrada index ($EE_{\text{estimated}}(N)$) of TUC_4C_8 nanosheet. Similarly, we compute the energy ($E_{\text{exact}}(N)$) and Estrada index ($EE_{\text{estimated}}(N)$) of naphthalene. We have observed some inequalities: the exact value of the energy of TUC_4C_8 nanosheet and naphthalene are both greater than the estimated value of TUC_4C_8 nanosheet and naphthalene, respectively.

(1). $E_{\text{exact}}(N) > E_{\text{estimated}}(N)$

(2) $E_{\text{exact}}(T) > E_{\text{estimated}}(T)$

This concludes that the error among the above-mentioned structures is always positive.

Similarly, the exact value of the Estrada index of TUC_4C_8 nanosheet and naphthalene are both smaller than the estimated value of TUC_4C_8 nanosheet and naphthalene, respectively.

(1). $EE_{\text{exact}}(N) < EE_{\text{estimated}}(N)$

(2) $EE_{\text{exact}}(T) < EE_{\text{estimated}}(T)$

This concludes that the error among the above-mentioned structures is always negative.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

Acknowledgments

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