

Euler-Sombor index of chemical graphs and its applications

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Abstract

Given a simple graph $\mathcal{A} = (V_{\mathcal{A}}, E_{\mathcal{A}})$. The Euler-Sombor index of $\mathcal{A}$ is given by

$$EU(\mathcal{A}) = \sum_{\tau\kappa \in E_{\mathcal{A}}} \sqrt{\eta(\tau)^2 + \eta(\kappa)^2 + \eta(\tau)\eta(\kappa)},$$

in which $\eta(c)$ is the degree of $c \in V_{\mathcal{A}}$.

In this paper, we focus on the chemical graphs which are simple graphs with property $\eta(\tau) \leq 4$ for any vertex $\tau \in V_{\mathcal{A}}$. We investigate the extremal problems of the *EU* index on the chemical graphs and find the sharp bounds for this index. Furthermore, we obtain the Euler-Sombor index for some nanostructures including Octagonal tiling $OT[p, q]$, $HAC_5 C_6 C_7[p, q]$ nanotube, titania $TiO_2[p, q]$ nanotube, and nanosheet $VC_5 C_7[p, q]$.

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1. Introduction

In this study, all graphs are simple graphs and consider $\mathcal{A} = (V_{\mathcal{A}}, E_{\mathcal{A}})$ as a graph where $V_{\mathcal{A}}$ denotes its set of vertices and $E_{\mathcal{A}}$ its set of edges. The degree of a vertex $z \in V_{\mathcal{A}}$ denotes by $\eta(z)$. A chemical graph is a simple graph with property $\eta(z) \leq 4$ for any vertex $z \in V_{\mathcal{A}}$.

A chemical graph can be associated with certain numerical descriptors known as topological indices. The descriptors are valuable tools in chemistry, pharmacology, and material science, offering a fast and informative way to

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analyze molecules and predict their properties. For a review of recent findings on the topological indices, see references [1-8] and their applications refer [9-17].

More recently, the Euler-Sombor index (denoted by EU) is introduced in [18] which is obtained using a new geometric approach and defined as

$$EU(\mathcal{A}) = \sum_{\tau\kappa \in E_{\mathcal{A}}} \sqrt{\eta(\tau)^2 + \eta(\kappa)^2 + \eta(\tau)\eta(\kappa)},$$

in which $\eta(c)$ is the degree of vertex c .

Tang et al. [18] analyzed the chemical applicability of the EU index. Gutman [19] investigated how the EU index correlates with the Sombor index in the context of graph theory. For recent results of the EU index, see [20, 21].

This paper investigates a new topological index of molecules called the Euler-Sombor index for chemical graphs. In particular, we aim to find the maximal and minimal values of the EU for these graphs in terms of order. In studies of nanostructures, some topological indices are computed and used to predict the behavior of these chemical structures [22-27]. In this work, we investigate four nanostructures such as Octagonal tiling $OT[p, q]$, $HAC_5C_6C_7[p, q]$ nanotube, titania $TiO_2[p, q]$ nanotube, and nanosheet $VC_5C_7[p, q]$. We compute EU for these structures and present numerical and graphical results.

2. Main Results

In this section, we present bounds for EU in chemical graphs and characterize the graphs attain to these bounds. To do this, some notations and preliminary concepts needed to prove the main theorems are stated as follows.

For a chemical graph $\mathcal{A}$ of order n and size m , let n_i be the cardinality of $\{w \in V_{\mathcal{A}} : \eta(w) = i\}$ and $\alpha_{i,j}$ be the cardinality of $\{(w, z) \in E_{\mathcal{A}} : \{\eta(w), \eta(z)\} = \{i, j\}\}$.

According to technique presented in [28], we consider

$$n = \sum_{(l,g) \in H} \alpha_{l,g} \left(\frac{l+g}{lg} \right), \quad (1)$$

in which $H = \{(l, g) : 1 \leq l \leq g \leq 4 \text{ and } l, g \in \mathbb{N}\}$.

According to the edge-partition method, we rewrite the Euler-Sombor index as follows

$$EU(\mathcal{A}) = \sum_{(l,g) \in H} \alpha_{l,g} \sqrt{l^2 + g^2 + lg}. \quad (2)$$

Let $K = \{(l, g) \in H : (l, g) \neq (4, 4)\}$. We have

$$\sqrt{l^2 + g^2 + lg} < 8\sqrt{3} \left(\frac{l+g}{lg} \right), \quad (3)$$

for any $(l, g) \in K$.

Theorem 2.1: For a chemical graph $\mathcal{A}$ of order n ,

$$EU(\mathcal{A}) \leq 8\sqrt{3}n.$$

Equality is achieved if and only if $\mathcal{A}$ is 4-regular graph.

Proof: Using the relations (1), (2) and (3), we get

$$\begin{aligned} EU(\mathcal{A}) &= 4\sqrt{3}\alpha_{4,4} + \sum_{(l,g) \in K} \alpha_{l,g} \sqrt{l^2 + g^2 + lg} \\ &= 8\sqrt{3} \left(n - \sum_{(l,g) \in K} \alpha_{l,g} \left(\frac{l+g}{lg} \right) \right) + \sum_{(l,g) \in K} \alpha_{l,g} \sqrt{l^2 + g^2 + lg} \\ &= 8\sqrt{3}n + \sum_{(l,g) \in K} \left(\sqrt{l^2 + g^2 + lg} - 8\sqrt{3} \left(\frac{l+g}{lg} \right) \right) \alpha_{l,g} \\ &\leq 8\sqrt{3}n. \end{aligned}$$

From the equality condition in the above relationship, we have

$$\sum_{(l,g) \in K} \left(\sqrt{l^2 + g^2 + lg} - 8\sqrt{3} \left(\frac{l+g}{lg} \right) \right) \alpha_{l,g} = 0.$$

Therefore, from the relation (3) we get $\alpha_{l,g} = 0$ for any $(l, g) \in K$. Consequently, $\mathcal{A}$ is a 4-regular graph. Conversely, let $\mathcal{A}$ be a 4-regular graph. Hence

$$EU(\mathcal{A}) = \sqrt{48}\alpha_{4,4} = \sqrt{48}m = \sqrt{48} \left(\frac{4n}{2} \right) = 8\sqrt{3}n.$$

Theorem 2.2: For a chemical graph $\mathcal{A}$ of order n ,

- i) if n is even, then $EU(\mathcal{A}) \geq \frac{\sqrt{3}}{2}n$. Equality is achieved if and only if $\mathcal{A} \cong \frac{n}{2}P_2$,
- ii) if n is odd, then $EU(\mathcal{A}) \geq \frac{n-3}{2}\sqrt{3} + 2\sqrt{7}$. Equality is achieved if and only if $\mathcal{A} \cong \frac{n-3}{2}P_2 \cup P_3$.

Proof:

- i) Let n be even and $P = \{(l, g) \in H : (l, g) \neq (1, 1)\}$. For any $(l, g) \in P$, we have

$$\sqrt{l^2 + g^2 + lg} > \frac{\sqrt{3}}{2} \left(\frac{p+q}{lg} \right). \quad (4)$$

From the relations (1), (2) and (4), we get

$$\begin{aligned} EU(\mathcal{A}) &= \sqrt{3}\alpha_{1,1} + \sum_{(l,g) \in P} \alpha_{l,g} \sqrt{l^2 + g^2 + lg} \\ &= \frac{\sqrt{3}}{2} \left(n - \sum_{(l,g) \in P} \alpha_{l,g} \left(\frac{l+g}{lg} \right) \right) + \sum_{(l,g) \in P} \alpha_{l,g} \sqrt{l^2 + g^2 + lg} \\ &= \frac{\sqrt{3}}{2}n + \sum_{(l,g) \in P} \left(\sqrt{l^2 + g^2 + lg} - \frac{\sqrt{3}}{2} \left(\frac{l+g}{lg} \right) \right) \alpha_{l,g} \\ &\geq \frac{1}{2}\sqrt{3}n. \end{aligned}$$

Suppose that $EU(\mathcal{A}) = \frac{\sqrt{3}}{2}n$. Hence Therefore, $\alpha_{l,g} = 0$ for any $(l, g) \in P$. It is straightforward to see that if n is even, then $\mathcal{A} \cong \frac{n}{2}P_2$. The converse holds trivially.

- ii) For an odd integer n , and under the assumption that $\mathcal{A}$ lacks isolated vertices, we derive the inequality $\alpha_{1,1} \leq \frac{n-3}{2}$.

Let $Q = \{(l, g) \in H: (l, g) \neq \{(1,1), (1,2)\}\}$. One can easily to check that for any $(l, g) \in Q$,

$$\sqrt{l^2 + g^2 + lg} > \frac{2\sqrt{7}}{3} \left(\frac{p+q}{lg} \right). \quad (5)$$

From the relations (1), (2) and (5), we have

$$\begin{aligned} EU(\mathcal{A}) &= \sqrt{3}\alpha_{1,1} + \sqrt{7}\alpha_{1,2} + \sum_{(l,g) \in Q} \alpha_{l,g} \sqrt{l^2 + g^2 + lg} \\ &= \left(\sqrt{3} - \frac{4\sqrt{7}}{3} \right) \alpha_{1,1} + \frac{2\sqrt{7}}{3} n + \sum_{(l,g) \in Q} \left(\sqrt{l^2 + g^2 + lg} - \frac{2\sqrt{7}}{3} \left(\frac{l+g}{lg} \right) \right) \alpha_{l,g} \\ &\geq \left(\sqrt{3} - \frac{4\sqrt{7}}{3} \right) \alpha_{1,1} + \frac{2\sqrt{7}}{3} n \\ &\geq \left(\sqrt{3} - \frac{4\sqrt{7}}{3} \right) \frac{n-3}{2} + \frac{2\sqrt{7}}{3} n \\ &= \frac{n-3}{2} \sqrt{3} + 2\sqrt{7}. \end{aligned}$$

Let $EU(\mathcal{A}) = \frac{n-3}{2} \sqrt{3} + 2\sqrt{7}$. Therefore, $\alpha_{1,1} = \frac{n-3}{2}$ and $\alpha_{l,g} = 0$ for any $(l, g) \in Q$. This clearly implies that $\mathcal{A} \cong \frac{n-3}{2} P_2 \cup P_3$. The converse is clear.

The next theorem follows directly from Theorem 2 in [1] and Theorem 2.1.

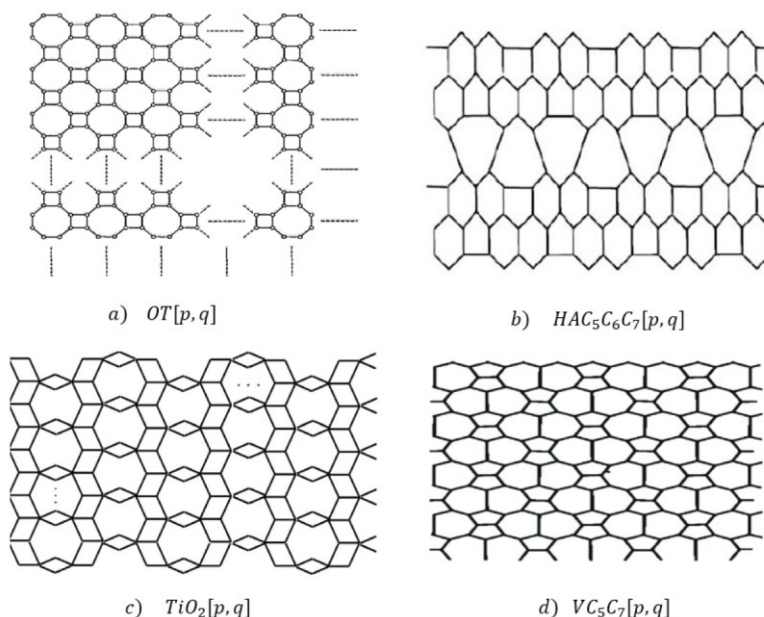
Theorem 2.: For a connected chemical graph $\mathcal{A}$ of order n ,

$$2\sqrt{3}(n-3) + 2\sqrt{7} \leq EU(\mathcal{A}) \leq 8\sqrt{3}n.$$

Equality holds in the left if and only if $\mathcal{A} \cong P_n$ and in the right if and only if $\mathcal{A}$ is 4-regular graph.

3. Euler-Sombor index for some nanostructures

Chemical graph theory models molecules using a graph structure. A molecular graph represents atoms as nodes and depicts chemical bonds between them as edges. Chemical graph theory employs topological indices to correlate the physicochemical properties of compounds. A key application of these indices lies in the development of quantitative structure-activity relationships (QSAR) models, which link molecular properties to biological activities. By establishing connections between molecular attributes and their corresponding behaviors, this field finds broad utility across physics, chemistry, and biology. In this section, we compute EU for four nanostructures including Octagonal tiling $OT[p, q]$, $HAC_5C_6C_7[p, q]$ nanotube, titania $TiO_2[p, q]$ nanotube, and nanosheet $VC_5C_7[p, q]$. We consider $V_{\mathcal{A}}(i) = \{w \in V_{\mathcal{A}}: \eta(c) = i\}$ and $E_{\mathcal{A}}(i, j) = \{ct \in E_{\mathcal{A}}: \eta(c) = i \text{ and } \eta(t) = j\}$ in a molecular graph $\mathcal{A}$.

**Figure 1**

Molecular graphs of nanostructures a) $OT[p, q]$, b) $HAC_5C_6C_7[p, q]$ nanotube, c) titania $TiO_2[p, q]$ nanotube, and d) nanosheet $VC_5C_7[p, q]$.

First, we calculate EU for the molecular graph $OT[p, q]$ with p denoting the horizontal octagon count and q indicating the vertical octagon count in every column (see Figure 1(a)).

Theorem 3.1: For a molecular graph $OT[p, q]$,

$$EU(OT[p, q]) = 4(5\sqrt{3} - 2\sqrt{19} + (\sqrt{19} - 5\sqrt{3})q + (\sqrt{19} + (9q - 5)\sqrt{3})p).$$

Proof: Consider $\mathcal{A}$ the molecular graph $OT[p, q]$ with $|V_{\mathcal{A}}(2)| = 4(q + p)$ and $|V_{\mathcal{A}}(3)| = 4(2pq - (p + q))$. Edge partitions of $\mathcal{A}$ are as follows.

$$\begin{aligned} E_{\mathcal{A}}(2, 2) &= \{ct \in E_{\mathcal{A}} : \eta(c) = 2 \text{ and } \eta(t) = 2\}, |E_{\mathcal{A}}(2, 2)| = 2(q + p + 2), \\ E_{\mathcal{A}}(2, 3) &= \{ct \in E_{\mathcal{A}} : \eta(c) = 2 \text{ and } \eta(t) = 3\}, |E_{\mathcal{A}}(2, 3)| = 4(q + p - 2), \\ E_{\mathcal{A}}(3, 3) &= \{ct \in E_{\mathcal{A}} : \eta(c) = 3 \text{ and } \eta(t) = 3\}, |E_{\mathcal{A}}(3, 3)| \\ &= 4(3pq - 2(p + q) + 1). \end{aligned} \quad (6)$$

Therefore, this graph contains $|V_{\mathcal{A}}| = \sum_{i=2}^3 |V_{\mathcal{A}}(i)| = 8pq$ vertices and $|E_{\mathcal{A}}| = \sum_{i \leq j} |E_{\mathcal{A}}(i, j)| = 2(6pq - (p + q))$ edges. Using the relation (2) and the cardinality of the edge partition in (6), we have

$$\begin{aligned} EU(\mathcal{A}) &= \sum_{(i, j) \in H} |E_{\mathcal{A}}(i, j)| \sqrt{i^2 + j^2 + ij} \\ &= |E_{\mathcal{A}}(2, 2)| \sqrt{12} + |E_{\mathcal{A}}(2, 3)| \sqrt{19} + |E_{\mathcal{A}}(3, 3)| \sqrt{27} \end{aligned}$$

$$\begin{aligned}
&= 4(p+q+2)\sqrt{3} + 4(q+p-2)\sqrt{19} + 12(3pq-2(p+q)+1)\sqrt{3} \\
&= 4(5\sqrt{3}-2\sqrt{19}+(\sqrt{19}-5\sqrt{3})q+(\sqrt{19}+(9q-5)\sqrt{3})p).
\end{aligned}$$

We consider the molecular graph $HAC_5C_6C_7[p, q]$ nanotube where p represents the pentagon count per row, with the vertices in the first three rows and edges repeating cyclically, and q indicates the number of repetitions (see Figure 1(b)).

Theorem 3.2: For a molecular graph $HAC_5C_6C_7[p, q]$,

$$EU(HAC_5C_6C_7[p, q]) = 2p(4\sqrt{19} + 3\sqrt{3}(-5 + 12q)).$$

Proof: Let $\mathcal{A}$ be the molecular graph $HAC_5C_6C_7[p, q]$. Edge partitions of $\mathcal{A}$ are as follows.

$$\begin{aligned}
E_{\mathcal{A}}(2,3) &= \{ct \in E_{\mathcal{A}}: \eta(c) = 2 \text{ and } \eta(t) = 3\}, |E_{\mathcal{A}}(2,3)| = 8p, \\
E_{\mathcal{A}}(3,3) &= \{ct \in E_{\mathcal{A}}: \eta(c) = 3 \text{ and } \eta(t) = 3\}, |E_{\mathcal{A}}(3,3)| = 2p(12q - 5). \quad (7)
\end{aligned}$$

Therefore, this graph contains $|V_{\mathcal{A}}| = 16pq$ vertices and $|E_{\mathcal{A}}| = \sum_{i \leq j} |E_{\mathcal{A}}(i, j)| = 24pq - 2p$ edges. From (7), we get

$$\begin{aligned}
EU(\mathcal{A}) &= \sum_{(i,j) \in H} |E_{\mathcal{A}}(i, j)| \sqrt{i^2 + j^2 + ij} \\
&= |E_{\mathcal{A}}(2,3)| \sqrt{19} + |E_{\mathcal{A}}(3,3)| \sqrt{27} \\
&= 8p\sqrt{19} + 6p(12q - 5)\sqrt{3} \\
&= 2p(4\sqrt{19} + 3\sqrt{3}(-5 + 12q)).
\end{aligned}$$

We consider the molecular graph $TiO_2[p, q]$ nanotube where p represents the pentagon count per row, with the vertices in the first three rows and edges repeating cyclically, and q indicates the number of repetitions (see Figure 1(c)).

Theorem 3.3: For a molecular graph $TiO_2[p, q]$,

$$EU(TiO_2[p, q]) = 2q((6\sqrt{7} + \sqrt{37} + \sqrt{39} - 7) + (21 + 2\sqrt{39})p).$$

Proof: Consider $\mathcal{A}$ the molecular graph $TiO_2[p, q]$ nanotube with $|V_{\mathcal{A}}(2)| = 2pq + 4q$, $|V_{\mathcal{A}}(3)| = 2pq$, $|V_{\mathcal{A}}(4)| = 2q$, and $|V_{\mathcal{A}}(5)| = 2pq$. Edge partitions of $\mathcal{A}$ are as follows.

$$\begin{aligned}
E_{\mathcal{A}}(2,4) &= \{ct \in E_{\mathcal{A}}: \eta(c) = 2 \text{ and } \eta(t) = 4\}, |E_{\mathcal{A}}(2,4)| = 6q, \\
E_{\mathcal{A}}(2,5) &= \{ct \in E_{\mathcal{A}}: \eta(c) = 2 \text{ and } \eta(t) = 5\}, |E_{\mathcal{A}}(2,5)| = 2q(2p + 1), \\
E_{\mathcal{A}}(3,4) &= \{ct \in E_{\mathcal{A}}: \eta(c) = 3 \text{ and } \eta(t) = 4\}, |E_{\mathcal{A}}(3,4)| = 2q, \\
E_{\mathcal{A}}(3,5) &= \{ct \in E_{\mathcal{A}}: \eta(c) = 3 \text{ and } \eta(t) = 5\}, |E_{\mathcal{A}}(3,5)| = 2q(3p - 1). \quad (8)
\end{aligned}$$

Therefore, $|V_{\mathcal{A}}| = 6(pq + q)$ and $|E_{\mathcal{A}}| = \sum_{i \leq j} |E_{\mathcal{A}}(i, j)| = 10pq + 8q$. From (8), we get

$$EU(\mathcal{A}) = \sum_{(i,j) \in H} |E_{\mathcal{A}}(i, j)| \sqrt{i^2 + j^2 + ij}$$

$$\begin{aligned}
&= |E_{\mathcal{A}}(2,4)|\sqrt{28} + |E_{\mathcal{A}}(2,5)|\sqrt{39} + |E_{\mathcal{A}}(3,4)|\sqrt{37} + |E_{\mathcal{A}}(3,5)|\sqrt{49} \\
&= 12q\sqrt{7} + 2q(2p+1)\sqrt{39} + 2q\sqrt{37} + 14q(3p-1) \\
&= 2q((6\sqrt{7} + \sqrt{37} + \sqrt{39} - 7) + (21 + 2\sqrt{39})p).
\end{aligned}$$

We consider the molecular graph of nanosheet $VC_5C_7[p, q]$ where p and q are denoted as the amount of pentagons found in the first row and the number of repetitions, respectively (see Figure 1(d)).

Theorem 3.4: For a molecular graph $VC_5C_7[p, q]$,

$$EU(VC_5C_7[p, q]) = 6p(2\sqrt{19} + 3\sqrt{3}(4q - 1)).$$

Proof: Consider $\mathcal{A}$ the molecular graph of nanosheet $VC_5C_7[p, q]$ with $|V_{\mathcal{A}}(2)| = 3(p + q)$ and $|V_{\mathcal{A}}(3)| = 16p$. Edge partitions of $\mathcal{A}$ are as follows.

$$\begin{aligned}
E_{\mathcal{A}}(2,3) &= \{ct \in E_{\mathcal{A}} : \eta(c) = 2 \text{ and } \eta(t) = 3\}, |E_{\mathcal{A}}(2,3)| = 12p, \\
E_{\mathcal{A}}(3,3) &= \{ct \in E_{\mathcal{A}} : \eta(c) = 3 \text{ and } \eta(t) = 3\}, |E_{\mathcal{A}}(3,3)| = 6p(4q - 1). \quad (9)
\end{aligned}$$

Therefore, $|V_{\mathcal{A}}| = 16pq + 6p$ and $|E_{\mathcal{A}}| = \sum_{i \leq j} |E_{\mathcal{A}}(i, j)| = 24pq + 6p$. Using (9), we get

$$\begin{aligned}
EU(\mathcal{A}) &= \sum_{(i,j) \in H} |E_{\mathcal{A}}(i, j)|\sqrt{i^2 + j^2 + ij} \\
&= |E_{\mathcal{A}}(2,3)|\sqrt{19} + |E_{\mathcal{A}}(3,3)|\sqrt{27} \\
&= 12p\sqrt{19} + 18p(4q - 1)\sqrt{3} \\
&= 6p(2\sqrt{19} + 3\sqrt{3}(4q - 1)).
\end{aligned}$$

Table 1
Euler-Sombor index values for molecular graphs of nanostructures.

$[p, q]$	$OT[p, q]$	$HAC_5C_6C_7[p, q]$	$TiO_2[p, q]$	$VC_5C_7[p, q]$
[1,1]	27.71	77.10	105.89	145.83
[2,2]	180.36	403.62	345.74	541.09
[3,2]	287.86	605.44	518.61	811.63
[3,3]	457.72	979.56	719.55	1185.75
[4,4]	859.78	1804.91	1227.32	2079.84
[5,5]	1386.56	2879.67	1869.05	3223.34

In Table 1, the values of EU for nanostructures including $OT[p, q]$, $HAC_5C_6C_7[p, q]$, $TiO_2[p, q]$, and $VC_5C_7[p, q]$ are provided. The results show that with increasing the parameters p and q , the Euler-Sombor index increases. The graphical representations of the values of the EU index of these nanostructures are depicted in Figure 2 for certain values of p and q . According to the finding, the highest and lowest values of the EU index are for nanostructures $VC_5C_7[p, q]$ and $OT[p, q]$, respectively.

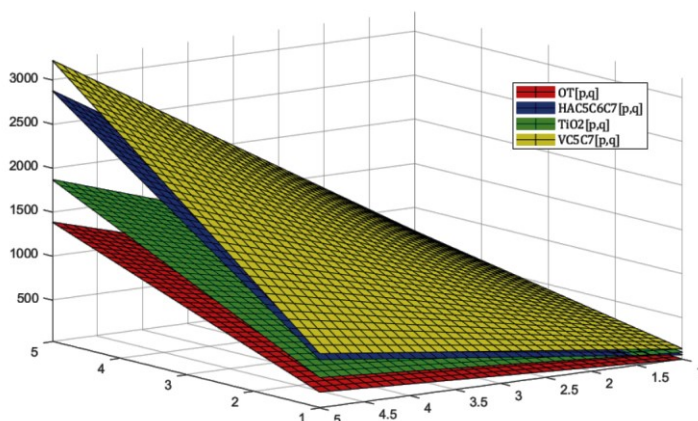


Figure 2

Graphical comparison of the EU index values for four nanostructures $OT[p, q]$, $HAC_5C_6C_7[p, q]$, $TiO_2[p, q]$, and $VC_5C_7[p, q]$.

4. Conclusion

In this paper, we considered a newly introduced topological index. We obtain sharp upper and lower bounds of this index on molecular graphs. For application, we considered four nanostructures including $OT[p, q]$, $HAC_5C_6C_7[p, q]$, $TiO_2[p, q]$, $VC_5C_7[p, q]$ and by investigating their molecular graphs computed this index. Our computational approach involved a combination of combinatorial, graph-theoretic, and analytical techniques. Specifically, we employed vertex and edge partitioning methods and degree-based calculations. To support these computations, MATLAB and Mathematica were utilized for numerical analysis, and MATLAB was used for the graphical representation of the results.

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