Journal of Discrete Mathematical Sciences & Cryptography
ISSN 0972-0529 (Print), ISSN 2169-0065 (Online)
Vol. 29 (2026), No. 1, pp. 49–64
DOI : 10.47974/JDMSC-2135

Graph Edge Hyper-Zagreb index : Applications and thermodynamic property predictions for linear acenes molecules

Zohreh Aliannejadi *
Somayeh Shafiee Alamoti †
Department of Mathematics
Islamic Azad University
South Tehran Branch
Deh Haghi Street
Pirouzi Street
Tehran
Iran

Abstract

This research explores the Edge Hyper-Zagreb index, a unique method of calculating graph indices by replacing vertex degrees with edge degrees. The edge degree is obtained by summing the degrees of the end vertices and subtracting 2. We analyze the Edge Hyper-Zagreb index for the Cartesian product and join of graphs and compute it for linear Acenes molecules with the formula ($C_{4n+2}\,H_{2n+4}$). Besides, we highlight the correlation between topological indices and the quantity of rings, using the Topological Indices Method (*TIM*) to predict the diverse thermodynamic characteristics of the Acenes family, like electron affinity, bond strength, heat of formation, and gap energy.

Subject Classification: *05C09, 05C12.*

Keywords: *Energy affinity of electrons, Bonding energy, Energy cap, Formation heat energy, Edge Hyper-Zagreb Graph index, Linear acenes molecules.*

1. Introduction

Molecular descriptors known as topological indices, or connectivity indices, are employed within the realms of mathematical chemistry,

* *ORCID-ID:* 0000-0001-6133-1047

* *E-mail:* z_alian@azad.ac.ir (Corresponding Author)
† *E-mail:* shafiee.s88@gmail.com

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molecular topology, and chemical graph theory. These numerical parameters are derived from a chemical compound's molecular graph, providing insights into the graph's topological characteristics [18]. Topological indices generally remain consistent across graphs and are instrumental in quantitative structure-activity relationships (*QSARs*), correlating molecules' biological activities or characteristics with their chemical structures, establishing a link between a compound's structure and its function [17].

To compute these indices, hydrogen-depleted molecular graphs are utilized, where atoms are depicted as vertices, and bonds as edges. The connections between atoms are illustrated using various topological matrices, such as distance or adjacency matrices. These matrices are then mathematically processed to yield a single numerical value, referred to as a graph invariant, graph-theoretical index, or topological index [14, 15]. As 2*D* descriptors, these indices can be conveniently calculated from molecular graphs and remain unaffected by the graph's depiction or labeling. An advantage of topological indices is that they do not require structural energy minimization of the chemical compound under investigation. These indices are valuable tools within the context of mathematical chemistry, molecular topology, and chemical graph theory, offering a reliable method for characterizing the topological attributes of molecular graphs.

Basic topological indices neglect double bonds, atom characteristics, and hydrogen atoms, as they only apply to connected undirected molecular graphs [23]. In contrast, advanced topological indices consider the hybridization status of atoms within the molecule [16]. Common indices include Hosoya, Wiener, Randićs molecular connectivity, Balaban's J index [7], and *TAU* descriptors [10]. Although individual indices may yield identical values for distinct molecular graphs, combining multiple indices can improve discriminatory capabilities.

ETA indices [24] were developed to enhance *TAU* descriptors. A topological index's ability to distinguish between graphs is crucial since individual indices may not differentiate certain molecular graphs. Creating a comprehensive superindex by merging indices can enhance this capability [9]. *QSARs* are statistical models that correlate the biological activity of substances, such as drugs and pollutants, with molecular structure and property descriptors. *QSARs* have applications in risk assessment, toxicity prediction, regulatory decision-making [28], and drug discovery [22].

Nanotechnology involves manipulating matter at the atomic, molecular, and supramolecular levels [29]. Initially focused on atomic and molecular manipulation for creating larger products, nanotechnology now enables production, manipulation, and utilization of nanomaterials [1, 2, 3, 4, 19]. Acenes and line graphs of nanotubes have gained interest due to their nanostructure dimensions [3, 7, 10, 15, 25, 27]. Developing reliable models for predicting heavier Acenes' properties is essential, and generating a topological index for chemical molecules is a promising approach [26].

This paper focuses on connected, finite, undirected graphs. The degree of vertex a in graph Γ, denoted as $d^*_\Gamma(a)$, represents the number of connected edges. Gutman and Trinajstić [20] pioneered the Zagreb indices in 1972, which marked a significant milestone in the study of molecular structure's influence on total φ electron energy. These indices comprise the first Zagreb index $M_1(\Gamma)$, calculating the sum of squared vertex degrees, and the second Zagreb index $M_2(\Gamma)$, summing the products of adjacent vertex pairs' degrees. Widely applied in chemical graph theory, the Zagreb indices have significantly enhanced the understanding of chemical compounds' properties and behavior. Their development has also laid the groundwork for additional topological indices that researchers employ to explore structure-property connections in diverse chemical systems.

Ashrafi et al. [6] introduced the first and second Zagreb coindices,

$$\overline{M}_1(\Gamma) = \sum_{ab \notin E(\Gamma)} (d^*_\Gamma(a) + d^*_\Gamma(b))$$

and

$$\overline{M}_2(\Gamma) = \sum_{ab \notin E(\Gamma)} (d^*_\Gamma(a).d^*_\Gamma(b)),$$

respectively. These indices were found to be related to the total φ-electron energy [20] and were developed to assess the level of branching in the carbon-atom skeleton [21]. The Zagreb index, or Zagreb group index, was later named in a review article [8]. Milicević et al. [5] reformulated the Zagreb indices considering edge-degrees rather than vertex-degrees, as below

$$EM_1(\Gamma) = \sum_{\alpha \in E(\Gamma)} (d^*_\Gamma(\alpha))^2 \quad EM_2(\Gamma) = \sum_{\alpha \sim \beta} (d^*_\Gamma(\alpha)).(d^*_\Gamma(\beta)),$$

in which $d^*_\Gamma(\alpha)$ signifies the degree of the edge α in Γ, which can be described as $d^*_\Gamma(\alpha) = d^*_\Gamma(a) + d^*_\Gamma(b) - 2$ with $\alpha = ab$ and $\alpha \sim \beta$ indicates

that the edges α and β are neighboring, i.e., both edges terminate at the same vertex in Γ.

Shirdel et al. [12] introduced a novel topological index, referred to as the Hyper-Zagreb index, specifically designed for a connected graph Γ as

$$HM(\Gamma) = \sum_{ab \in E(\Gamma)} (d^*_\Gamma(a) + d^*_\Gamma(b))^2.$$

Now, We would like to define the Edge Hyper-Zagreb index as:

Definition 1.1: The Edge Hyper-Zagreb index of graph Γ for every α and $\beta \in E(\Gamma)$ is introduced as

$$EHM(\Gamma) = \sum_{\alpha \sim \beta \in E(\Gamma)} (d^*_\Gamma(\alpha) + d^*_\Gamma(\beta))^2.$$

2. Cartesian Product and Join of Graphs

In the following section, we explore the behavior of the *EHM* index under the Cartesian product and join of graphs. We consider only connected, finite and simple graphs, denoted by Γ and Ω with sets of vertex $V(\Gamma)$ and $V(\Omega)$ and sets of edge $E(\Gamma)$ and $E(\Omega)$, respectively. In addition, we symbolize $|V(\Gamma)| = n_\Gamma$, $|E(\Gamma)| = m_\Gamma$ and $|V(\Omega)| = n_\Omega$, $|E(\Omega)| = m_\Omega$.

The join of $\Gamma + \Omega$ of graphs Γ and Ω is a graph with $V(\Gamma) \cup V(\Omega)$ as its vertices and edge set $E(\Gamma) \cup E(\Omega) \cup \{ab \mid a \in V(\Gamma)$ and $b \in V(\Omega)\}$. The degree of a vertex a of $\Gamma + \Omega$ is given by

$$d^*_{(\Gamma+\Omega)}(a) = \begin{cases} d^*_\Gamma(a) + n_\Omega, a \in V(\Gamma) \\ d^*_\Omega(a) + n_\Gamma, a \in V(\Omega). \end{cases}$$

The Cartesian product $\Gamma \times \Omega$ of graphs Γ and Ω contains $V(\Gamma \times \Omega) = V(\Gamma) \times V(\Omega)$ as its vertices and (a,b) (a',b') is an edge of $\Gamma \times \Omega$ if $a = a'$ and $bb' \in E(\Omega)$, or $aa' \in E(\Gamma)$ and $b = b'$.

Theorem 2.1: *The EHM index of* $\Gamma + \Omega$ *is equal to:*

$$\begin{aligned} EHM(\Gamma + \Omega) = {} & 2EM_1(\Gamma) + 16n_\Omega(M_1(\Gamma) - 2m_\Gamma) + 16n_\Omega^2 m_\Gamma \\ & + 2EM_2(\Gamma) + 2EM_1(\Omega) + 16n_\Gamma(M_1(\Omega) - 2m_\Omega) \\ & + 16n_\Gamma^2 m_\Omega + 2EM_2(\Omega) + 2n_\Omega M_1(\Gamma) + 2n_\Gamma M_1(\Omega) \\ & + 32m_\Gamma m_\Omega + 8(2n_\Gamma + 2n_\Omega - 4)(n_\Gamma m_\Omega + n_\Omega m_\Gamma) \\ & + 4n_\Gamma n_\Omega(2n_\Gamma + 2n_\Omega - 4)^2 + 8{m_\Gamma}^2 + 8{m_\Omega}^2. \end{aligned}$$

Proof: Let $\alpha = ab$ and $\beta = bc$ be two adjacent edges in $E(\Gamma + \Omega)$. Then we have

$$\begin{aligned}
EHM(\Gamma+\Omega) &= \sum_{\alpha\sim\beta\in E(\Gamma+\Omega)}(d^*_{\Gamma+\Omega}(\alpha)+d^*_{\Gamma+\Omega}(\beta))^2\\
&= \sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma+\Omega}(\alpha)+d^*_{\Gamma+\Omega}(\beta))^2\\
&\quad+\sum_{\alpha\sim\beta\in E(\Omega)}(d^*_{\Gamma+\Omega}(\alpha)+d^*_{\Gamma+\Omega}(\beta))^2\\
&\quad+\sum_{\alpha\sim\beta\in\{\alpha\sim\beta|\alpha\in E(\Gamma),\beta\in E(\Omega)\}}(d^*_{\Gamma+\Omega}(\alpha)+d^*_{\Gamma+\Omega}(\beta))^2.\\
&= A1 + A_2 + A_3.
\end{aligned}$$

We consider

$$\begin{aligned}
A_1 &= \sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma+\Omega}(\alpha)+d^*_{\Gamma+\Omega}(\beta))^2\\
&= \sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma+\Omega}(a)+d^*_{\Gamma+\Omega}(b)-2+d^*_{\Gamma+\Omega}(b)+d^*_{\Gamma+\Omega}(c)-2)^2\\
&= \sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma}(a)+d^*_{\Gamma}(b)+2n_\Omega-2+d^*_{\Gamma}(b)+d^*_{\Gamma}(c)+2n_\Omega-2)^2\\
&= \sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma}(a)+d^*_{\Gamma}(b)-2+d^*_{\Gamma}(b)+d^*_{\Gamma}(c)-2+4n_\Omega)^2\\
&= \sum_{\alpha\sim\beta\in E(\Gamma)}((d^*_{\Gamma}(a)+d^*_{\Gamma}(b)-2)^2+(d^*_{\Gamma}(b)+d^*_{\Gamma}(c)-2)^2\\
&\quad+16n_\Omega^2+2(d^*_{\Gamma}(a)+d^*_{\Gamma}(b)-2)(d^*_{\Gamma}(b)+d^*_{\Gamma}(c)-2)\\
&\quad+8n_\Omega(d^*_{\Gamma}(a)+d^*_{\Gamma}(b)-2)+8n_\Omega(d^*_{\Gamma}(b)+d^*_{\Gamma}(c)-2))\\
&= \sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma}(a)+d^*_{\Gamma}(b)-2)^2\\
&\quad+8n_\Omega\sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma}(a)+d^*_{\Gamma}(b)-2)\\
&\quad+16\sum_{\alpha\sim\beta\in E(\Gamma)}n_\Omega^2+\sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma}(b)+d^*_{\Gamma}(c)-2)^2\\
&\quad+8n_\Omega\sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma}(b)+d^*_{\Gamma}(c)-2)\\
&\quad+2\sum_{\alpha\sim\beta\in E(\Gamma)}(d^*_{\Gamma}(a)+d^*_{\Gamma}(b)-2)(d^*_{\Gamma}(b)+d^*_{\Gamma}(c)-2)\\
&= EM_1(\Gamma)+8n_\Omega(M_1(\Gamma)-2m_\Gamma)+16n_\Omega^2m_\Gamma\\
&\quad+EM_1(\Gamma)+8n_\Omega(M_1(\Gamma)-2m_\Gamma)+2EM_2(\Gamma)\\
&= 2EM_1(\Gamma)+16n_\Omega(M_1(\Gamma)-2m_\Gamma)+16n_\Omega^2m_\Gamma+2EM_2(\Gamma).
\end{aligned}$$

Similarly,

$$\begin{aligned}
A_2 &= \sum_{\alpha\sim\beta\in E(\Omega)}(d^*_{\Gamma+\Omega}(\alpha)+d^*_{\Gamma+\Omega}(\beta))^2\\
&= \sum_{\alpha\sim\beta\in E(\Omega)}(d^*_{\Gamma+\Omega}(a)+d^*_{\Gamma+\Omega}(b)-2+d^*_{\Gamma+\Omega}(b)+d^*_{\Gamma+\Omega}(c)-2)^2\\
&= \sum_{\alpha\sim\beta\in E(\Omega)}(d^*_{\Omega}(a)+d^*_{\Omega}(b)+2n_\Gamma-2+d^*_{\Omega}(b)+d^*_{\Omega}(c)+2n_\Gamma-2)^2\\
&= \sum_{\alpha\sim\beta\in E(\Omega)}(d^*_{\Omega}(a)+d^*_{\Omega}(b)-2+d^*_{\Omega}(b)+d^*_{\Omega}(c)-2+4n_\Gamma)^2\\
&= \sum_{\alpha\sim\beta\in E(\Omega)}((d^*_{\Omega}(a)+d^*_{\Omega}(b)-2)^2+(d^*_{\Omega}(b)+d^*_{\Omega}(c)-2)^2+16n_\Gamma^2\\
&\quad+2(d^*_{\Omega}(a)+d^*_{\Omega}(b)-2)(d^*_{\Omega}(b)+d^*_{\Omega}(c)-2)\\
&\quad+8n_\Gamma(d^*_{\Omega}(a)+d^*_{\Omega}(b)-2)+8n_\Gamma(d^*_{\Omega}(b)+d^*_{\Omega}(c)-2))
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{\alpha\sim\beta\in E(\Omega)}(d^*_\Omega(a)+d^*_\Omega(b)-2)^2\\
&+8n_\Gamma\sum_{\alpha\sim\beta\in E(\Omega)}(d^*_\Omega(a)+d^*_\Omega(b)-2)\\
&+16\sum_{\alpha\sim\beta\in E(\Omega)}n_\Gamma^2+\sum_{\alpha\sim\beta\in E(\Omega)}(d^*_\Omega(b)+d^*_\Omega(c)-2)^2\\
&+8n_\Gamma\sum_{\alpha\sim\beta\in E(\Omega)}(d^*_\Omega(b)+d^*_\Omega(c)-2)\\
&+2\sum_{\alpha\sim\beta\in E(\Omega)}(d^*_\Omega(a)+d^*_\Omega(b)-2)(d^*_\Omega(b)+d^*_\Omega(c)-2)\\
&= EM_1(\Omega)+8n_\Gamma(M_1(\Omega)-2m_\Omega)+16n_\Gamma^2m_\Omega\\
&+EM_1(\Omega)+8n_\Gamma(M_1(\Omega)-2m_\Omega)+2EM_2(\Omega)\\
&= 2EM_1(\Omega)+16n_\Gamma(M_1(\Omega)-2m_\Omega)+16n_\Gamma^2m_\Omega+2EM_2(\Omega).
\end{aligned}
$$

Finally,

$$
\begin{aligned}
A_3 &= \sum_{\alpha\sim\beta\in\{\alpha\sim\beta|\alpha\in E(\Gamma),\beta\in E(\Omega)\}}(d^*_{\Gamma+\Omega}(\alpha)+d^*_{\Gamma+\Omega}(\beta))^2\\
&= \sum_{\alpha\sim\beta\in\{\alpha\sim\beta|\alpha\in E(\Gamma),\beta\in E(\Omega)\}}(d^*_{\Gamma+\Omega}(a)+d^*_{\Gamma+\Omega}(b)-2+d^*_{\Gamma+\Omega}(b)+d^*_{\Gamma+\Omega}(c)-2)^2\\
&= \sum_{a,b\in V(\Gamma),b,c\in V(\Omega)}(d^*_\Gamma(a)+n_\Omega+d^*_\Omega(b)+n_\Gamma-2+d^*_\Gamma(b)+n_\Omega+d^*_\Omega(c)+n_\Gamma-2)^2\\
&= \sum_{a,b\in V(\Gamma),b,c\in V(\Omega)}((d^*_\Gamma(a)+d^*_\Omega(b))+(d^*_\Gamma(b)+d^*_\Omega(c))+(2n_\Omega+2n_\Gamma-4)^2\\
&= \sum_{a,b\in V(\Gamma),b,c\in V(\Omega)}((d^*_\Gamma(a)^2+d^*_\Omega(b)^2+2d^*_\Gamma(a)d^*_\Omega(b))+(d^*_\Gamma(b)^2+d^*_\Omega(c)^2\\
&+2d^*_\Gamma(b)d^*_\Omega(b))+(2n_\Omega+2n_\Gamma-4)^2+2(d^*_\Gamma(a)+d^*_\Omega(b))(d^*_\Gamma(b)+d^*_\Omega(c))\\
&+2(d^*_\Gamma(a)+d^*_\Omega(b))(2n_\Omega+2n_\Gamma-4)+2(d^*_\Gamma(b)+d^*_\Omega(a))(2n_\Omega+2n_\Gamma-4)\\
&= n_\Omega M_1(\Gamma)+n_\Gamma M_1(\Omega)+8m_\Gamma m_\Omega+n_\Omega M_1(\Gamma)+n_\Gamma M_1(\Omega)+8m_\Gamma m_\Omega\\
&+4n_\Gamma n_\Omega(2n_\Gamma+2n_\Omega-4)^2+4(2n_\Gamma+2n_\Omega-4)(n_\Gamma m_\Omega+n_\Omega m_\Gamma)+4(2n_\Gamma\\
&+2n_\Omega-4)(n_\Gamma m_\Omega+n_\Omega m_\Gamma)+8m_\Gamma m_\Omega+8m_\Gamma m_\Omega+8{m_\Gamma}^2+8{m_\Omega}^2\\
&= 2n_\Omega M_1(\Gamma)+2n_\Gamma M_1(\Omega)+32m_\Gamma m_\Omega\\
&+8(2n_\Gamma+2n_\Omega-4)(n_\Gamma m_\Omega+n_\Omega m_\Gamma)\\
&+4n_\Gamma n_\Omega(2n_\Gamma+2n_\Omega-4)^2+8{m_\Gamma}^2+8{m_\Omega}^2.
\end{aligned}
$$

Theorem 2.2: *Adding A_1, A_2 and A_3, we obtain the desired result.*

The EHM index of $\Gamma\times\Omega$ is given by

$$
\begin{aligned}
EHM(\Gamma\times\Omega) &= 2(n_\Gamma EM_1(\Omega)+8m_\Gamma M_1(\Omega)+4m_\Omega M_1(\Gamma)\\
&+n_\Omega EM_1(\Gamma)+8m_\Omega M_1(\Gamma)+4m_\Gamma M_1(\Omega)-32m_\Gamma m_\Omega).
\end{aligned}
$$

Proof: Let $(a,b)\,(a',b')$ and $(a',b')\,(a'',b'')$ be two adjacent edges in $EHM(\Gamma\times\Omega)$. Then we have:

$$
EHM(\Gamma\times\Omega)=\sum_{(a,b)(a',b')\sim(a',b')(a'',b'')\in E(\Gamma\times\Omega)}(d^*_{\Gamma\times\Omega}(a,b)(a',b')+d^*_{\Gamma\times\Omega}(a',b')(a'',b''))^2
$$

$$
\begin{aligned}
&= \sum_{(a,b)(a',b')\sim(a',b')(a'',b'')\in E(\Gamma\times\Omega)}(d^*_{\Gamma\times\Omega}(a,b)+d^*_{\Gamma\times\Omega}(a',b')-2\\
&+d^*_{\Gamma\times\Omega}(a',b')+d^*_{\Gamma\times\Omega}(a'',b'')-2)^2\\
&=\sum_{(a,b)(a,b'),bb'\in E(\Omega)}(d^*_{\Gamma\times\Omega}(a,b)+d^*_{\Gamma\times\Omega}(a,b')-2)^2\\
&+\sum_{(a,b)(a',b),aa'\in E(\Gamma)}(d^*_{\Gamma\times\Omega}(a,b)+d^*_{\Gamma\times\Omega}(a',b)-2)^2\\
&+\sum_{(a',b')(a',b''),b'b''\in E(\Omega)}(d^*_{\Gamma\times\Omega}(a',b')+d^*_{\Gamma\times\Omega}(a',b'')-2)^2\\
&+\sum_{(a',b')(a'',b'),a'a''\in E(\Gamma)}(d^*_{\Gamma\times\Omega}(a',b')+d^*_{\Gamma\times\Omega}(a'',b')-2)^2\\
&=A_1+A_2+A_3+A_4.
\end{aligned}
$$

We consider

$$
\begin{aligned}
A_1&=\sum_{(a,b)(a,b'),bb'\in E(\Omega)}(d^*_{\Gamma\times\Omega}(a,b)+d^*_{\Gamma\times\Omega}(a,b')-2)^2\\
&=\sum_{a\in V(\Gamma)}\sum_{bb'\in E(\Omega)}(2d^*_{\Gamma}(a)+d^*_{\Omega}(b)+d^*_{\Omega}(b')-2)^2\\
&=4\sum_{bb'\in E(\Omega)}\sum_{a\in V(\Gamma)}(d^*_{\Gamma}(a)^2)\\
&+\sum_{a\in V(\Gamma)}\sum_{bb'\in E(\Omega)}(d^*_{\Omega}(b)+d^*_{\Omega}(b')-2)^2\\
&+4\sum_{a\in V(\Gamma)}d^*_{\Gamma}(a)\sum_{bb'\in E(\Omega)}(d^*_{\Omega}(b)+d^*_{\Omega}(b')-2)\\
&=n_{\Gamma}EM_1(\Omega)+8m_{\Gamma}M_1(\Omega)+4m_{\Omega}M_1(\Gamma)-16m_{\Gamma}m_{\Omega}.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
A_2&=\sum_{(a,b)(a',b),aa'\in E(\Gamma)}(d^*_{\Gamma\times\Omega}(a,b)+d^*_{\Gamma\times\Omega}(a',b)-2)^2\\
&=\sum_{b\in V(\Omega)}\sum_{aa'\in E(\Gamma)}(2d^*_{\Omega}(b)+d^*_{\Gamma}(a)+d^*_{\Gamma}(a')-2)^2\\
&=4\sum_{aa'\in E(\Gamma)}\sum_{b\in V(\Omega)}(d^*_{\Omega}(b)^2)\\
&+\sum_{b\in V(\Omega)}\sum_{aa'\in E(\Gamma)}(d^*_{\Gamma}(a)+d^*_{\Gamma}(a')-2)^2\\
&+4\sum_{b\in V(\Omega)}d^*_{\Omega}(b)\sum_{aa'\in E(\Gamma)}(d^*_{\Gamma}(a)+d^*_{\Gamma}(a')-2)\\
&=n_{\Omega}EM_1(\Gamma)+8m_{\Omega}M_1(\Gamma)+4m_{\Gamma}M_1(\Omega)-16m_{\Gamma}m_{\Omega}.
\end{aligned}
$$

Similarly again,

$$
\begin{aligned}
A_3&=\sum_{(a',b')(a',b''),b'b''\in E(\Omega)}(d^*_{\Gamma\times\Omega}(a',b')+d^*_{\Gamma\times\Omega}(a',b'')-2)^2\\
&=\sum_{a'\in V(\Gamma)}\sum_{b'b''\in E(\Omega)}(2d^*_{\Gamma}(a')+d^*_{\Omega}(b')+d^*_{\Omega}(b'')-2)^2\\
&=4\sum_{b'b''\in E(\Omega)}\sum_{a'\in V(\Gamma)}(d^*_{\Gamma}(a')^2)\\
&+\sum_{a'\in V(\Gamma)}\sum_{b'b''\in E(\Omega)}(d^*_{\Omega}(b')+d^*_{\Omega}(b'')-2)^2\\
&+4\sum_{a'\in V(\Gamma)}d^*_{\Gamma}(a')\sum_{b'b''\in E(\Omega)}(d^*_{\Omega}(b')+d^*_{\Omega}(b'')-2)\\
&=n_{\Gamma}EM_1(\Omega)+8m_{\Gamma}M_1(\Omega)+4m_{\Omega}M_1(\Gamma)-16m_{\Gamma}m_{\Omega}.
\end{aligned}
$$

Finally,

$$\begin{aligned}
A_4 &= \sum_{(a',b')(a'',b'),a'a''\in E(\Gamma)}(d^*_{\Gamma\times\Omega}(a',b')+d^*_{\Gamma\times\Omega}(a'',b')-2)^2\\
&= \sum_{b'\in V(\Omega)}\sum_{a'a''\in E(\Gamma)}(2d^*_{\Omega}(b')+d^*_{\Gamma}(a')+d^*_{\Gamma}(a'')-2)^2\\
&= 4\sum_{a'a''\in E(\Gamma)}\sum_{b'\in V(\Omega)}(d^*_{\Omega}(b')^2)\\
&\quad +\sum_{b'\in V(\Omega)}\sum_{a'a''\in E(\Gamma)}(d^*_{\Gamma}(a')+d^*_{\Gamma}(a'')-2)^2\\
&\quad +4\sum_{b'\in V(\Omega)}d^*_{\Omega}(b')\sum_{a'a''\in E(\Gamma)}(d^*_{\Gamma}(a')+d^*_{\Gamma}(a'')-2)\\
&= n_{\Omega}EM_1(\Gamma)+8m_{\Omega}M_1(\Gamma)+4m_{\Gamma}M_1(\Omega)-16m_{\Gamma}m_{\Omega}.
\end{aligned}$$

By adding A_1, A_2, A_3 and $+A_4$, the desired result follows.

3. Methods and Theory

In this section, we are going to compute the EHM index for the family of linear Acenes $(C_{4n+2}H_{2n+4})$ molecule, (FIGURE 1).

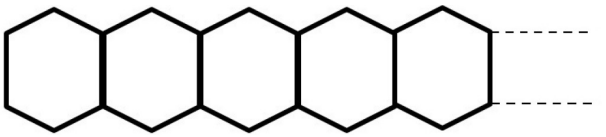

Figure 1

Linear Acenes Molecular Graph

Theorem 3.1: We presume that Γ represents a linear Acenes $(C_{4n+2}H_{2n+4})$ molecule. The EHM index can be calculated as follow:

$$EHM(\Gamma) = 4(85n-62).$$

Proof: Let's assume Γ represents a simple graph within the Acenes family. The rings set divide into two partitions according to outer (pendant) rings and inner rings. Now, we divide rings again according to the degree of edges as follow (see FIGURE 2 and FIGURE 3):

(i) degree of edges in outer rings. So, we have

$$E'_1 = \{\alpha\sim\beta\in E(\Gamma)\,|\,d^*_\alpha = d^*_\beta = 2\},$$

$$E'_2 = \{\alpha\sim\beta\in E(\Gamma)\,|\,d^*_\alpha = 2, d^*_\beta = 3\} \text{ and}$$

$$E'_3 = \{\alpha\sim\beta\in E(\Gamma)\,|\,d^*_\alpha = 3, d^*_\beta = 4\}.$$

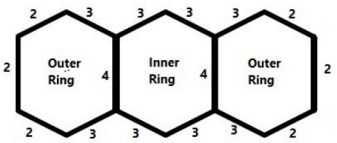

Figure 2
Phenantherene Molecular Graph

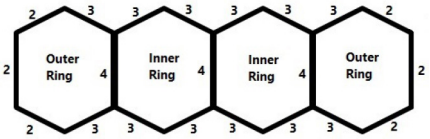

Figure 3
Chrysene Molecular Graph

(ii) degree of edges in inner rings. So, we obtain

$$E_4' = \{\alpha \sim \beta \in E(\Gamma) \mid d_\alpha^* = d_\beta^* = 3\} \text{ and}$$

$$E_5' = \{\alpha \sim \beta \in E(\Gamma) \mid d_\alpha^* = 3, d_\beta^* = 4\}.$$

(iii) degree of edges between outer and inner rings. Then, we attain

$$E_6' = \{\alpha \sim \beta \in E(\Gamma) \mid d_\alpha^* = d_\beta^* = 3\}.$$

Now, we investigate the statement by induction on the number of rings that it is indicated by n. According to FIGURE 1 and FIGURE 2, we can compute $|E_1'|,...,|E_6'|$ for $n = 3$ and $n = 4$.

If $n = 3$, then

$$|E_1'(\Gamma)| = 4, |E_2'(\Gamma)| = 4, |E_3'(\Gamma)| = 4, |E_4'(\Gamma)| = 2, |E_5'(\Gamma)| = 4 \text{ and } |E_6'(\Gamma)| = 4.$$

So, we can conclude $EHM(\Gamma)$ as follow:

$$EHM(\Gamma) = \sum_{\alpha\sim\beta\in E_i'(\Gamma)} (d_\alpha^* + d_\beta^*)^2, \text{ for } 1 \leqslant i \leqslant 6 \Rightarrow$$

$$\begin{aligned} EHM(\Gamma) &= \sum_{\alpha\sim\beta\in E_1'}(\Gamma)(d_\alpha^* + d_\beta^*)^2 + \sum_{\alpha\sim\beta\in E_3'}(\Gamma)(d_\alpha^* + d_\beta^*)^2 + \sum_{\alpha\sim\beta\in E_4'}(\Gamma)(d_\alpha^* + d_\beta^*)^2 \\ &\quad + \sum_{\alpha\sim\beta\in E_5'}(\Gamma)(d_\alpha^* + d_\beta^*)^2 + \sum_{\alpha\sim\beta\in E_6'}(\Gamma)(d_\alpha^* + d_\beta^*)^2 \\ &= 4(2+2)^2 + 4(2+3)^2 + 4(3+4)^2 + 2(3+3)^2 + 4(3+4)^2 + 4(3+3)^2 \\ &= 772. \end{aligned}$$

If $n = 4$, then

$$|E_1'(\Gamma)| = 4, |E_2'(\Gamma)| = 4, |E_3'(\Gamma)| = 4, |E_4'(\Gamma)| = 4, |E_5'(\Gamma)| = 8 \text{ and } |E_6'(\Gamma)| = 6.$$

Furthermore, same as previous calculations $EHM(\Gamma)$ for $n = 3$, we can verify $EHM(\Gamma)$ for $n = 4$. Hence, $EHM(\Gamma) = 1112$.

We proceed under the assumption that the claim is valid for any number of rings fewer than n, where n is greater than 4.

We saw that $|E_1'(\Gamma)| = |E_2'(\Gamma)| = |E_3'(\Gamma)| = 4$ are constant for all edges in outer rings. So,

$$EHM(\Gamma) = \sum_{\alpha\sim\beta\in E_i'(\Gamma)}(d_\alpha^* + d_\beta^*)^2 = 360 \text{ for } 1 \leqslant i \leqslant 3$$

and

$$|E_4'(\Gamma)| = 2(n-2), |E_5'(\Gamma)| = 4(n-2) \text{ and } |E_6'(\Gamma)| = 2(n-1),$$

in which n is the number of rings. Hence, the EHM index of Acenes $(C_{4n+2}H_{2n+4})$ is equal to

$$EHM(\Gamma) = \sum_{\alpha\sim\beta\in E_i'(\Gamma)}(d_\alpha^* + d_\beta^*)^2, \text{ for } 1 \leqslant i \leqslant 6 \Rightarrow$$

$$\begin{aligned} EHM(\Gamma) &= 360 + \sum_{\alpha\sim\beta\in E_4'(\Gamma)}(d_\alpha^* + d_\beta^*)^2 + \sum_{\alpha\sim\beta\in E_5'(\Gamma)}(d_\alpha^* + d_\beta^*)^2 \\ &\quad + \sum_{\alpha\sim\beta\in E_6'(\Gamma)}(d_\alpha^* + d_\beta^*)^2 \\ &= 360 + 2(n-2)(6)^2 + 4(n-2)(7)^2 + 2(n-1)(6)^2 \\ &= 4(85n - 62). \end{aligned}$$

Finally, the proof is completed.

4. Results

Equation $EHM(A) = 4(85n - 62)$ was used to calculate the EHM index for 8 elements of the Acenes family, which are then displayed in TABLE 1.

Table 1

The *EHM* index for the initial eight linear Acenes molecules

Chemical Formula	IUPAC Name	$EHM(\Gamma)$
$C_{10}H_8$	Benzene	432
$C_{14}H_{10}$	Naphthalene	772
$C_{18}H_{12}$	Anthracene	1112
$C_{22}H_{14}$	Tetracene	1452
$C_{26}H_{16}$	Pentacene	1792
$C_{30}H_{18}$	Hexacene	2132
$C_{34}H_{20}$	Heptacene	2472
$C_{36}H_{22}$	Optacene	2812

We conducted calculations for Gibbs Energy (GE), Heat of formation $(H.oF)$, as well as Electro-optical characteristics like gap energy (E_g) and electron affinity energy (E_{ea}) in the Acenes family using empirical data to examine the thermodynamic properties. These results were then compared against established sources, as detailed in TABLE 2 [11, 13].

Table 2

(GE), $(H.oF)$, (E_g) and (E_{ea}) energy

Chemical Formula	$H.of(Kj/mol)$	$GE(Kj/mol)$	E_g	E_{ea}
$C_{10}H_8$	80.83	121.68	–0.32	4.09
$C_{14}H_{10}$	177.87	252.38	–0.05	4.19
$C_{18}H_{12}$	274.91	383.08	–0.29	3.73
$C_{22}H_{14}$	371.95	513.78	0.4	3.7
$C_{26}H_{16}$	468.99	644.48	0.57	3.47
$C_{30}H_{18}$	566.03	775.18	0.64	3.5
$C_{34}H_{20}$	633.07	905.88	0.73	3.44
$C_{36}H_{22}$	760.11	1036.58	0.84	3.36

FIGURES 4, 5, 6 and 7 illustrate the values of E_{ea}, E_g, $H.oF$, and GE for linear Acenes in relation to the EHM index, reflecting the findings of this study.

FIGURES 4 and 5 demonstrate the precise calculation of E_g and E_{ea} using the $EHM(A)$ index variations within the Acenes family.

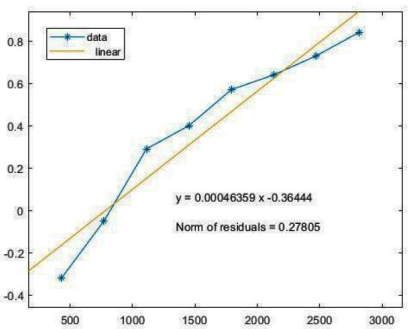

Figure 4

Electron affinity energy

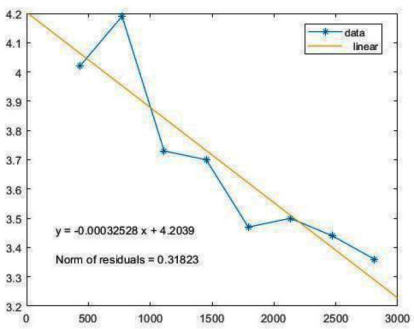

Figure 5

Gap energy

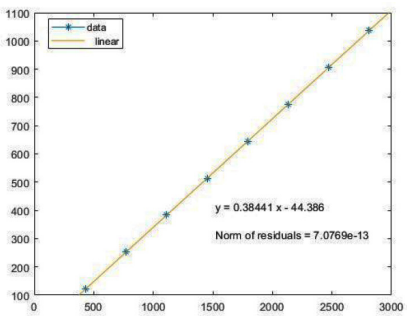

Figure 6
Gipps energy

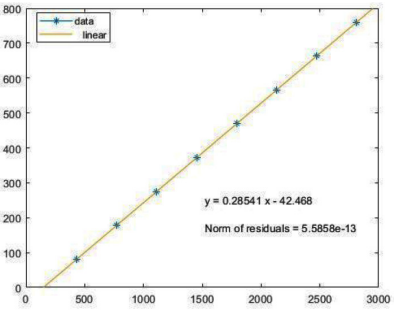

Figure 7
Heat of formation energy

These forecasts can be made using a pair of equations:

$$E_{ea} = 0.00046359EHM(\Gamma) - 0.36444 \qquad (4-1),$$

$$E_g = -0.00032528EHM(\Gamma) + 4.2039 \qquad (4-2).$$

FIGURES (6) and (7) demonstrate the effectiveness of the $EHM(\Gamma)$ index in predicting GE and $H.oF$ within the linear Acenes family, with an R^2 value of 1. The corresponding equation is provided below

$$GE = 0.38441EHM(\Gamma) - 44.386 \qquad (4-3),$$

$$E_g = -0.00032528EHM(\Gamma) + 4.2039 \qquad (4-4).$$

5. Conclusion

In TABLE 3, we state the values of E_G, E_{ea}, GE, and $H.oF$ for the Acenes family using the TIM method. This table highlights the reliability of the TIM method by comparing the results with the reference values from TABLE 2. The TIM method, along with the EHM index, allows for accurate prediction of various physical and chemical properties within the Acenes family, saving time and resources compared to traditional theoretical and experimental approaches that often yield only approximate results. Moving forward, several heavier members of the Acenes family will undergo analysis using the TIM method. Equations $(4-1)$, $(4-2)$, and $(4-4)$ have been employed to forecast the energies of E_G, E_{ea}, GE, and $H.oF$ with the outcomes detailed in TABLE 4.

Table 3

Calculation (*GE*), (*H.oF*), (E_g), and (E_{ea}) energy of first eight Acenes family by *TIM* method

Chemical Formula	*H.of*	*GE*	E_g	E_{ea}
$C_{10}H_8$	80.82912	121.67912	–0.16412912	4.06337904
$C_{14}H_{10}$	177.86852	252.37852	–0.00650852	3.95278384
$C_{18}H_{12}$	274.90792	383.07792	0.15111208	3.84218864
$C_{22}H_{14}$	371.94732	513.77732	0.30873268	3.73159344
$C_{26}H_{16}$	468.98672	644.47672	0.46635328	3.62099824
$C_{30}H_{18}$	566.02612	775.17612	0.62397388	3.51040304
$C_{34}H_{20}$	633.06552	905.87552	0.78159448	3.39980784
$C_{36}H_{22}$	760.10492	1036.57492	0.93921508	3.28921264

Table 4

Prediction (*GE*), (*H.oF*), (E_g) and (E_{ea}) energy for Acenes family

Chemical Formula	*n*	*EHM*(Γ)	*H.oF*	*GE*	E_{ea}	E_g
$C_{42}H_{24}$	10	3152	80.82912	121.67912	–0.16412912	4.06337904
$C_{46}H_{26}$	11	3492	177.86852	252.37852	–0.00650852	3.95278384
$C_{50}H_{28}$	12	3832	274.90792	383.07792	0.15111208	3.84218864
$C_{54}H_{30}$	13	4172	371.94732	513.77732	0.30873268	3.73159344
$C_{58}H_{32}$	14	4512	468.98672	644.47672	0.46635328	3.62099824
$C_{62}H_{34}$	15	4852	566.02612	775.17612	0.62397388	3.51040304
$C_{66}H_{36}$	16	5192	663.06552	905.87552	0.78159448	3.39980784
$C_{70}H_{38}$	17	5532	760.10492	1036.57492	0.93921508	3.28921264

References

[1] A. A. Khakpoor and B. Aghahi Keshe, "A Model for Computing Gap Energy and Electron Affinity Energy of Carbon Nanostructures", *J. of Chemical and Material Engineerin*, vol. 4, no. 1, pp. 8-12 (2016).

[2] A. A. Khakpoor and B. Aghahi Keshe, "Nano structures and Its Thermodynamic Properties Using *TIM*", *J. of Material Science and Chemical Engineering*, vol. 3, pp. 1-6 (2015).

[3] A. A. Khakpoor and B. Aghahi Keshe, "Physical and Electro-Optical Properties of Rylenes as Nanostructures Using Topological Indices Method", *Journal of Nanoelectronics and Optoelectronics*, vol. 11, no. 3, pp. 280-283 (2016).

[4] A. A. Khakpoor, "Prediction Electronic and Physical Properties of Nano Structures; Topological Index Method", *International Journal of Advanced Research*, vol. 3, pp. 1536-1540 (2015).

[5] A. Milicević and S. N. Trinajstić, "On reformulated Zagreb indices", *Mol. Divers.*, vol. 8, pp. 393-399 (2004).

[6] A. R. Ashrafi, T. Došlić and A. Hamzeh, "The Zagreb coindices of graph operations", *Discrete Appl. Math.*, vol. 158, pp. 1571-1578 (2010).

[7] A. R. Katritzky, M. Karelson and R. Petrukhin, *Topological Descriptors* (2002).

[8] A. T. Balaban, I. Motoc, D. Bonchev and O. Mekenyan, "Topological indices for structure-activity correlations", *Top. Curr. Chem.*, vol. 114, pp. 21-55 (1983).

[9] D. Bonchev, O. Mekenyan and N. Trianjstić, "Isomer discrimination by topological information approach", *Journal of Computational Chemistry*, vol. 2, no. 2, pp. 127-148 (1981).

[10] D. K. Pal, C. Sengupta and A. U. De, "A new topochemical descriptor (*TAU*) in molecular connectivity concept", *Part I--Aliphatic compounds. Indian J. Chem.*, vol. 27, pp. 734-739 (1988).

[11] E. S. Kadantsev, M. J. Stott and A. Rubio, Electronic Strutcure and Ecitations in Oligoace from ab Initio Calculations, *The Jornal of Chemical Physics*, vol. 124, no. 13, pp. 134901 (2006).

[12] G. H. Shirdel, H. Rezapour and A. M. Sayadi, "The hyper-Zagreb index of graph operation", *Iranian Journal of Mathematical Chemistry*, vol. 4, no. 2, pp. 213-220 (2013).

[13] G. Malloci, G. Mulas, G. Cappellini and C. Joblin, "Time Dependent Density Functional Study of the Electronic Spectra of Oligoacenes in the Charge States –1, 0, +1 and +2", *Chemical Physics*, vol. 340, pp. 43-58 (2007).

[14] H. González-Díaz, S. Vilar, L. Santana and E. Uriarte, "Medicinal chemistry and bioinformatics-current trends in drugs discovery with

networks topological indices", *Current Topics in Medicinal Chemistry*, vol. 7, no. 10, pp. 101529 (2007).

[15] H. González-Díaz, Y, González-Díaz, L. Santana, F. M. Uberia and E. Uriarte, "Proteomics, networks and connectivity indices", *Proteomics*, vol. 8, no. 4, pp. 750-778 (2008).

[16] H. Haruo, "Topological index, A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons", *Bulletin of the Chemical Society of Japan*, vol. 44, no. 9, pp. 2232-2339 (1971).

[17] H, Lowell, H. Kier and B. Lemont, *Molecular connectivity in chemistry and drug research*, Boston: Academic Press (1976).

[18] H. Timmerman, R. Todeschini, V. Consonni, R. Mannhold and H. Kubinyi, *Handbook of Molecular Descriptors*. Weinheim: Wiley-VCH (2002).

[19] I. Ballade and A. Buzdin, *Thermodynamic Properties of Ferro magnet/ Superconductor/Ferro magnet Nanostructures*, Physical Review, B.67 (2003).

[20] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons", *Chemical Physics Letters*, vol. 17, no. 4, pp. 535-538 (1972).

[21] I. Gutman, B. Ru. i., N. Trinajstić and C. F. Wilcox, "Graph theory and molecular orbits, XII. Acyclic polyenes", *Jornal of Chemical Physics*, vol. 62, pp. 3399-3405 (1975).

[22] J. C. Dearden, "In silico prediction of drug toxicity", *Journal of Computer-Aided Molecular Design*, vol. 17, pp. 119-127 (2003).

[23] K. R. Bruce, *Chemical applications of topology and graph theory* (1983).

[24] K. Roy and G. Ghosh, "Extended Topochemical Atom (*ETA*) Indices in the Valence Electron Mobile (*VEM*) Environment as Tools for *QSAR/QSPR* Studies", *Internet Electronic Journal of Molecular Design*, vol. 2, no. 9, pp. 599-620 (2003).

[25] M. S. Y. Alsharafi, A. Q. Alameri and Y. Zeren, "The second Hyper-Zagreb index of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes", *Journal of Discrete Mathematical Sciences and Cryptography*, vol. 27, no. 3, pp. 915-928 (2024).

[26] N. Trinajstić, *Chemical Graph Theory*, 2nd Edition, CRC Press, Boca Raton (1992).

[27] S. Shafiee Alamotie, M. Alaeiyan and A.Gilani, "Studying Thermodynamic Properties of Linear Acnes Molecules ($C_{(4n+2)}H_{(2n+4)}$) ", *Journal of Discrete Mathematical Sciences and Cryptography*, vol. 22, no. 7, pp. 1261-1268 (2019).

[28] W. Tong, H. Hong, Q. Xie, L. Shi, H. Fang and R. Perkins, "Assessing *QSAR* Limitations-A Regulatory Perspective", *Current Computer-Aided Drug Design*, vol. 1, no. 2, pp. 195-205 (2005).

[29] Z. L. Wang, "Zinc Oxide Nanostructure, Growth, Properties and Applications", *Journal of Physics: Condesed Matter*, vol. 16, pp. 829-858 (2004).

Received March, 2024