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Topological Characterization and Predictive Modeling of Graph Energy in Ionic Covalent Organic Frameworks

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ABSTRACT: Covalent organic frameworks (COFs) are crystalline materials composed of covalently bonded organic ligands with chemically permeable structures. Their crystallization is achieved by balancing thermal reversibility with the dynamic nature of the frameworks. Ionic covalent organic frameworks (ICOFs) are a subclass that incorporates ions in positive, negative, or zwitterionic forms into the frameworks. In particular, spiroborate-derived linkages enhance both the structural diversity and functionality of ICOFs. Unlike electroneutral COFs, ICOFs can be tailored by adjusting the types and arrangements of ions, influencing their formation mechanisms and physical properties. This study focuses on analyzing the graph-based structural characteristics of ICOFs with spiroborate linkages. We compute graph based entropy using hybrid topological descriptors that capture both local and global structural patterns. Furthermore, statistical regression models are developed to predict graph energies of larger-dimensional ICOF structures based on these descriptors. To ensure the robustness and accuracy of our results, we validated our findings using a pseudocode algorithm specifically designed for computing degree-based topological indices. This computational validation confirms the consistency of the derived descriptors and supports their applicability in quantitative structure-property relationship (QSPR) modeling. Overall, this approach provides valuable insights for future applications in material design and property prediction within the framework of ICOFs.

KEYWORDS: Vertex degree topological indices; ionic covalent organic frameworks; entropies; QSPR models

1 Introduction

Covalent organic frameworks are crystalline materials with a porous structure, formed by organic molecular building blocks made up of light elements, which are interconnected through covalent bonds [1,2]. COFs can form crystalline structures with permanent porosity, enabling organic reactions to occur without altering their properties [3]. The structural adaptability of COFs enables their use in a wide range of applications, including gas separation, drug discovery, heterogeneous catalysis, and energy conversion [4,5]. A defining feature of COFs is their uniquely predictable skeleton structures, which distinguish them from other porous polymeric materials [6]. The design of COFs with structural arrangements and tailored pore sizes relies on the strategic choice of linkers and molecular building units [7]. The polymerization process combines covalent bonds with noncovalent interactions, resulting in well-organized, extended crystalline frameworks. The crystallization of COFs successfully resolves the persistent challenge of crystallizing covalent solids. This is achieved by carefully balancing thermodynamic and kinetic factors during the reversible formation of covalent bonds, which is vital for producing extended crystalline structures [8]. Concurrently,



advances in ion-regulated design, particularly the incorporation of multivalent ions [9,10], zwitterionic groups [11], and spatial ion-binding architectures [12,13], have significantly enhanced the performance of ICOFs in terms of selective ion adsorption, ion-exchange capacity, and long-range ionic conductivity, especially under conditions of high ionic competition and dynamic operating environments [14].

The structure of a covalent organic framework is influenced by the size, arrangement, and connectivity of the linkers. COFs with boronate, spiroborate, imine, hydrazone, triazine, and benzyl nitrile linkages have been synthesized through polycondensation reactions between organic precursors [15]. Among these linkers, the spiroborates, derived from boronic acid, are ionic compounds known for their exceptional hydrolytic resistance and durability in aqueous, methanolic, and alkaline conditions [16]. Their ionic properties make spiroborate-linked COFs promising candidates for ion-conductive materials. These linkages are easily formed by condensing polyols with alkali tetraborate or boric acid, or through transesterification between borates and polyols under thermodynamically controlled conditions. They have also found widespread use in the synthesis of macrocycles, facilitating a wide range of applications, including electrolytes, sensors, catalysts, and hosts for neutral molecules or ions [17–19]. Recent developments in ionic covalent organic frameworks have highlighted a wide range of synthetic strategies, particularly leveraging dynamic covalent chemistry to achieve tunable architectures and enhanced energy functionalities [20–23].

This study investigates the topological characterization of ionic covalent organic frameworks (ICOFs) via spiroborate linkages, incorporating sp^3 hybridized boron anionic centers and tunable counteranions [24] as depicted in Fig. 1. ICOFs are formed by their repeating ionic units and crystalline structures, providing high ionic conductivity [25–27]. By merging the properties of porous ionic polymers (PiPs) with COFs, they maintain atomic periodicity and porosity while introducing oppositely charged groups via electrostatic interactions or ion exchange [28]. Their adaptable structures, organized channels, and abundant charged sites make them highly promising for applications such as purification, ion transport, sensing, catalysis, and energy retention [29–32]. With permanent porosity and customizable architectures, ICOFs are highly suitable for selective trace element extraction, efficient ion transport, and sustained ionic flow, positioning them as ideal candidates for energy devices and material innovations [33].

Topological descriptors serve as a means to characterize the molecular graphs of ICOF, with degree-based descriptors reflecting atom valency through vertex degrees at bond ends [34,35], and potentially being used to quantify ICOFs through QSPR and QSAR analyses [36–39]. Degree-based topological indices (TIs) are key graph invariants derived from various graph properties [40] which are fundamentally grounded in the vertex degree, representing the number of edges connected to a vertex. To refine this traditional degree-based TIs, neighborhood degree-based TIs, which sum the degrees of a vertex's adjacent vertices, are being developed as a more effective measure [41–44]. These descriptors are widely used in areas such as molecular modeling and applied materials research, delivering valuable insights across a broad range of disciplines [45–49]. In the context of ICOFs, these descriptors provide a rigorous framework for understanding structure–property relationships that influence critical functionalities such as ion transport, adsorption, and energy storage [50–54]. In information theory, Shannon's entropy plays a crucial role in quantifying system uncertainty. Graph entropy measures, particularly those derived from degree descriptors, are widely used in graph theory to assess the complexity and diversity of molecular graphs [55–57]. Its versatility across fields such as biology and chemistry makes it an essential tool for analyzing complex systems [58–60]. In parallel, topological descriptors and entropy-based analyses have gained traction in quantifying structure–property relationships in porous and crystalline frameworks [61–64]. This evolving literature forms the foundation for our graph-theoretic approach, which complements recent machine-learning-based models and contributes to a deeper understanding of structure-driven energy properties in ICOFs.

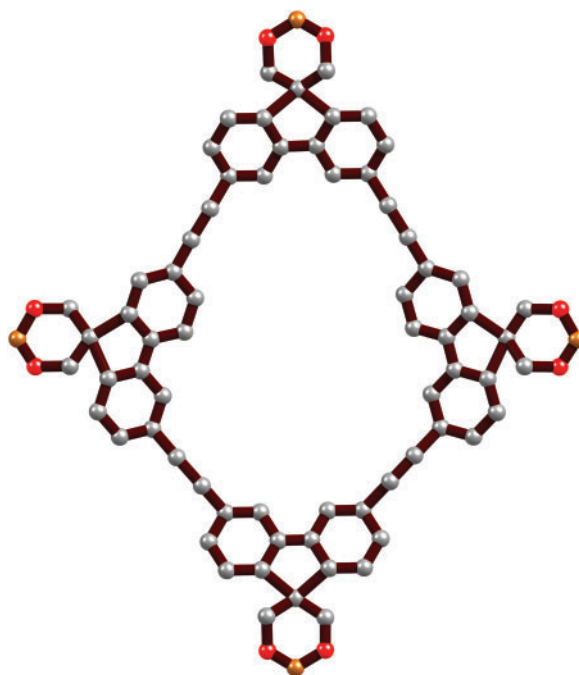


Figure 1: The building block of ICOF is composed of carbon atoms depicted in grey, boron atoms in yellow, and oxygen atoms in red

The Hückel molecular orbital (HMO) theory is frequently used to calculate the total π -electron energy in alternant hydrocarbon frameworks, which is a key quantum-chemical feature of conjugated molecules. The π -electron energy and the graph-based energy for alternant hydrocarbons are generally correlated, although this relationship is not always valid for all molecular graphs. By applying the same approach used for graphs composed entirely of carbon atoms, this method can be modified to include graphs with heteroatoms [65,66] through the incorporation of external validation. While the current study employs linear regression models due to their simplicity and strong predictive performance, alternative nonlinear models such as exponential regressions can also be explored to capture more complex dependencies [67]. Additionally, recent developments including the thermodynamically consistent deep energy method [68] and machine learning interatomic potentials [69] demonstrate the potential of machine learning techniques for accurate energy prediction in complex materials. These approaches offer promising avenues for future research. This study involved calculating topological descriptors and entropy values for ICOFs, comparing entropy at the bond level, and applying regression models to predict graph energy.

2 Computational Methods

The ionic covalent organic framework (ICOF), characterized by spiroborate linkages, can be represented as a molecular graph, where the vertex set $V(\text{ICOF})$ corresponds to the atoms, and the edge set $E(\text{ICOF})$ represents the bonds. The molecular graph of ICOF as shown in Fig. 1 is depicted in Fig. 2, in which all the atoms are considered as vertices and the bonds as edges.

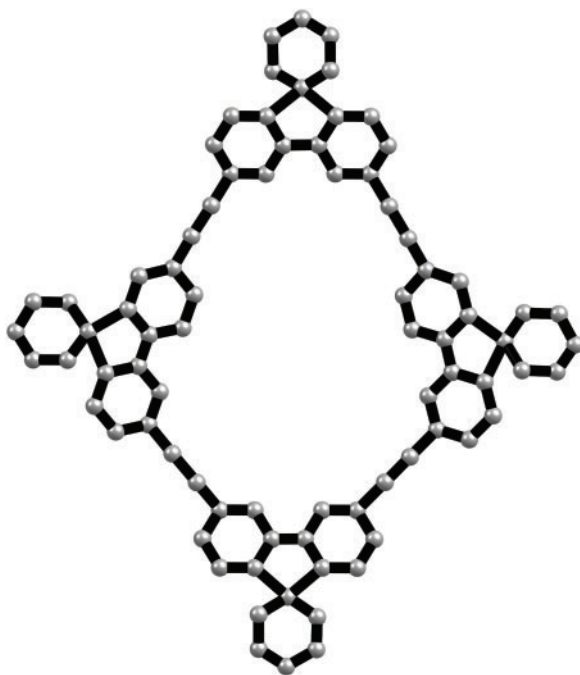


Figure 2: The molecular graph of ICOF

In this framework, the degree of a vertex $g \in V(\text{ICOF})$, expressed as $d_{\text{ICOF}}(g)$, refers to the number of bonds connected to g . The degree-sum, represented as $s_{\text{ICOF}}(g)$, is the total of the degrees of all atoms adjacent to g . That is, $s_{\text{ICOF}}(g) = \sum_{h \in N_{\text{ICOF}}(g)} d_{\text{ICOF}}(h)$ where $N_{\text{ICOF}}(g) = \{h \in V(\text{ICOF}) \mid gh \in E(\text{ICOF})\}$. Let $d_{(f,u)} = |\{gh \in E(\text{ICOF}) : f = d_{\text{ICOF}}(g) \text{ and } u = d_{\text{ICOF}}(h)\}|$ and $s_{(f,u)} = |\{gh \in E(\text{ICOF}) : f = s_{\text{ICOF}}(g) \text{ and } u = s_{\text{ICOF}}(h)\}|$. The edge classes, determined by $d_{(f,u)}$ and $s_{(f,u)}$, are grouped into the sets $D(\text{ICOF})$ and $S(\text{ICOF})$, respectively. The index function Υ is used to define the additive and multiplicative forms of topological descriptors, as outlined below [70–73].

$$\Upsilon^d(\text{ICOF}) = \sum_{d_{(f,u)} \in D(\text{ICOF})} d_{(f,u)} \Upsilon(f, u)$$

$$\Upsilon^{d^*}(\text{ICOF}) = \prod_{d_{(f,u)} \in D(\text{ICOF})} d_{(f,u)} \Upsilon(f, u)$$

$$\Upsilon^s(\text{ICOF}) = \sum_{s_{(f,u)} \in S(\text{ICOF})} s_{(f,u)} \Upsilon(f, u)$$

$$\Upsilon^{s^*}(\text{ICOF}) = \prod_{s_{(f,u)} \in S(\text{ICOF})} s_{(f,u)} \Upsilon(f, u)$$

The index function Υ is exponentiated to its own value to derive the self-powered forms of the topological descriptors [74–76].

$$\Upsilon^{dp}(\text{ICOF}) = \sum_{d_{(f,u)} \in D(\text{ICOF})} d_{(f,u)} \Upsilon(f, u)^{\Upsilon(f, u)}$$

$$\Upsilon^{dp^*}(\text{ICOF}) = \prod_{d_{(f,u)} \in D(\text{ICOF})} d_{(f,u)} \Upsilon(f, u)^{\Upsilon(f, u)}$$

$$\begin{aligned} Y^{sp}(\text{ICOF}) &= \sum_{s(f,u) \in S(\text{ICOF})} s(f,u) Y(f,u)^{Y(f,u)} \\ Y^{sp*}(\text{ICOF}) &= \prod_{s(f,u) \in S(\text{ICOF})} s(f,u) Y(f,u)^{Y(f,u)} \end{aligned}$$

The hybrid descriptors, along with the index function $Y(f, u)$, are provided below [77–80].

- $M_1(f, u) = f + u$ (First Zagreb)
- $M_2(f, u) = fu$ (Second Zagreb)
- $HM(f, u) = (f + u)^2$ (Hyper Zagreb)
- $AZ(f, u) = \left(\frac{fu}{f+u-2}\right)^3$ (Augmented Zagreb)
- $BM(f, u) = f + u + fu$ (Bi-Zagreb)
- $TM(f, u) = f^2 + u^2 + fu$ (Tri-Zagreb)
- $GBM(f, u) = \frac{\sqrt{fu}}{f+u+fu}$ (Geometric – Bi-Zagreb)
- $GTM(f, u) = \frac{\sqrt{fu}}{f^2+u^2+fu}$ (Geometric – Tri-Zagreb)
- $BMG(f, u) = \frac{(f+u+fu)}{\sqrt{fu}}$ (Bi-Zagreb – Geometric)
- $TMG(f, u) = \frac{f^2+u^2+fu}{\sqrt{fu}}$ (Tri-Zagreb – Geometric)
- $TMA(f, u) = \frac{2(f^2+u^2+fu)}{f+u}$ (Tri-Zagreb – Arithmetic)
- $BMA(f, u) = \frac{2(f+u+fu)}{f+u}$ (Bi-Zagreb – Arithmetic)

As we see from the definitions of topological descriptors, the classification of edge classes does not consider the specific types of atoms at their terminal points. However, it is essential to distinguish between the three types of atoms that form the basis of ionic covalent organic frameworks. To enhance the partitions based on $d(f, u)$ and $s(f, u)$, we introduce weight functions that incorporate both atom and bond contributions. The function Φ represents atom weights, while Γ denotes bond weights. To be more specific, Φ_B refers to the weight assigned to atom B, whereas Γ_{BC} represents the weight function for the bond between atoms B and C.

Shannon's entropy method is used to define a structural information function for the bonds in ICOF. A high entropy value signifies greater complexity or disorder, while a low entropy value indicates more order and regularity. The following form is used to define the entropy of the ICOF structure using Y as the structural information function on $E(\text{ICOF}) = \{c_1, c_2, \dots, c_m\}$ as shown below.

$$\begin{aligned} I_Y(\text{ICOF}) &= - \sum_{k=1}^m \frac{Y(c_k)}{\sum_{x=1}^m Y(c_x)} \log \left(\frac{Y(c_k)}{\sum_{x=1}^m Y(c_x)} \right) \\ &= \log \left(\sum_{k=1}^m Y(c_k) \right) - \frac{1}{\sum_{k=1}^m Y(c_k)} \log \left(\prod_{k=1}^m Y(c_k)^{Y(c_k)} \right) \end{aligned}$$

The modified entropy approach, which replaces the multiplicative form with a scalar multiplicative form, is outlined below [57,81].

$$I_Y(\text{ICOF}) = \log(Y(\text{ICOF})) - \frac{1}{Y(\text{ICOF})} \log(Y^{p*}(\text{ICOF}))$$

The adjacency matrix of an ICOF determines its spectrum through its eigenvalues, which are denoted as $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$, arranged in descending order. Collectively, these eigenvalues form the eigen-spectrum

of the ICOF. As given below, the graph energy [82], represented as $E_\pi(\text{ICOF})$ and expressed in β -units, is obtained by adding the non-negative values of the ICOF's eigenvalues.

$$E_\pi(\text{ICOF}) = \sum_{i=1}^n |\lambda_i|$$

3 Results and Discussion

The structural configuration of ionic covalent organic frameworks, with an emphasis on comparing their topological features using entropy information is explored in this section. The COFs featuring spiroborate linkages are depicted in a parallelogram peripheral shape, achieved by arranging the ionic COF units in a $p \times r$ grid-like pattern, where $p, r \geq 1$, as illustrated in Fig. 3. The ICOF is composed of $78pr - 5p - 5r$ vertices and $96pr - 8p - 8r$ edges, respectively.

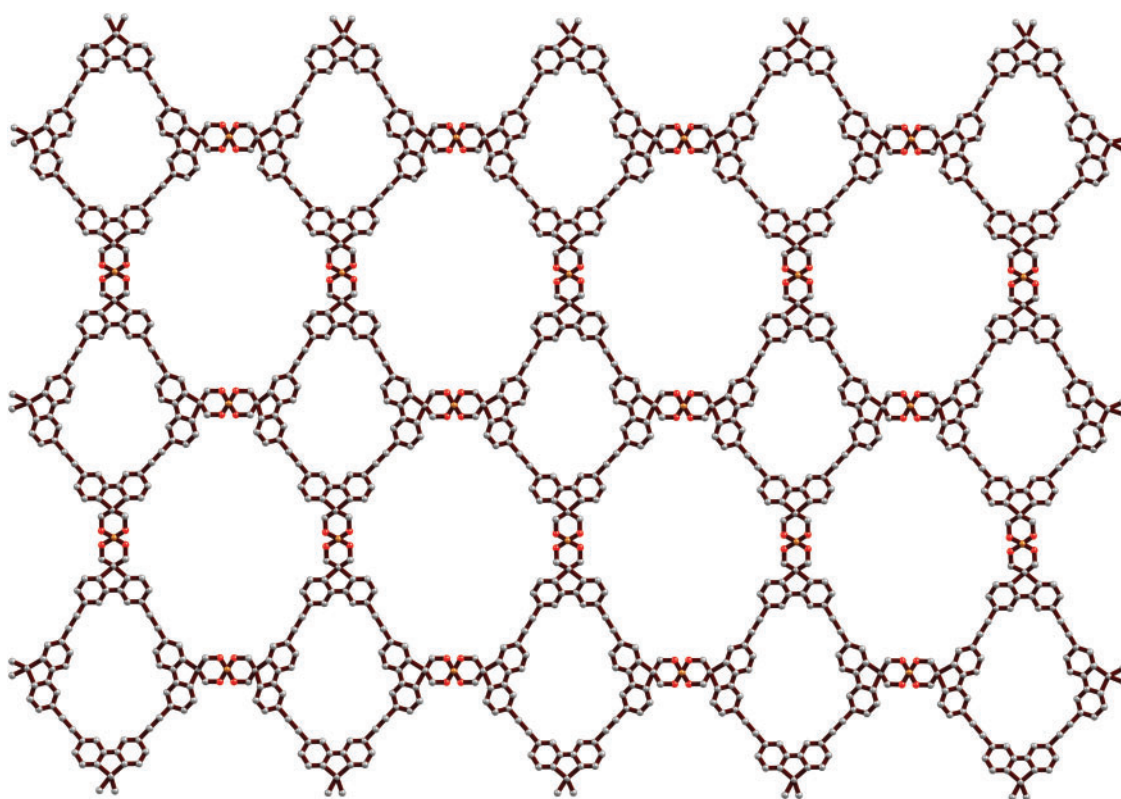


Figure 3: ICOF in parallelogram of dimensions (3,5)

The bond classes of ICOF are distributed over the set $\{B-O, O-C, C-C\}$ with their corresponding bond degree classes being $\{(1,4), (2,2), (2,3), (2,4), (3,3), (3,4)\}$ while degree-sum bond classes are $\{(4,8), (5,5), (5,6), (5,9), (6,6), (6,8), (6,10), (8,8), (8,9), (9,10)\}$. The bond classification of ICOFs is identified, and their numerical values are shown in Tables 1 and 2.

Table 1: ICOF(p, r) bonds are classified according to degree classes

Bond A–B	$(d_{\text{ICOF}}(\text{A}), d_{\text{ICOF}}(\text{B}))$	Frequency	
		Degrees	ICOF(p, r)
B–O	$(\Phi_B + \Phi_C, 4\Phi_O)$	2–4	$8pr - 4p - 4r$
O–C	$(2\Phi_C, \Phi_B + \Phi_C)$	2–2	$8pr - 4p - 4r$
C–C	$(\Phi_C, 4\Phi_C)$	1–4	$4p + 4r$
	$(2\Phi_C, 2\Phi_C)$	2–2	$12pr$
	$(2\Phi_C, 3\Phi_C)$	2–3	$40pr$
	$(2\Phi_C, 4\Phi_C)$	2–4	$8pr - 4p - 4r$
	$(3\Phi_C, 3\Phi_C)$	3–3	$12pr$
	$(3\Phi_C, 4\Phi_C)$	3–4	$8pr$

Table 2: ICOF(p, r) bonds are classified according to degree-sum classes

Bond A–B	$(s_{\text{ICOF}}(\text{A}), s_{\text{ICOF}}(\text{B}))$	Frequency	
		Degree-sums	ICOF(p, r)
B–O	$(4\Phi_B + 2\Phi_C, 8\Phi_O)$	6–8	$8pr - 4p - 4r$
O–C	$(4\Phi_C + 2\Phi_O, 4\Phi_B + 2\Phi_C)$	6–6	$8pr - 4p - 4r$
C–C	$(4\Phi_C, 8\Phi_C)$	4–8	$4p + 4r$
	$(5\Phi_C, 5\Phi_C)$	5–5	$12pr$
	$(5\Phi_C, 6\Phi_C)$	5–6	$16pr$
	$(5\Phi_C, 9\Phi_C)$	5–9	$8pr$
	$(6\Phi_C, 6\Phi_C)$	6–6	$8pr$
	$(6\Phi_C, 8\Phi_C)$	6–8	$8pr$
	$(6\Phi_C, 10\Phi_C)$	6–10	$8pr - 4p - 4r$
	$(8\Phi_C, 8\Phi_C)$	8–8	$4pr$
	$(8\Phi_C, 9\Phi_C)$	8–9	$8pr + 4p + 4r$
	$(9\Phi_C, 10\Phi_C)$	6–10	$8pr - 4p - 4r$

The degree and degree-sum-based descriptors for ICOF((p, r)) are calculated using the following equations with respect to Y .

$$\begin{aligned}
 Y^d(\text{ICOF}(p, r)) &= (8pr - 4p - 4r)\Gamma_{\text{BO}}Y(4\Phi_O, \Phi_B + \Phi_C) + (8pr - 4p - 4r)\Gamma_{\text{OC}}Y(2\Phi_C, \Phi_B + \Phi_C) \\
 &\quad + (4p + 4r)\Gamma_{\text{CC}}Y(\Phi_C, 4\Phi_C) + (12pr)\Gamma_{\text{CC}}Y(2\Phi_C, 2\Phi_C) + (40pr)\Gamma_{\text{CC}}Y(2\Phi_C, 3\Phi_C) \\
 &\quad + (8pr - 4p - 4r)\Gamma_{\text{CC}}Y(2\Phi_C, 4\Phi_C) + (12pr)\Gamma_{\text{CC}}Y(3\Phi_C, 3\Phi_C) + (8pr)\Gamma_{\text{CC}}Y(3\Phi_C, 4\Phi_C) \\
 Y^s(\text{ICOF}(p, r)) &= (8pr - 4p - 4r)\Gamma_{\text{BO}}Y(4\Phi_B + 2\Phi_C, 8\Phi_O) + (8pr - 4p - 4r)\Gamma_{\text{OC}}Y(4\Phi_C + 2\Phi_O, 4\Phi_B + 2\Phi_C) \\
 &\quad + (4p + 4r)\Gamma_{\text{CC}}Y(4\Phi_C, 8\Phi_C) + (12pr)\Gamma_{\text{CC}}Y(5\Phi_C, 5\Phi_C) + (16pr)\Gamma_{\text{CC}}Y(5\Phi_C, 6\Phi_C) \\
 &\quad + (8pr)\Gamma_{\text{CC}}Y(5\Phi_C, 9\Phi_C) + (8pr)\Gamma_{\text{CC}}Y(6\Phi_C, 6\Phi_C) + (8pr)\Gamma_{\text{CC}}Y(6\Phi_C, 8\Phi_C) \\
 &\quad + (8pr - 4p - 4r)\Gamma_{\text{CC}}Y(6\Phi_C, 10\Phi_C) + (4pr)\Gamma_{\text{CC}}Y(8\Phi_C, 8\Phi_C) \\
 &\quad + (8pr + 4p + 4r)\Gamma_{\text{CC}}Y(8\Phi_C, 9\Phi_C) + (8pr - 4p - 4r)\Gamma_{\text{CC}}Y(9\Phi_C, 10\Phi_C)
 \end{aligned}$$

By setting the atom and bond weights to unity, the above two equations can be simplified in the following form.

$$\begin{aligned} Y^d(\text{ICOF}(p, r)) &= (4p + 4r)Y(1, 4) + (8pr - 4p - 4r)Y(2, 2) + (12pr)Y(2, 2) + (40pr)Y(2, 3) \\ &\quad + (16pr - 8p - 8r)Y(2, 4) + (12pr)Y(3, 3) + (8pr)Y(3, 4) \\ Y^s(\text{ICOF}(p, r)) &= (4p + 4r)Y(4, 8) + (12pr)Y(5, 5) + (16pr)Y(5, 6) + (8pr)Y(5, 9) + (16pr - 4p - 4r)Y(6, 6) \\ &\quad + (16pr - 4p - 4r)Y(6, 8) + (8pr - 4p - 4r)Y(6, 10) + (4pr)Y(8, 8) + (8pr + 4p + 4r)Y(8, 9) \\ &\quad + (8pr - 4p - 4r)Y(9, 10) \end{aligned}$$

We now illustrate the computation of the index $M_1(\text{ICOF})$ of dimension $(2, 2)$ as shown below.

$$\begin{aligned} M_1^d(\text{ICOF}(2, 2)) &= 16 \times (1 + 4) + 64 \times (2 + 2) + 160 \times (2 + 3) + 32 \times (2 + 4) + 48 \times (3 + 3) + 32 \times (3 + 4) \\ &= 16 \times (5) + 64 \times (4) + 160 \times (5) + 32 \times (6) + 48 \times (6) + 32 \times (7) \\ &= 1840 \\ M_1^s(\text{ICOF}(2, 2)) &= 16 \times (4 + 8) + 48 \times (5 + 5) + 64 \times (5 + 6) + 32 \times (5 + 9) + 48 \times (6 + 6) + 48 \times (6 + 8) \\ &\quad + 16 \times (6 + 10) + 16 \times (8 + 8) + 48 \times (8 + 9) + 16 \times (9 + 10) \\ &= 16 \times (12) + 48 \times (10) + 64 \times (11) + 32 \times (14) + 48 \times (12) + 48 \times (14) + 16 \times (16) + 16 \times (16) \\ &\quad + 48 \times (17) + 16 \times (19) \\ &= 4704 \end{aligned}$$

We now derive the numerical expressions for the topological descriptors of $\text{ICOF}(p, r)$, with the resulting expressions presented in simplified form, $Y^\#(\text{ICOF}) = \{Y^d(\text{ICOF}), Y^s(\text{ICOF})\}$.

Result 1. *The topological descriptors for ICOF are algebraically expressed for $p, r \geq 2$.*

1. $M_1^\#(\text{ICOF}(p, r)) = \{(504pr - 44p - 44r), (1304pr - 128p - 128r)\}$
2. $M_2^\#(\text{ICOF}(p, r)) = \{(652pr - 64p - 64r), (4516pr - 520p - 520r)\}$
3. $HM^\#(\text{ICOF}(p, r)) = \{(2720pr - 252p - 252r), (18416pr - 2096p - 2096r)\}$
4. $AZ^\#(\text{ICOF}(p, r)) = \{((1710559pr)/2000 - (2336p)/27 - (2336r)/27), ((31743354508473967412051pr)/5091288592416768000 - (293250748539392650537p)/377132488327168000 - (293250748539392650537r)/377132488327168000)\}$
5. $BM^\#(\text{ICOF}(p, r)) = \{(1156pr - 108p - 108r), (5820pr - 648p - 648r)\}$
6. $TM^\#(\text{ICOF}(p, r)) = \{(2068pr - 188p - 188r), (13900pr - 1576p - 1576r)\}$
7. $GBM^\#(\text{ICOF}(p, r)) = \{(pr(150480\sqrt{2} + \sqrt{3}(239400\sqrt{2} + 55440) + 487179) - p(75240\sqrt{2} + 7315) - r(75240\sqrt{2} + 7315)/65835), (pr(\sqrt{5}(2343382253520\sqrt{2} + \sqrt{3}(4153311636320\sqrt{2} + 2240602330120) + 4329299417520) + 5739970014240\sqrt{2} + 10986179167040\sqrt{3} + 43787771251488) - p(\sqrt{5}(\sqrt{2}1171691126760 + 1120301165060\sqrt{3}) - 6740116304600\sqrt{2} + 2746544791760\sqrt{3} + 5321430534035) - r(\sqrt{5}(1171691126760\sqrt{2} + 1120301165060\sqrt{3}) - 6740116304600\sqrt{2} + 2746544791760\sqrt{3} + 5321430534035)/10642861068070)\}$
8. $GTM^\#(\text{ICOF}(p, r)) = \{(2(pr(8436\sqrt{2} + \sqrt{3}(15540\sqrt{2} + 3192) + 34447) - p(4218\sqrt{2} + 2109) - r(4218\sqrt{2} + 2109)/14763), (pr(\sqrt{5}(\sqrt{3}(473118780960\sqrt{2} + 219662291160) + 238305216240\sqrt{2} + 427686845040) + 595213950240\sqrt{2} + 1163616461280\sqrt{3} + 4993045912673) - p(290904115320\sqrt{3} - 682015984650\sqrt{2} + \sqrt{5}(119152608120\sqrt{2} + 109831145580\sqrt{3}) + 597969570380) - r(290904115320\sqrt{3} - 682015984650\sqrt{2} + \sqrt{5}(119152608120\sqrt{2} + 109831145580\sqrt{3}) + 597969570380)/2690863066710)\}$

9. $BMG^{\#}(\text{ICOF}(p, r)) = \{(2(pr(84\sqrt{2} + \sqrt{3}(110\sqrt{2} + 38) + 210) - p(42\sqrt{2} - 3) - r(42\sqrt{2} - 3)/3), (pr(890\sqrt{2} + 1240\sqrt{3} + \sqrt{5}(436\sqrt{2} + \sqrt{3}(328\sqrt{2} + 304) + 472) + 3780) - p(310\sqrt{3} - 775\sqrt{2} + \sqrt{5}(218\sqrt{2} + 152\sqrt{3}) + 480) - r(310\sqrt{3} - 775\sqrt{2} + \sqrt{5}(218\sqrt{2} + 152\sqrt{3}) + 480)/15)\}$
10. $TMG^{\#}(\text{ICOF}(p, r)) = \{(2(pr(168\sqrt{2} + \sqrt{3}(190\sqrt{2} + 74) + 342) - p(84\sqrt{2} - 27) - r(84\sqrt{2} - 27)/3), (pr(2170\sqrt{2} + 2960\sqrt{3} + \sqrt{5}(1084\sqrt{2} + \sqrt{3}(728\sqrt{2} + 784) + 1208) + 8460) - p(740\sqrt{3} - 1925\sqrt{2} + \sqrt{5}(542\sqrt{2} + 392\sqrt{3}) + 1080) - r(740\sqrt{3} - 1925\sqrt{2} + \sqrt{5}(542\sqrt{2} + 392\sqrt{3}) + 1080)/15)\}$
11. $TMA^{\#}(\text{ICOF}(p, r)) = \{((6460pr)/3 - 128p - 128r), ((230462pr)/45 - (4163p)/9 - (4163r)/9)\}$
12. $BMA^{\#}(\text{ICOF}(p, r)) = \{((4012pr)/3 - 96p - 96r), ((115934pr)/45 - (2123p)/9 - (2123r)/9)\}$

The numerical values for the dimensions of ICOFs are computed using mathematical expressions derived from prior results, as presented in Table 3, and are further validated using the pseudocode algorithm for computing degree-based topological indices, as presented in Algorithm 1. These values are essential for determining the frameworks entropy levels such that the multiplicative self-powered descriptors are available. The algebraic expressions for these descriptors are given below.

1. $Y^{dp^*}(\text{ICOF}(p, r)) = Y_{\alpha}(4915200p^6r^5 - 3440640p^6r^4 + 491520p^6r^3 + 4915200p^5r^6 - 6881280p^5r^5 + 1474560p^5r^4 - 3440640p^4r^6 + 1474560p^4r^5 + 491520p^3r^6)$
2. $Y^{sp^*}(\text{ICOF}(p, r)) = Y_{\beta}(3221225472p^{10}r^9 - 3221225472p^{10}r^8 + 201326592p^{10}r^7 + 704643072p^{10}r^6 - 251658240p^{10}r^5 + 25165824p^{10}r^4 + 3221225472p^9r^{10} - 6442450944p^9r^9 + 603979776p^9r^8 + 2818572288p^9r^7 - 1258291200p^9r^6 + 150994944p^9r^5 - 3221225472p^8r^{10} + 603979776p^8r^9 + 4227858432p^8r^8 - 2516582400p^8r^7 + 377487360p^8r^6 + 201326592p^7r^{10} + 2818572288p^7r^9 - 2516582400p^7r^8 + 503316480p^7r^7 + 704643072p^6r^{10} - 1258291200p^6r^9 + 377487360p^6r^8 - 251658240p^5r^{10} + 150994944p^5r^9 + 25165824p^4r^{10})$

where we used $D = \{(1, 4), (2, 2), (2, 3), (2, 4), (3, 3), (3, 4)\}$, $S = \{(4, 8), (5, 5), (5, 6), (5, 9), (6, 6), (6, 8), (6, 10), (8, 8), (8, 9), (9, 10)\}$ such that $Y_{\alpha} = \prod_{(f,u) \in D} Y(f, u)^{Y(f,u)}$, $Y_{\beta} = \prod_{(f,u) \in S_1} Y(f, u)^{Y(f,u)}$.

The formulas based on topological and self-powered descriptors are used to derive entropy expressions, resulting in more complex formulations. An illustrative computation of the modified Shannon entropy for ICOF(3,3), using the M_1^d index, is presented below.

$$I_{M_1^d}(\text{ICOF}(3,3)) = \log(4272) - \left(\frac{1}{4272}\right) \times \log(1006157168640 \times (4)^4 \times 2(5)^5 \times 2(6)^6 \times (7)^7) = 8.3401$$

We have now correlated the topological index and entropy values for the case where the dimensions $p = r$. Among the degree-based indices, the bi-Zagreb-geometric index is the most effective for modeling the logarithmic regression model of ICOF, as shown below with the correlation (r), F-value (F) and standard error (Se),

$$I_{BMG^d}(\text{ICOF}(p, r)) = 1.0072 \log(BMG^d) - 0.0757, \quad r = 1, \quad F = 50.08743672, \quad Se = 3773.59342.$$

Extending this approach, QSPR models could be formulated when experimental physicochemical data for ICOF become available.

Table 3: Topological descriptor values for ICOF(p, r) based on degree and degree-sum

γ		ICOF														
		$p = 1$					$p = 2$					$p = 3$				
		$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$	$r = 2$	$r = 3$	$r = 4$	$r = 5$	$r = 4$	$r = 3$	$r = 4$	$r = 5$	$r = 4$	$r = 5$
d	s															
M_1	416	876	1336	1796	2256	1840	2804	3768	4732	4272	5740	7208	7712	9684	12,160	
	1048	2224	3400	4576	5752	4704	7184	9664	12,144	10,968	14,752	18,536	19,840	24,928	31,320	
M_2	524	1112	1700	2288	2876	2352	3592	4832	6072	5484	7376	9268	9920	12,464	15,660	
	3476	7472	11,468	15,464	19,460	15,984	24,496	33,008	41,520	37,524	50,552	63,580	68,096	85,640	107,700	
HM	2216	4684	7152	9620	12,088	9872	15,060	20,248	25,436	22,968	30,876	38,784	41,504	52,132	65,480	
	14,224	30,544	46,864	63,184	79,504	65,280	100,016	134,752	169,488	153,168	206,320	259,472	277,888	349,456	439,440	
AZ	682,2425	1451	2219.8	2988.5	3757.3	3075	4699.1	6323.1	7947.2	7178.4	9657.7	12,137	12,992	16,327	20,517	
	4679.7	10,137	15,594	21,051	26,509	21,829	33,521	45,213	56,905	51,448	69,375	87,302	93,537	117,700	148,100	
BM	940	1988	3036	4084	5132	4192	6396	8600	10,804	9756	13,116	16,476	17,632	22,148	27,820	
	4524	9696	14,868	20,040	25,212	20,688	31,680	42,672	53,664	48,492	65,304	82,116	87,936	110,568	139,020	
TM	1692	3572	5452	7332	9212	7520	11,468	15,416	19,364	17,484	23,500	29,516	31,584	39,668	49,820	
	10,748	23,072	35,396	47,720	60,044	49,296	75,520	101,744	127,968	115,644	155,768	195,892	209,792	263,816	331,740	
GBM	17,5436	36,8145	56,0855	75,3564	94,6273	77,0837	117,353	157,6222	197,8914	178,6205	239,888	301,1555	322,1538	404,4197	507,6838	
	9,6093	20,0257	30,4421	40,8586	51,275	41,6657	63,3058	84,9458	106,5859	96,1695	129,0331	161,8968	173,1204	217,2077	272,5186	
GTM	10,0011	21,0959	32,1908	43,2857	54,3806	44,3796	67,6632	90,9468	114,2304	103,1355	138,6079	174,0802	186,2689	233,93	293,7798	
	4,1337	8,6166	13,0995	17,5824	22,0653	17,9315	27,2464	36,5613	45,8762	41,3933	55,5403	69,6872	74,5192	93,4981	117,3091	
BMG	367,5079	772,6137	1177.7	1582.8	1987.9	1620.4	2468.2	3316	4163.9	3758.7	5049.3	6339.8	6782.5	8515.7	10,692	
	679,7671	1439.5	2199.2	2958.9	3718.6	3038.8	4638.1	6237.5	7836.8	7077.1	9516.1	11,955	12,795	16,073	20,191	
TMG	659,7165	1380.6	2101.5	2822.5	3543.4	2883.7	4386.7	5889.7	7392.7	6671.8	8956.9	11,242	12,024	15,091	18,941	
	1604.4	3400.2	5196	6991.8	8787.6	7183.2	10,966	14,749	18,532	16,737	22,507	28,277	30,264	38,022	47,767	
TMA	1897.3	3922.7	5948	7973.3	9998.7	8101.3	12,280	16,459	20,637	18,612	24,944	31,276	33,429	41,915	52,553	
	4196.3	8855.1	13,514	18,173	22,832	18,635	28,415	38,196	47,976	43,317	58,219	73,120	78,242	98,265	123,410	
BMA	1145.3	2386.7	3628	4869.3	6110.7	4965.3	7544	10,123	12,701	11,460	15,376	19,292	20,629	25,883	32,473	
	2104.5	4445	6785.4	9125.8	11,466	9361.7	14,278	19,195	24,112	21,771	29,265	36,758	39,334	49,403	62,049	

As a result, entropy values of topological descriptors based on degree and degree-sum are calculated by equating their dimensions, setting $p = r$ in their configurations to ensure that entropy values are measured on a consistent scale. Among these, the geometric-tri-Zagreb index exhibits the highest entropy, whereas the hyper-Zagreb index displays the lowest entropy. To ensure consistency in comparing entropies across ICOF configurations, the values are scaled relative to the total number of bonds in each structure, accounting for variations caused by their fixed dimensions. This scaling facilitates a direct comparison of degree and degree-sum entropies across different ICOF configurations. For ICOF(3,3), the scaled entropy based on M_1 is calculated as $8.3401/816 = 0.0102$. Table 4 shows that ICOF^s consistently exhibits higher entropy values than ICOF^d, as illustrated in Fig. 4. These results reveal that scaled entropies decrease asymptotically as the dimensions of p and r increase.

Table 4: Scaled entropy values for ICOF(p, r) based on degree and degree-sum

Y	$p = r = 3$		$p = r = 4$		$p = r = 5$		$p = r = 6$	
	ICOF ^d	ICOF ^s	ICOF ^d	ICOF ^s	ICOF ^d	ICOF ^s	ICOF ^d	ICOF ^s
M_1	0.010221	0.011354	0.006073	0.006708	0.004051	0.004456	0.002908	0.003189
M_2	0.010525	0.012841	0.006243	0.007539	0.00416	0.004986	0.002984	0.003555
HM	0.01227	0.014542	0.007213	0.008488	0.004775	0.005589	0.003409	0.003973
AZ	0.010856	0.013221	0.006427	0.007776	0.004277	0.005122	0.003064	0.00365
BM	0.011229	0.013152	0.006634	0.007712	0.004407	0.005096	0.003154	0.003631
TM	0.011937	0.014201	0.007028	0.008298	0.004658	0.005469	0.003327	0.003889
GBM	0.006178	0.005085	0.003862	0.003321	0.002659	0.002338	0.001951	0.001738
GTM	0.005371	0.003345	0.003444	0.002501	0.002403	0.001866	0.001778	0.001432
BMG	0.010065	0.010822	0.005986	0.006411	0.003996	0.004268	0.00287	0.003058
TMG	0.010764	0.011865	0.006374	0.006993	0.004242	0.004637	0.00304	0.003314
TMA	0.01201	0.013016	0.007065	0.007633	0.00468	0.005044	0.003342	0.003595
BMA	0.011423	0.012184	0.006739	0.00717	0.004474	0.00475	0.0032	0.003391

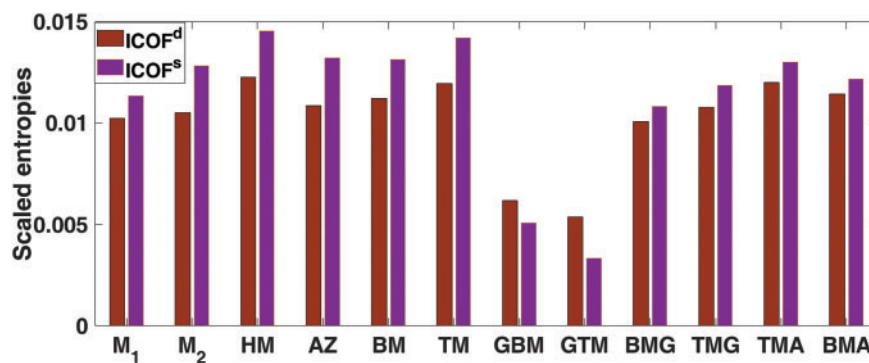


Figure 4: Bar diagram of scaled entropy for ICOF(3,3) based on various descriptors

Algorithm 1: Computation of topological indices from an adjacency matrix

1: **Input:** Adjacency matrix A of a simple undirected graph (from **newGRAPH** software).

2: **Output:** Dictionary *indices* of computed topological indices.

Vertex Degree Calculation

3: $n \leftarrow$ number of vertices in A

4: $deg \leftarrow [0, \dots, 0]$

▷ Array of size n

5: **for** $i \leftarrow 0$ to $n - 1$ **do**

6: $deg[i] \leftarrow \sum_{j=0}^{n-1} A[i][j]$

▷ Sum row i to count degree of vertex i

7: **end for**

Initialize Topological Indices

8: $M_1, M_2, HM, AZ, BM, TM, GBM, GTM, BMG, TMG, BMA, TMA \leftarrow 0$

Edge Processing and Index Updates

9: **for** $u \leftarrow 0$ to $n - 2$ **do**

10: **for** $v \leftarrow u + 1$ to $n - 1$ **do**

▷ Avoid double-counting of edges

11: **if** $A[u][v] = 1$ **then**

▷ Edge exists between u and v

12: $f \leftarrow deg[u], g \leftarrow deg[v]$

▷ Degrees of endpoints

13: First Zagreb Index: $M_1 \leftarrow M_1 + (f + g)$

14: Second Zagreb Index: $M_2 \leftarrow M_2 + (f \cdot g)$

15: Hyper Zagreb Index: $HM \leftarrow HM + (f + g)^2$

16: **if** $f + g \neq 2$ **then**

▷ Avoid division by zero

17: Augmented Zagreb Index: $AZ \leftarrow AZ + \left(\frac{f \cdot g}{f + g - 2} \right)^3$

18: **end if**

19: Bi-Zagreb Index: $BM \leftarrow BM + (f + g + f \cdot g)$

20: Tri-Zagreb Index: $TM \leftarrow TM + (f^2 + g^2 + f \cdot g)$

21: Geometric Bi-Zagreb: $GBM \leftarrow GBM + \frac{\sqrt{f \cdot g}}{f + g + f \cdot g}$

22: Geometric Tri-Zagreb: $GTM \leftarrow GTM + \frac{\sqrt{f \cdot g}}{f^2 + g^2 + f \cdot g}$

23: Bi-Zagreb Geometric: $BMG \leftarrow BMG + \frac{f + g + f \cdot g}{\sqrt{f \cdot g}}$

24: Tri-Zagreb Geometric: $TMG \leftarrow TMG + \frac{f^2 + g^2 + f \cdot g}{\sqrt{f \cdot g}}$

25: Bi-Zagreb Arithmetic: $BMA \leftarrow BMA + \frac{2 \cdot (f + g + f \cdot g)}{f + g}$

26: Tri-Zagreb Arithmetic: $TMA \leftarrow TMA + \frac{2 \cdot (f^2 + g^2 + f \cdot g)}{f + g}$

27: **end if**

28: **end for**

29: **end for**

30: **return** *indices*

4 Modeling of Graph Energy

In this section, we develop linear regression models for producing the graph energies of ICOFs using the topological indices that were determined in the preceding section. The relationship between a graph's structural characteristics and the overall π -electron energy in molecules is examined through graph energy. McClelland's theory for calculating E_π is a groundbreaking contribution to the field of total π -electron energy. As an effective computational substitute for complex quantum chemistry methods, McClelland introduced the formula $E_\pi(G) \approx 0.91 \times \sqrt{2|V(G)||E(G)|}$, which provides a straightforward method for estimating

the total π -electron energy [83,84]. While McClelland's formula offers a fast and simple approximation of π -electron energy based solely on the number of vertices and edges in a molecular graph, it does not capture the full complexity of electronic interactions in large or highly conjugated systems. As the size and structural intricacy of ICOFs increase, the limitations of this approach become more evident. For example, as shown in Table 5, for ICOF(5,5), the actual graph energy is 2653.47942, whereas McClelland's estimate is 2701.9, resulting in a discrepancy of approximately 48.4 units. To address this, our work incorporates regression models based on topological descriptors, which better reflect structural nuances and provide energy estimates that more closely align with spectral values [85–88]. In this paper, we compute graph energies using the well-known platform newGRAPH, a comprehensive tool designed to facilitate and advance research in graph theory.

Table 5: ICOF Graph energy and McClelland's energy

ICOF(p, r)	E_π	McClelland's E_π
ICOF(1,1)	91.27135	94.9196
ICOF(1,2)	191.83738	198.0709
ICOF(1,3)	292.40342	301.2196
ICOF(1,4)	392.96945	404.3678
ICOF(1,5)	493.53548	507.5157
ICOF(2,2)	402.25846	412.5904
ICOF(2,3)	612.67951	627.1056
ICOF(2,4)	823.10056	841.6196
ICOF(2,5)	1033.52161	1056.1
ICOF(3,3)	932.95552	952.9851
ICOF(3,4)	1253.23153	1278.9
ICOF(3,5)	1573.50754	1604.7
ICOF(4,4)	1683.36251	1716.1
ICOF(4,5)	2113.49348	2153.3
ICOF(5,5)	2653.47942	2701.9

The eigen-spectrum and graph energy for specific dimensions of ICOFs were calculated using the machine-generated package [89] in conjunction with McClelland's graph energy as shown in Table 5. A linear regression model, $E_\pi(\text{ICOF}) = a(Y(\text{ICOF})) + b$, was developed to predict graph energy based on topological descriptor values. In this equation, a and b are constants and parameters related to statistics, such as correlation (r), standard error (Se), and F -value, are incorporated.

The bi-Zagreb-geometric index is the most effective for modeling linear regression models of ICOFs using degree descriptors, whereas the tri-Zagreb-arithmetic index yields the highest accuracy for degree-sum descriptors, as shown below.

$$\begin{aligned}
 E_\pi(\text{ICOF}(p, r)) &= 0.24816806778517(BMG^d) + 0.146261847, \\
 r &= 0.999999999, F = 4611352006, Se = 0.041570275 \\
 E_\pi(\text{ICOF}(p, r)) &= 0.0214883975178587(TMA^s) + 2.072468999, \\
 r &= 0.999999825, F = 37225220.86, Se = 0.462677438
 \end{aligned}$$

The geometric-tri-Zagreb and bi-Zagreb-geometric indices exhibit higher entropy values due to their strong topological structural relevance, allowing them to effectively capture the intricate connectivity and branching patterns of ICOF frameworks. This enhances their capacity to reflect the spectral and energetic characteristics of these materials.

Given that the computation of graph energy through spectral methods involves eigenvalue analysis, which becomes increasingly complex and resource-intensive for large molecular structures, we developed linear regression models based on topological descriptors as a practical alternative. These models enable efficient estimation of graph energies without the need for full spectral decomposition. As shown in Table 6, the predicted values closely approximate the actual spectral energies, with minimal error (e.g., an error of only 0.089 units for ICOF-P(6,1)). Although minor discrepancies are observed, the models offer a computationally efficient and scalable approach for estimating graph energies in complex systems. This predictive framework serves as a useful tool for large-scale applications, where exact spectral calculations may be impractical.

Table 6: Comparison of original and predicted ICOF energies based on degree and degree-sum descriptors

ICOF-P(p,r)	E_π	Predicted E_π by BMG^d	Predicted by TMA^s
ICOF-P(6,1)	594.10152	594.0124481	592.7885168
ICOF-P(6,2)	1243.94266	1243.890167	1243.156356
ICOF-P(6,3)	1893.78356	1893.743069	1893.524195
ICOF-P(6,4)	2543.62445	2543.620789	2543.935011
ICOF-P(6,5)	3193.46535	3193.572958	3194.17392

The graph energy of ICOFs is predicted using degree and degree-sum descriptors, based on the regression equations outlined earlier. As shown in Table 6, these predicted values are compared with the original E_π values and depicted in Fig. 5.

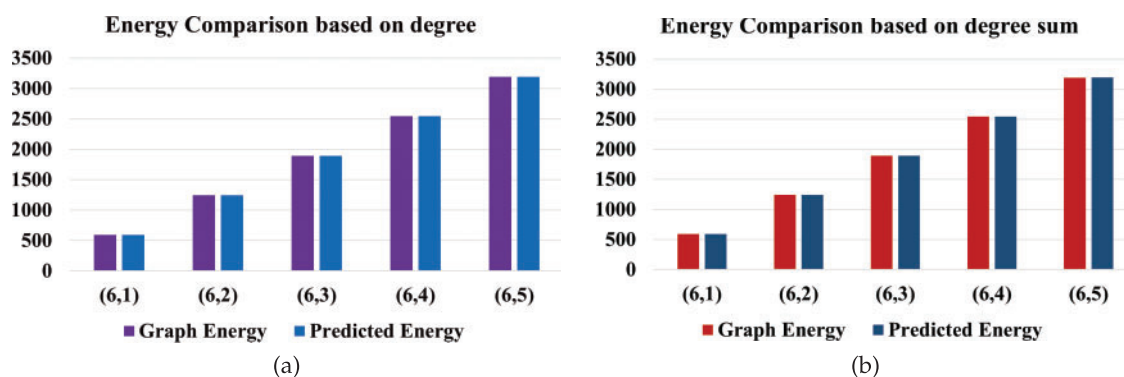


Figure 5: Graph energy prediction using (a) degree and (b) degree-sum

5 Conclusion

We have discussed the topological descriptors and entropies of ICOFs with parallelogram configurations. Our analysis, using scaled entropy measures, demonstrated that degree-based entropy reveals a

higher level of informational disorder than degree-sum entropy, offering a more comprehensive understanding of the structural arrangement. To further enhance computational efficiency, we developed a set of optimized linear regression models specifically designed to predict graph energy across ICOF frameworks of varying dimensions. By refining these models, we were able to significantly reduce the computational complexity while maintaining high predictive accuracy. The results not only expand our understanding of the structural diversity within ICOF frameworks but also provide valuable insights into the relationship between framework dimensions and graph energy. These findings open new avenues for future research by providing a robust framework for exploring ICOF properties and guiding the design of advanced materials in this domain.

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Availability of Data and Materials: All data generated during this work are included in this paper.

Ethics Approval: Not applicable.

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