Research Article

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Entropy measures of the metal–organic network via topological descriptors

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Abstract: A family of chemical compounds known as metal–organic networks (MONs) is composed mainly of clusters of metal ions with organic ligands. It can increase volatility or make substances soluble in organic solvents. By using these salient features, organic compounds generate applications in material sciences for sol–gel processing. A graph’s entropy is utilized as a complexity indicator and is interpreted as the structural information content of the graph. Investigating the entropies of relationship systems is a common occurrence in discrete mathematics, computer science, information theory, statistics, chemistry, and biology. In this article, we investigated the degree-based entropies: geometric arithmetic entropy, atom bond connectivity entropy, general Randić entropy, and general sum connectivity entropy for MONs. Furthermore, we created tables for all expressions by using 1–10 values for the s parameter of these entropies.

Keywords: metal–organic network, entropy, organic ligands, topological indices

1 Introduction

Chemical graph theory (CGT) is a subfield of mathematical chemistry that explores chemical phenomena computationally using the techniques of graph theory. In CGT, theoretical chemistry and graph theory are merged. It also connects to the nontrivial applications of graph theory for mitigating molecular issues (Gao et al., 2018). Hydrogen, oxygen, and nitrogen are the three elements that make up the core of the earth. One of the upcoming energy sources is hydrogen (Yang et al., 2009). Among the numerous gases, hydrogen lacks smell, which makes it nearly impossible for humans to trace any leaks. The US Energy Department’s current rules focus on the tool’s detection accuracy, requiring it to find 1% of the volume of unscented molecular hydrogen in the air within just 60 s (Wasson et al., 2019, Yanyan and Xiuping, 2013). With the help of palladium (Pd) nanowires, created a rapid molecular hydrogen detector with metal nodes and organic ligands known as a metal–organic network (MON). In just 7 s, this gadget must detect hydrogen leaks with an intensity of less than 1%. Furthermore, MONs manifest a very salient physio-chemical characteristic in creating composites with various materials (Ahmed and Jhung, 2014), exchanging ions (Kim et al., 2012), attaching active groups (Hwang et al., 2008), and modifying organic ligands (Eddaoudi et al., 2002).

A topological invariant is a numeric value that is associated with the chemical structure and helps predict the modeling of quantitative structure property relationship/quantitative structure activity relationship for any chemical structure. From logic and biology to physics and engineering, entropy has been a rigorous and transcendental method in a variety of fields of research. Information entropy was first conceived by Shannon (1948) in communication theory. In information theory, it serves as a structural descriptor to evaluate the complexity of chemical structures. A measure of a system’s uncertainty is known as the entropy of a probability distribution, too. Entropy was later applied to chemical networks and graphs. It was created to assess the usefulness of analysis in graphs and chemical networks. Rashevsky (1955), Trucco (1956), and Mowshowitz (1968) were the first to define and analyse the entropy of graphs.

Let $\Gamma(r, t)$ be a simple and connected graph with order $r$ and size $t$. The degree of any vertex $p \in V(\Gamma)$ is the number of vertices that are adjacent to vertex $p$, and it is written as $\chi_p$. For more understanding of the terminologies and symbols of graph theory, read the studies of Wilson (1996) and Deo (1990).
In a molecular graph, vertices and edges are considered atoms and bonds, respectively. Several topological indices of MONs and some interesting molecular structures are reported in Kashif et al. (2021) and Liu et al. (2022). Dehmer and Mowshowitz (2011) presented a comprehensive survey on graph entropies. Zhang et al. (2022) computed the entropy of ceria oxide via topological indices. Imran et al. (2021) calculated the edge-weighted graph entropies of various shapes of carbon nanotubes. Ghorbani et al. (2020) studied the characteristics of entropies for the chemical structure known as fullerenes. Koam et al. (2022) investigated the entropy measures of y-junction-related nanostructures. Ghani et al. (2022) reported some computations of entropies for boric acid \((HBO_3)_3\) layers. Manzoor et al. (2022) determined the exact expressions of entropy values for isomeric natural polymers. Wang et al. (2021) obtained some degree-based entropy expressions for silicon carbide compounds. For more studies, one can refer to Manzoor et al. (2020a,b,c) and Liu et al. (2023a,b).

2 Definitions

Mathematicians define some topological descriptors and graph entropies that are very useful for our computation.

2.1 Degree-based topological invariants

Das et al. (2011) introduced the geometric arithmetic index, which is defined as

\[
\text{GA}(\Gamma) = \sum_{pq \in E(\Gamma)} \frac{X_p X_q}{X_p + X_q}
\]

(1)

Xing et al. (2011) defined the atom bond connectivity (ABC) index, which is written as

\[
\text{ABC}(\Gamma) = \sum_{pq \in E(\Gamma)} \frac{X_p X_q - X_p + X_q}{X_p + X_q}
\]

(2)

Li and Shi (2008) surveyed on a general Randić index, which is defined as

\[
\text{R}_{\alpha}(\Gamma) = \sum_{pq \in E(\Gamma)} (X_p X_q)^{\alpha}
\]

(3)

It is also called a product connectivity index. We are interested in the values of \(\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}\). We can observe that if \(\alpha = 1\), then it is converted into the second Zagreb index.

Zhou and Trinajstić (2010) derived the expression of the general sum connectivity index, which is written as

\[
\text{SC}_{\alpha}(\Gamma) = \sum_{pq \in E(\Gamma)} (X_p + X_q)^{\alpha}
\]

(4)

We are interested in the values of \(\alpha = 1, 2, \frac{1}{2}, -\frac{1}{2}\). We can observe that if \(\alpha = 1, 2\), then it is converted into the first Zagreb index and the hyper Zagreb index, respectively.

2.2 Edge weight-based entropies

Chen et al. (2014) investigated the definition of entropy in relation to an edge-weighted graph. Let \(\Gamma = (V(\Gamma); E(\Gamma); \psi(pq))\) be an edge-weighted entropy for graph \(\Gamma\), in which \(V(\Gamma), E(\Gamma), \psi(pq)\) represent the vertex set, edge set, and the edge weight of edge \((pq)\), respectively. Its mathematical expression can be written as

\[
E_\psi(\Gamma) = -\sum_{p'q' \in E(\Gamma)} \frac{\psi(p'q')}{\sum_{pq \in E(\Gamma)} \psi(pq)} \log \frac{\psi(p'q')}{\sum_{pq \in E(\Gamma)} \psi(pq)}
\]

(5)

2.2.1 Geometric arithmetic entropy

If \(\psi(pq) = \frac{X_p X_q}{X_p + X_q}\), then

\[
\sum_{pq \in E(\Gamma)} \psi(pq) = \sum_{pq \in E(\Gamma)} \frac{X_p X_q}{X_p + X_q} = \text{GA}(\Gamma)
\]

Now, Eq. 5 is converted into a new expression called a geometric arithmetic entropy (Manzoor et al., 2020a,b,c):

\[
E_{\text{GA}}(\Gamma) = \log(\text{GA}(\Gamma))
\]

- \frac{1}{\text{GA}(\Gamma)} \log \left[ \prod_{pq \in E(\Gamma)} \frac{X_p X_q}{X_p + X_q} \right]

(6)

2.2.2 ABC entropy reduced to a new expression

If \(\psi(pq) = \sqrt[\frac{X_p + X_q - \frac{2}{\sqrt{X_p X_q}}}{X_p X_q}}\), then

\[
\sum_{pq \in E(\Gamma)} \psi(pq) = \sum_{pq \in E(\Gamma)} \sqrt[\frac{X_p + X_q - \frac{2}{\sqrt{X_p X_q}}}{X_p X_q}}
\]

Now, Eq. 5 is converted into a new expression called an ABC entropy (Manzoor et al., 2020a,b,c):
2.2.3 General Randic’ entropy

If \( \psi(pq) = (x_p x_q)^a \), then

\[
\sum_{pq \in E(\Gamma)} \psi(pq) = \sum_{pq \in E(\Gamma)} (x_p x_q)^a
\]

Now, Eq. 5 is reduced to a new expression called a general Randic’ entropy (Manzoor et al., 2020):

\[
E_{R_a}(\Gamma) = \log(R_a(\Gamma)) - \frac{1}{R_a(\Gamma)} \log \left( \prod_{pq \in E(\Gamma)} \left( \frac{x_p + x_q - 2}{x_p x_q} \right)^{a(x_p x_q)} \right)
\]

(7)

2.2.4 General sum connectivity entropy

If \( \psi(pq) = (x_p + x_q)^a \), then

\[
\sum_{pq \in E(\Gamma)} \psi(pq) = \sum_{pq \in E(\Gamma)} (x_p + x_q)^a
\]

Now, Eq. 5 is reduced into a new expression called a general sum connectivity entropy (Manzoor et al., 2020a,b,c; Afzal et al., 2020):

\[
E_{SC_a}(\Gamma) = \log(SC_a(\Gamma)) - \frac{1}{SC_a(\Gamma)} \log \left( \prod_{pq \in E(\Gamma)} (x_p + x_q)^{a(x_p + x_q)} \right)
\]

(9)

3 MON

In this section, we will determine the chemical structure of the MON. As shown in Figure 1, the MON is made of metals and organic ligands. The networks MON\(_1\) and MON\(_2\) are created by combining the fundamental metal organic structures. The larger vertex in the MON\(_1\) is connected to another one by zeolite imidazole. Likewise, the smaller organic metal vertex in the MON\(_2\) is linked to the other vertex. The first MON\(_1\) and the second MON\(_2\) are shown in Figure 2(a) and (b), respectively. For dimension \( s \geq 2 \), the order and size of both MONs are \( 48s \) and 72s – 12, respectively.

In MON\(_1\), there are four types of vertices with degrees 2, 3, 4, and 6, but in MON\(_2\), there are three types of vertices with degrees 2, 3, and 4. The edge partition of MON\(_1\) and MON\(_2\) w.r.t. the degree of end vertices is given in Tables 1 and 2, respectively.

4 Main results

In this section, we present the computation of some graph entropies for the first and second MONs.

**Theorem 1.** (Hong et al., 2020) If MON\(_1\) and MON\(_2\) are the first and second MONs, respectively, then

\[
\text{GA(MON}_1\text{)} = 66.4833 + 22.1132
\]

\[
\text{GA(MON}_2\text{)} = 70.9482 - 13.0480
\]

**Theorem 2.** (Hong et al., 2020) If MON\(_1\) and MON\(_2\) are the first and second MONs, respectively, then

\[
\text{ABC(MON}_1\text{)} = \left( \frac{60}{\sqrt{2}} + \frac{12}{\sqrt{3}} \right)s - \frac{12}{\sqrt{3}}
\]

\[
\text{ABC(MON}_2\text{)} = \left( \frac{24}{\sqrt{2}} + 6 \sqrt{\frac{5}{3}} + 3\sqrt{6} + 16 \right)s
\]

\[
+ \left( \frac{36}{\sqrt{2}} - 6 \sqrt{\frac{5}{3}} - 3\sqrt{6} - 16 \right)
\]

**Theorem 3.** (Kashif et al., 2021) If MON\(_1\) and MON\(_2\) are the first and second MONs, respectively, then
Theorem 4. If $MON_1$ and $MON_2$ are the first and second MONs, respectively, then

$$E_{GA}(MON_1) = \log[66.4833s + 22.1132] - \log[66.4833s + 22.1132].$$

Table 1: Edge partition of $MON_1$ w.r.t. the degrees of end nodes

<table>
<thead>
<tr>
<th>$(u_p, x_q)$</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2,3)</td>
<td>36</td>
</tr>
<tr>
<td>(2,4)</td>
<td>12(s + 1)</td>
</tr>
<tr>
<td>(2,6)</td>
<td>24(s - 1)</td>
</tr>
<tr>
<td>(4,6)</td>
<td>12(s - 1)</td>
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</tbody>
</table>

Table 2: Edge partition of $MON_2$ w.r.t. the degrees of end nodes

<table>
<thead>
<tr>
<th>$(u_p, x_q)$</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2,3)</td>
<td>12(s + 2)</td>
</tr>
<tr>
<td>(2,4)</td>
<td>12(s + 1)</td>
</tr>
<tr>
<td>(3,3)</td>
<td>24(s - 1)</td>
</tr>
<tr>
<td>(3,4)</td>
<td>12(s - 1)</td>
</tr>
<tr>
<td>(4,4)</td>
<td>12(s - 1)</td>
</tr>
</tbody>
</table>

$$R_d(MON_1) = 6^6 36 + 12^2 24(s - 1) + 8^3 12(3s - 1) + 12^4 12(s - 1)$$

$$R_d(MON_2) = 6^6 12(s + 2) + 8^3 12(s + 1) + 9^2 24(s - 1) + 12^4 12(s - 1) + 16^3 12(s - 1)$$

Theorem 5. Let $MON_1$ be the first MON with $s \geq 2$ and $E_{GA}$ be the geometric arithmetic entropy. Then,

$$E_{GA}(MON_1) = \log[66.4833s + 22.1132] - \log[66.4833s + 22.1132].$$

Proof. The expression of the topological invariant of the geometric arithmetic index is given by Eq. 1, and the result of this index for the structure of $MON_1$ is presented in Theorem 1. Now to investigate the geometric arithmetic entropy for the network $MON_1$, using Eq. 1 and edge partition from Table 1 in the expression of geometric arithmetic entropy $E_{GA}$, which is defined in Eq. 6, we will obtain the desired result as follows: \qed
Theorem 6. Let MON₁ be a first MON with $s \geq 2$ and $E_{ABC}$ be the atom bond connectivity (ABC) entropy. Then,

$$E_{ABC}(MON₁) = \log \left( \frac{60 \sqrt{2} + 12 \sqrt{3}}{\sqrt{2} \sqrt{3}} s - \frac{12}{\sqrt{3}} \right) - \log \left( \frac{1}{\sqrt{2}} \sqrt{\frac{36}{2}} \sqrt{\frac{12(3s-1)}{2}} \sqrt{\frac{24(s-1)}{2}} \sqrt{\frac{12(s-1)}{2}} \right) - \frac{60 \sqrt{2} + 12 \sqrt{3}}{\sqrt{2} \sqrt{3}} s - \frac{12}{\sqrt{3}}$$

Proof. The expression of the topological invariant of the ABC index is given by Eq. 2, and the result of this index for the network of MON₁ is given in Theorem 2. Now to investigate the ABC entropy for the structure MON₁, using Eq. 2 and edge partition from Table 1 in the expression of ABC entropy $E_{ABC}$, which is defined in Eq. 7, we will achieve the desired result as follows:

$$E_{ABC}(MON₁) = \log \left( \frac{60 \sqrt{2} + 12 \sqrt{3}}{\sqrt{2} \sqrt{3}} s - \frac{12}{\sqrt{3}} \right) - \log \left( \frac{1}{\sqrt{2}} \sqrt{\frac{36}{2}} \sqrt{\frac{12(3s-1)}{2}} \sqrt{\frac{24(s-1)}{2}} \sqrt{\frac{12(s-1)}{2}} \right) - \frac{60 \sqrt{2} + 12 \sqrt{3}}{\sqrt{2} \sqrt{3}} s - \frac{12}{\sqrt{3}}$$

which is our required result.

Theorem 7. Let MON₁ be a first MON with $s \geq 2$ and $E_{R₁}$ be the general Randic' entropy. Then,

$$E_{R₁}(MON₁) = \log \left( 6^{3} \cdot 36 + 12^{2} \cdot 24(s - 1) + 8^{4} \cdot 12(3s - 1) + 24^{4} \cdot 12(s - 1) \right)$$

Proof. The expression of the topological invariant of the general Randic' index is given by Eq. 3, and the result of this index for the network MON₁ is given in Theorem 3. Now to investigate the general Randic' entropy for the structure MON₁, using Eq. 3 and edge partition from Table 1 in the expression of general Randic' entropy $E_{R₁}$, which is defined in Eq. 8, we will obtain the desired outcome as follows:

$$E_{R₁}(MON₁) = \log \left( 6^{3} \cdot 36 + 12^{2} \cdot 24(s - 1) + 8^{4} \cdot 12(3s - 1) + 24^{4} \cdot 12(s - 1) \right)$$
Theorem 8. Let $\text{MON}_1$ be a first MON with $s \geq 2$ and $E_{SC_1}$ be the general sum connectivity entropy. Then,

$$E_{SC_1}(\text{MON}_1) = \log[5^3 36 + 6^4 12(s - 1) + 8^4 12(s - 1) + 10^4 12(s - 1)]$$

which is our required expression.

Proof. The expression of the topological invariant of the general sum connectivity index is given by Eq. 4, and the result of this index for the network $\text{MON}_1$ is given in Theorem 4. Now, to investigate the general sum connectivity entropy for the network $\text{MON}_1$, using Eq. 4 and edge partition from Table 1 in the expression of the general sum connectivity entropy $E_{SC_1}$, which is defined in Eq. 9, we will achieve the desired result as follows:

$$E_{GA}(\text{MON}_1) = \log[70.9482s - 13.0480]$$

result of this index for the network $\text{MON}_1$ is given in Theorem 4. Now, to investigate the general sum connectivity entropy for the structure $\text{MON}_1$, using Eq. 4 and edge partition from Table 1 in the expression of the general sum connectivity entropy $E_{SC_1}$, which is defined in Eq. 9, we will achieve the desired expression as follows:

$$E_{SC_1}(\text{MON}_1) = \log[5^3 36 + 6^4 12(s - 1) + 8^4 12(s - 1) + 10^4 12(s - 1)]$$

which is our required result.

Theorem 9. Let $\text{MON}_2$ be a second MON with $s \geq 2$ and $E_{GA}$ be the geometric arithmetic entropy. Then,

$$E_{GA}(\text{MON}_2) = \log[70.9482s - 13.0480]$$

Proof. The expression of the topological invariant of the geometric arithmetic index is given by Eq. 1, and the result of this index for the structure $\text{MON}_2$ is presented in Theorem 1. Now, to investigate the geometric arithmetic entropy for the network $\text{MON}_2$, using Eq. 1 and edge partition from Table 2 in the expression of the geometric arithmetic entropy $E_{GA}$, which is defined in Eq. 6, we will achieve the desired result as follows:

$$E_{GA}(\text{MON}_2) = \log[70.9482s - 13.0480]$$
Table 3: Numerical analysis of some graph entropies for the network $MON_1$

<table>
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<th>$E_{GA}$</th>
<th>$E_{ABC}$</th>
<th>$E_{R_1}$</th>
<th>$E_{R^{-1}}$</th>
<th>$E_{R_1^2}$</th>
<th>$E_{R^{-1}_2}$</th>
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Table 4: Numerical analysis of some graph entropies for the network $MON_2$

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Theorem 10. Let \( \text{MON}_2 \) be a second MON with \( s \geq 2 \) and \( E_{\text{ABC}} \) be the ABC entropy. Then,

\[
E_{\text{ABC}}(\text{MON}_2) = \log \left( \frac{24}{\sqrt{2}} + 6 \sqrt{\frac{5}{3}} + 3 \sqrt{6} + 16 \right) s + \left( \frac{36}{\sqrt{2}} - 6 \sqrt{\frac{5}{3}} - 3 \sqrt{6} - 16 \right)
\]

Proof. The expression of the topological invariant of the ABC index is given by Eq. 2, and the result of this index for the network \( \text{MON}_2 \) is given in Theorem 2. Now, to investigate the ABC entropy for the structure \( \text{MON}_2 \), using Eq. 2 and edge partition from Table 2 in the expression of ABC entropy \( E_{\text{ABC}} \), which is defined in Eq. 7, we will achieve the desired result as follows:

\[
E_{\text{ABC}}(\text{MON}_2) = \log \left( \frac{24}{\sqrt{2}} + 6 \sqrt{\frac{5}{3}} + 3 \sqrt{6} + 16 \right) s + \left( \frac{36}{\sqrt{2}} - 6 \sqrt{\frac{5}{3}} - 3 \sqrt{6} - 16 \right)
\]

which is our required result.

Theorem 11. Let \( \text{MON}_2 \) be a second MON with \( s \geq 2 \) and \( E_{\overline{R}} \) be the general Randic' entropy. Then,

\[
E_{\overline{R}}(\text{MON}_2) = \log \left[ 6^s 12(8^s 12(s + 2) + 8^s 12(s + 1) + 9^s 24(s - 1) + 12^s 12(s - 1) + 16^s 12(s - 1)) \right]
\]

Proof. The expression of the topological invariant of the general Randic' index is given by Eq. 3, and the result of this index for the network \( \text{MON}_2 \) is given in Theorem 3. Now, to investigate the general Randic' entropy for the structure \( \text{MON}_2 \), using Eq. 3 and edge partition from Table 2 in the expression of general Randic' entropy \( E_{\overline{R}} \), which is defined in Eq. 8, we will achieve the desired result as follows:

\[
E_{\overline{R}}(\text{MON}_2) = \log \left[ 6^s 12(8^s 12(s + 2) + 8^s 12(s + 1) + 9^s 24(s - 1) + 12^s 12(s - 1) + 16^s 12(s - 1)) \right]
\]
Figure 3: Comparison of $E_{GA}$ and $E_{ABC}$ for MON$_1$.

Figure 4: Comparison of $E_{R_1}$, $E_{R_{1/2}}$, $E_{R_{1}}$, and $E_{R_{1/2}}$ for MON$_1$.

Figure 5: Comparison of $E_{SC_1}$, $E_{SC_2}$, $E_{SC_1}$, and $E_{SC_{1/2}}$ for MON$_1$. 
Figure 6: Comparison of $E_{GA}$ and $E_{ABC}$ for MON$_2$.

Figure 7: Comparison of $E_{R1}$, $E_{R1/2}$, $E_{R1}$, and $E_{R1/2}$ for s.

Figure 8: Comparison of $E_{SC1}$, $E_{SC2}$, $E_{SC1/2}$, and $E_{SC1/2}$ for MON$_2$. 
which is our required expression.

**Theorem 12.** Let $MON_2$ be a second $MON$ with $s \geq 2$ and $E_{SCs}$ is the general sum connectivity entropy. Then,

$$E_{SCs}(MON_2) = \log[5^612(s + 2) + 6^612(s + 1) + 6^624(s - 1) + 7^612(s - 1) + 8^612(s - 1) - \log(5^{612}(s + 2) + 6^{612}(s + 1) + 6^{624}(s - 1) + 7^{612}(s - 1) + \sum_{\lambda = 1}^{s - 1} (8^{612}(s - 1)\lambda)]$$

$$= \log[5^{612}(s + 2) + 6^{612}(s + 1) + 6^{624}(s - 1) + 7^{612}(s - 1) + 8^{612}(s - 1) - \log(5^{612}(s + 2) + 6^{612}(s + 1) + 6^{624}(s - 1) + 7^{612}(s - 1) + \sum_{\lambda = 1}^{s - 1} (8^{612}(s - 1)\lambda)]$$

**Proof.** The expression of the topological invariant of the general sum connectivity index is given by Eq. 4, and the result of this index for the network $MON_1$ is given in Theorem 4. Now, to investigate the general sum connectivity entropy for the structure $MON_1$, using Eq. 4 and edge partition from Table 2 in the expression of general sum connectivity entropy $E_{SCs}$, which is defined in Eq. 9, we will achieve the desired expression as follows:

$$E_{SCs}(MON_2) = \log[5^{612}(s + 2) + 6^{612}(s + 1) + 6^{624}(s - 1) + 7^{612}(s - 1) + 8^{612}(s - 1) - \log(5^{612}(s + 2) + 6^{612}(s + 1) + 6^{624}(s - 1) + 7^{612}(s - 1) + \sum_{\lambda = 1}^{s - 1} (8^{612}(s - 1)\lambda)]$$

which is our required result.

5 Discussion and comparison

Since edge-weighted entropy is widely used in many fields of science, including chemistry, biology, pharmaceuticals, and computers, chemists benefit from the numerical and graphical display of these estimated outcomes. In this section, we have numerically determined some important edge-weighted entropies for ten values of parameter of networks $MON_1$ and $MON_2$ by using the above new results (Tables 3 and 4). We can clearly see that when the $s$ value increases, all the values of entropies are in ascending order. Graphical comparisons between entropies are presented in Figures 3–8.

6 Conclusion

We have investigated the edge-weighted entropies: geometric arithmetic entropy, ABC entropy, general Randic' entropy, and general sum connectivity entropy for the $MON_1$ and $MON_2$ structures. We also calculated numerical values of these entropies in Tables 3 and 4. By using these tables, we established Figures 3–8 for a comparison that are very useful for the physico-chemical properties of MONs. Researchers can obtain the remaining graph entropies for MONs and other chemical structures as a future project.

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**Conflict of interest:** Authors state no conflict of interest.

**Data availability statement:** The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

**References**


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