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# Characterization of entropy measures with connection number based indices of boric acid hydrogen-bonded 2D lattice sheets

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The cut method is a computational approach utilized to predict the fundamental activities of physicochemical properties of chemical networks, also called topological indices. The connection number is a new idea, that gives interesting and good results of the topological indices (TIs) and entropy measures (EMs) for structural representation of chemical compounds and networks. The physical density of chemical networks is characterized by these indices. In this paper, we determined the computational results for indices based on connection numbers for a two-dimensional lattice sheet of hydrogen-bonded boric acid. Boric acid, an inorganic compound, is not very harmful when applied to the skin or consumed. Finally, graphical and numerical comparisons of topological numbers including the number of borate hydrogen-bonded double lattice forms are also included in this study.

**Keywords** Connection numbers, Entropy measures, Topological indices, Boric acid hydrogen-bonded 2D lattice sheet

In mathematical chemistry, chemical graph theory uses graph theory to explore the topological structure or networks of chemical compounds. Chemical graph theory is fruitful in many areas of mathematical chemistry. Atoms and their bonds in a chemical structure are represented by the vertices and edges of the chemical graph, respectively. Graph theory is crucial for predicting molecular structure using the Topological Index (TI)<sup>1</sup>. TI's research is important for drug research and provides insight into molecular behaviour and properties. These parameters derived from molecular imaging provide a numerical approximation of specific molecular features that are non-uniform in image migration. Their importance lies in the ability to measure the difference between physical or chemical processes based on changes in molecular structure. The TI's assist in the numerical evaluation of molecular structures, providing a real way to measure physicochemical and structural properties prior to compound production<sup>2</sup>. By examining changes in index values, researchers can capture connections or expectations between molecular structures and desired functions or properties, such as mutagenicity or carcinogenicity, given by<sup>3</sup>.

The hypothetical work has significant ability to streamline drug design processes, identifying potent anti-HIV agents<sup>4</sup>, anti-cancer compounds<sup>5</sup>, lowering support on costly trial-and-error synthesis approaches. The flexibility of topological indices increases theoretical explorations, advancing in organic synthesis planning, compound classification, and bioactivity estimations. While these techniques have indicated varying degrees of success, ongoing innovations in chemical and topological knowledge, linked with the incorporation of information technology, are estimated to improve their reliability and efficiency in the future.

This article related with the application of entropy measures and other topological indices in molecular descriptors to assess structure-function relationships of different molecules and materials. It discusses recent improvements in entropy measures and their connection with other topological indices, such as information theoretic indices. The aim is to determine the appropriate topological indices and their entropy measures for some molecular structures. Graphs are very important for characterizing and studying molecules and atoms, with vertices and edges, denoting atoms and bonds. The analysis of graph complication via entropy has been

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considered by various disciplines, including computer science, statistical physics, chemistry, and life sciences. Entropy measures have been used in several research areas, including chemical sciences, mathematical information theory, social sciences, ecology, health sciences, and genetics.

The Randic index—formerly known as the branching index—is especially helpful for determining how much a saturated hydrocarbon's carbon atom framework is branching. The first and second Zagreb indices were first introduced in<sup>6</sup> by Gutman and Transjistic, who utilized them to explain branching problems. The study of chirality<sup>7</sup>, molecular complexity<sup>8,9</sup>, ZE isomerism<sup>10</sup>, and benzenoid hydrocarbons<sup>11</sup> includes the fields in which these Zagreb indices and their different types are used. Furthermore, the overall Zagreb indices are used to find multilinear regression models<sup>12,13</sup>. According to<sup>14,15</sup>, the connection between the *ABC* index and the thermodynamic properties of alkanes are considerable. To learn more about the calculation of graph topological indices, see<sup>16–19</sup>.

Recently a new concept, the connection number based indices are introduced and the researchers have started working on these connection number based TIs rapidly. Tang et al.<sup>20</sup> and Ali et al.<sup>21</sup> determined exact values of connection number based indices and their modified versions for subdivision-related operations on graphs. Cao et al.<sup>22</sup> gave the upper bounds for connection based Zagreb indices of product-related graphs. Ahmad et al.<sup>23</sup> exact values of connection number based indices for Backbone DNA Networks. The connection number based indices for cellular neural networks<sup>24</sup>, wheel related graphs<sup>25</sup>, triangular chain structures<sup>26</sup> and Skin Cancer Drugs<sup>27</sup> are calculated. Further article related to connection number indices are listed in<sup>28–30</sup>.

In the discipline of topological indices, entropy measures are being used more and more because they provide practical information on the information content and fundamental complexity of molecular networks<sup>31</sup>. The measurement of fundamental complexity and multiplicity in molecular graphs is one of the most familiar utilities of entropy measures in topological indices<sup>32</sup>. The degree of disorder or uncertainty in molecular structures can be determined using entropy-based indices; this degree of uncertainty is normally associated with properties like molecular stability, reactivity, and biological activity<sup>33</sup>. Several entropy metrics have been particularly constructed to be used with topological indices<sup>34</sup>. Additionally, entropy metrics in topological indices are helpful in a variety of fields, including bioinformatics, materials science, chemoinformatics, and drug discovery, see<sup>35–37</sup>. The concept of entropy was introduced by Chen et al.<sup>38</sup>, and is defined as

$$ENT_{\Omega} = \sum_{\wp \Im \in E(G)} \frac{\Omega(\wp \Im)}{\sum_{\wp \Im \in E(G)} \Omega(\wp \Im)} \log \left\{ \frac{\Omega(\wp \Im)}{\sum_{\wp \Im \in E(G)} \Omega(\wp \Im)} \right\}. \quad (1.1)$$

1. The first Zagreb connection index entropy: if  $\Omega(\wp \Im) = (\xi_{\wp} + \xi_{\Im})$ . Then

$$FZCI(G) = \sum_{\wp \Im \in E(G)} (\xi_{\wp} + \xi_{\Im}) = \sum_{\wp \Im \in E(G)} \Omega(\wp \Im), \quad (1.2)$$

By using this equation in Eq. (1.1), we get the first Zagreb connection index entropy:

$$ENT_{FZCI(G)} = \log(FZCI(G)) - \frac{1}{FZCI(G)} \log \left\{ \prod_{\wp \Im \in E(G)} [\xi_{\wp} + \xi_{\Im}]^{\xi_{\wp} + \xi_{\Im}} \right\}. \quad (1.3)$$

2. The second Zagreb connection index entropy: if  $\Omega(\wp \Im) = (\xi_{\wp} \times \xi_{\Im})$ . Then

$$SZCI(G) = \sum_{\wp \Im \in E(G)} (\xi_{\wp} \times \xi_{\Im}) = \sum_{\wp \Im \in E(G)} \Omega(\wp \Im), \quad (1.4)$$

By using this equation in Eq. (1.1), we get the second Zagreb connection index entropy:

$$ENT_{SZCI(G)} = \log(SZCI(G)) - \frac{1}{SZCI(G)} \log \left\{ \prod_{\wp \Im \in E(G)} [\xi_{\wp} \times \xi_{\Im}]^{\xi_{\wp} \times \xi_{\Im}} \right\}. \quad (1.5)$$

The remaining entropies were found in<sup>34,39</sup>, that are defined as:

3. The Randić connection index entropy: if  $\Omega(\wp \Im) = \left( \frac{1}{\sqrt{\xi_{\wp} \times \xi_{\Im}}} \right)$ . Then

$$RC(G) = \sum_{\wp\mathfrak{Z} \in E(G)} \left( \frac{1}{\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}} \right) = \sum_{\wp\mathfrak{Z} \in E(G)} \Omega(\wp\mathfrak{Z}), \quad (1.6)$$

By using this equation in Eq. (1.1), we get the Randić connection index entropy:

$$ENT_{RC(G)} = \log(RC(G)) - \frac{1}{RC(G)} \log \left\{ \prod_{\wp\mathfrak{Z} \in E(G)} \left[ \frac{1}{\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}} \right]^{\frac{1}{\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}} \right\}. \quad (1.7)$$

4. The sum connectivity connection index entropy: if  $\Omega(\wp\mathfrak{Z}) = \left( \frac{1}{\sqrt{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right)$ . Then

$$SCCI(G) = \sum_{\wp\mathfrak{Z} \in E(G)} \left( \frac{1}{\sqrt{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right) = \sum_{\wp\mathfrak{Z} \in E(G)} \Omega(\wp\mathfrak{Z}), \quad (1.8)$$

By using this equation in Eq. (1.1), we get the sum connectivity connection index entropy:

$$ENT_{SCCI(G)} = \log(SCCI(G)) - \frac{1}{SCCI(G)} \log \left\{ \prod_{\wp\mathfrak{Z} \in E(G)} \left( \frac{1}{\sqrt{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right)^{\frac{1}{\sqrt{\xi_{\wp} + \xi_{\mathfrak{Z}}}}} \right\}. \quad (1.9)$$

5. The atom-bond connectivity connection index entropy: if  $\Omega(\wp\mathfrak{Z}) = \sqrt{\frac{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2}{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}$ . Then

$$ABCCI(G) = \sum_{\wp\mathfrak{Z} \in E(G)} \sqrt{\frac{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2}{\xi_{\wp} \times \xi_{\mathfrak{Z}}}} = \sum_{\wp\mathfrak{Z} \in E(G)} \Omega(\wp\mathfrak{Z}), \quad (1.10)$$

By using this equation in Eq. (1.1), we get the atom-bond connectivity connection index entropy:

$$ENT_{ABCCI(G)} = \log(ABCCI(G)) - \frac{1}{ABCCI(G)} \log \left\{ \prod_{\wp\mathfrak{Z} \in E(G)} \left( \sqrt{\frac{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2}{\xi_{\wp} \times \xi_{\mathfrak{Z}}}} \right)^{\sqrt{\frac{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2}{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}} \right\}. \quad (1.11)$$

6. The geometric-arithmetic connection index entropy: if  $\Omega(\wp\mathfrak{Z}) = \frac{2\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}}$ . Then

$$GACI(G) = \sum_{\wp\mathfrak{Z} \in E(G)} \frac{2\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}} = \sum_{\wp\mathfrak{Z} \in E(G)} \Omega(\wp\mathfrak{Z}), \quad (1.12)$$

By using this equation in Eq. (1.1), we get the geometric-arithmetic connection index entropy:

$$ENT_{GACI(G)} = \log(GACI(G)) - \frac{1}{GACI(G)} \log \left\{ \prod_{\wp\mathfrak{Z} \in E(G)} \left( \frac{2\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}} \right)^{\frac{2\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right\}. \quad (1.13)$$

7. the augmented Zagreb connection index entropy: if  $\Omega(\wp\mathfrak{Z}) = \left( \frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2} \right)^3$ . Then

$$AZCI(G) = \sum_{\wp\mathfrak{Z} \in E(G)} \left( \frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2} \right)^3 = \sum_{\wp\mathfrak{Z} \in E(G)} \Omega(\wp\mathfrak{Z}), \quad (1.14)$$

By using this equation in Eq. (1.1), we get the augmented Zagreb connection index entropy:

$$ENT_{AZCI(G)} = \log(AZCI(G)) - \frac{1}{AZCI(G)} \log \left\{ \prod_{\wp \Im \in E(G)} \left( \left( \frac{\xi_{\wp} \times \xi_{\Im}}{\xi_{\wp} + \xi_{\Im} - 2} \right)^3 \left( \frac{\xi_{\wp} \times \xi_{\Im}}{\xi_{\wp} + \xi_{\Im} - 2} \right)^3 \right) \right\}. \quad (1.15)$$

8. The symmetric division degree connection index entropy: if  $\Omega(\wp \Im) = \left( \frac{\xi_{\wp}^2 + \xi_{\Im}^2}{\xi_{\wp} \times \xi_{\Im}} \right)$ . Then

$$SDDCI(G) = \sum_{\wp \Im \in E(G)} \left( \frac{\xi_{\wp}^2 + \xi_{\Im}^2}{\xi_{\wp} \times \xi_{\Im}} \right) = \sum_{\wp \Im \in E(G)} \Omega(\wp \Im), \quad (1.16)$$

By using this equation in Eq. (1.1), we get the symmetric division degree connection index entropy:

$$ENT_{SDDCI(G)} = \log(SDDCI(G)) - \frac{1}{SDDCI(G)} \log \left\{ \prod_{\wp \Im \in E(G)} \left( \frac{\xi_{\wp}^2 + \xi_{\Im}^2}{\xi_{\wp} \times \xi_{\Im}} \right)^{\frac{\xi_{\wp}^2 + \xi_{\Im}^2}{\xi_{\wp} \times \xi_{\Im}}} \right\}. \quad (1.17)$$

9. The harmonic connection index entropy: if  $\Omega(\wp \Im) = \left( \frac{2}{\xi_{\wp} + \xi_{\Im}} \right)$ . Then

$$HCI(G) = \sum_{\wp \Im \in E(G)} \left( \frac{2}{\xi_{\wp} + \xi_{\Im}} \right) = \sum_{\wp \Im \in E(G)} \Omega(\wp \Im), \quad (1.18)$$

By using this equation in Eq. (1.1), we get the harmonic connection index entropy:

$$ENT_{HCI(G)} = \log(HCI(G)) - \frac{1}{HCI(G)} \log \left\{ \prod_{\wp \Im \in E(G)} \left( \frac{2}{\xi_{\wp} + \xi_{\Im}} \right)^{\frac{2}{\xi_{\wp} + \xi_{\Im}}} \right\}. \quad (1.19)$$

10. The inverse sum connection index entropy: if  $\Omega(\wp \Im) = \left( \frac{\xi_{\wp} \times \xi_{\Im}}{\xi_{\wp} + \xi_{\Im}} \right)$ . Then

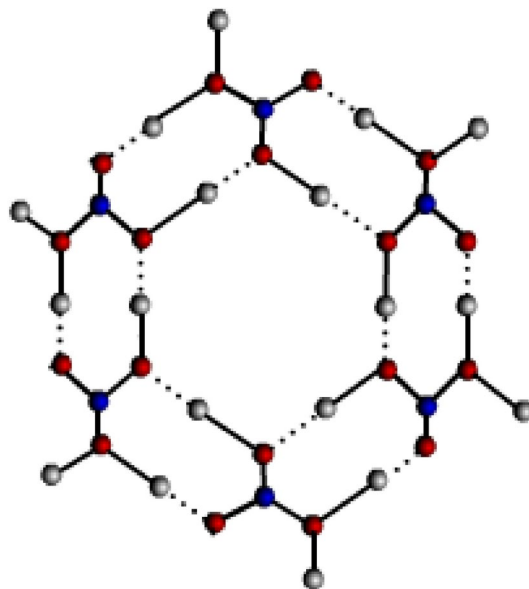
$$ISCI(G) = \sum_{\wp \Im \in E(G)} \left( \frac{\xi_{\wp} \times \xi_{\Im}}{\xi_{\wp} + \xi_{\Im}} \right) = \sum_{\wp \Im \in E(G)} \Omega(\wp \Im), \quad (1.20)$$

By using this equation in Eq. (1.1), we get the inverse sum connection index entropy:

$$ENT_{ISCI(G)} = \log(ISCI(G)) - \frac{1}{ISCI(G)} \log \left\{ \prod_{\wp \Im \in E(G)} \left( \frac{\xi_{\wp} \times \xi_{\Im}}{\xi_{\wp} + \xi_{\Im}} \right)^{\frac{\xi_{\wp} \times \xi_{\Im}}{\xi_{\wp} + \xi_{\Im}}} \right\}. \quad (1.21)$$

## Main results

In this study, we determined the TIs and entropy measures based on connection numbers for the structure of boric acid. Boric acid, is well known an inorganic compound used for cleaning and food preservation, its chemical formula  $H_3BO_3$  or  $B(OH)_3$ , also known by several names such as orthoboric acid, boracic acid, hydrogen borate, and acidum boricum, it has been utilized since ancient Greece<sup>40,41</sup>. This flexible material is used in many different productions, such as the production of jewellery, LCD displays, nuclear reactors, pH-regulating buffers in swimming pools, lubricants and flame retardants. The importance of boric acid in the discipline of inorganic chemistry cannot be exaggerated<sup>40,41</sup>. The solubility of the chemical is significantly influenced by temperature. In order to control neutron reactivity in the core of the reactor, boric acid is dissolved in the reactor coolant and acts as a soluble neutron absorber, soluble poison, or chemical shim<sup>42</sup>. The existence of a high boron level shows the commencement of a fuel cycle and acts to balance additional reactivity within the core<sup>43</sup>. Fuel burn-up, temperature changes, core reactivity, and the build-up of additional poisons such as xenon and samarium all influence to the quantity being decreased throughout the fuel cycle<sup>44</sup>. The first crystals of boric acid were constructed by Wilhelm Hornberg in 1702, who named it sal sedativum Hombergi (sedative salt of Hornberg).



**Fig. 1.** Unit cell of boric acid hydrogen-bonded 2D lattice sheets.

$(\xi_\varphi, \xi_\mathfrak{S})$	No. of Edges
(2,3)	$2p + 4q + 2$
(3,3)	$2p + 6q + 6$
(3,4)	$4p + 4q - 4$
(3,5)	$4p + 8q + 4$
(4,4)	$24pq + 2p + 6q - 6$
(4,5)	$2p + 4q + 2$
(4,6)	$12pq - 6$

**Table 1.** The edge partition of  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$  based on the connection numbers of the end vertices.

In the construction of boric acid, planar  $\text{BO}_3$  units are bonded by hydrogen bonds, forming a polymeric layer structure, boric acid is considered as a 2D sheet in the Fig. 2, for further detail<sup>45</sup>.

In this section, we computed topological indices for the boric acid hydrogen-bonded 2D lattice sheets using the data from the edge partition with connection numbers. The Fig. 1 is a graph of Unit cell boric acid hydrogen-bonded 2D lattice sheets. Let the graph  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$  be a boric acid hydrogen-bonded 2D lattice sheets with  $E_{\varphi,\mathfrak{S}}$  are edges with end vertices have connection number  $\xi_\varphi$  and  $\xi_\mathfrak{S}$ . The order and size of the graph  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$  are  $28pq + 14p + 28q$  and  $36pq + 16p + 32q - 2$ . We partitioned the edges based on the connection numbers of the end vertices are as follows: 2, 3; 3, 3; 3, 4; 3, 5; 4, 4; 4, 5; 4, 6. Now, we determine the cardinalities of these edge partitions. The number of edges of each type  $(\xi_\varphi, \xi_\mathfrak{S})$  are shown in Table 1

### Topological indices

By using the values of Table 1, the first Zagreb connection index calculated as:

$$\begin{aligned}
 FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) &= \sum_{\varphi\mathfrak{S} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} (\xi_\varphi + \xi_\mathfrak{S}) \\
 &= (2p + 4q + 2)(2 + 3) + (2p + 6q + 6)(3 + 3) + (4p + 4q - 4)(3 + 4) + (4p + 8q + 4)(3 + 5) \\
 &\quad + (24pq + 2p + 6q - 6)(4 + 4) + (2p + 4q + 2)(4 + 5) + (12pq - 6)(4 + 6) \\
 &= 312pq + 116p + 232q - 40
 \end{aligned} \tag{2.22}$$

By using the values of Table 1, the second Zagreb connection index calculated as:

$$\begin{aligned}
SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} (\xi_{\wp} \times \xi_{\mathfrak{Z}}) \\
&= (2p+4q+2)(2 \times 3) + (2p+6q+6)(3 \times 3) + (4p+4q-4)(3 \times 4) + (4p+8q+4)(3 \times 5) \\
&\quad + (24pq+2p+6q-6)(4 \times 4) + (2p+4q+2)(4 \times 5) + (12pq-6)(4 \times 6) \\
&= 672pq + 210p + 422q - 122
\end{aligned} \tag{2.23}$$

By using the values of Table 1, the Randić connection index calculated as:

$$\begin{aligned}
RC(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \left( \frac{1}{\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}} \right) \\
&= (2p+4q+2)\left(\frac{1}{\sqrt{2 \times 3}}\right) + (2p+6q+6)\left(\frac{1}{\sqrt{3 \times 3}}\right) + (4p+4q-4)\left(\frac{1}{\sqrt{3 \times 4}}\right) + (4p+8q+4)\left(\frac{1}{\sqrt{3 \times 5}}\right) \\
&\quad + (24pq+2p+6q-6)\left(\frac{1}{\sqrt{4 \times 4}}\right) + (2p+4q+2)\left(\frac{1}{\sqrt{4 \times 5}}\right) + (12pq-6)\left(\frac{1}{\sqrt{4 \times 6}}\right) \\
&= \left(6 + \frac{4\sqrt{6}}{3}\right)pq + \left(\frac{\sqrt{6}}{3} + \frac{7}{6} + \frac{2\sqrt{3}}{3} + \frac{4\sqrt{15}}{15} + \frac{\sqrt{5}}{5}\right)p + \left(\frac{2\sqrt{6}}{3} + \frac{7}{2} + \frac{2\sqrt{3}}{3} + \frac{8\sqrt{15}}{15} + \frac{2\sqrt{5}}{5}\right)q \\
&\quad - \frac{\sqrt{6}}{6} + \frac{1}{2} - \frac{2\sqrt{3}}{3} + \frac{4\sqrt{15}}{15} + \frac{\sqrt{5}}{5} \\
&= 8.4495pq + 4.6179p + 9.2477q + 0.41702
\end{aligned} \tag{2.24}$$

By using the values of Table 1, the sum Connectivity connection index calculated as:

$$\begin{aligned}
SCCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \left( \frac{1}{\sqrt{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right) \\
&= (2p+4q+2)\left(\frac{1}{\sqrt{2+3}}\right) + (2p+6q+6)\left(\frac{1}{\sqrt{3+3}}\right) + (4p+4q-4)\left(\frac{1}{\sqrt{3+4}}\right) + (4p+8q+4)\left(\frac{1}{\sqrt{3+5}}\right) \\
&\quad + (24pq+2p+6q-6)\left(\frac{1}{\sqrt{4+4}}\right) + (2p+4q+2)\left(\frac{1}{\sqrt{4+5}}\right) + (12pq-6)\left(\frac{1}{\sqrt{4+6}}\right) \\
&= \left(6\sqrt{2} + \frac{8\sqrt{10}}{5}\right)pq + \left(\frac{2\sqrt{5}}{5} + \frac{\sqrt{6}}{3} + \frac{4\sqrt{7}}{7} + \frac{3\sqrt{2}}{2} + \frac{2}{3}\right)p + \left(\frac{4\sqrt{5}}{5} + \sqrt{6} + \frac{4\sqrt{7}}{7} + \frac{7\sqrt{2}}{2} + \frac{4}{3}\right)q \\
&\quad + \frac{2\sqrt{5}}{5} + \sqrt{6} - \frac{4\sqrt{7}}{7} - \frac{\sqrt{2}}{2} + \frac{2}{3} - \frac{3\sqrt{10}}{5} \\
&= 12.280015pq + 6.0108p + 12.033q - 0.1058
\end{aligned} \tag{2.25}$$

By using the values of Table 1, the atom-bond connectivity connection index calculated as:

$$\begin{aligned}
ABCCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \sqrt{\frac{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2}{\xi_{\wp} \times \xi_{\mathfrak{Z}}}} \\
&= (2p+4q+2)\sqrt{\frac{2+3-2}{2 \times 3}} + (2p+6q+6)\sqrt{\frac{3+3-2}{3 \times 3}} + (4p+4q-4)\sqrt{\frac{3+4-2}{3 \times 4}} \\
&\quad + (4p+8q+4)\sqrt{\frac{3+5-2}{3 \times 5}} + (24pq+2p+6q-6)\sqrt{\frac{4+4-2}{4 \times 4}} + (2p+4q+2)\sqrt{\frac{4+5-2}{4 \times 5}} \\
&\quad + (12pq-6)\sqrt{\frac{4+6-2}{4 \times 6}} \\
&= \left(6\sqrt{6} + \frac{16\sqrt{3}}{3}\right)pq + \left(\sqrt{2} + \frac{4}{3} + \frac{2\sqrt{15}}{3} + \frac{4\sqrt{10}}{5} + \frac{\sqrt{6}}{2} + \frac{\sqrt{35}}{5}\right)p \\
&\quad + \left(2\sqrt{2} + 4 + \frac{2\sqrt{15}}{3} + \frac{8\sqrt{10}}{5} + \frac{3\sqrt{6}}{2} + \frac{2\sqrt{35}}{5}\right)q + \sqrt{2} + 4 - \frac{2\sqrt{15}}{3} + \frac{4\sqrt{10}}{5} - \frac{3\sqrt{6}}{2} + \frac{\sqrt{35}}{5} - 2\sqrt{3} \\
&= 21.6251pq + 10.267p + 20.510q - 0.5932
\end{aligned} \tag{2.26}$$

By using the values of Table 1, the Geometric-arithmetic connection index calculated as:

$$\begin{aligned}
GACI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \frac{2\sqrt{\xi_{\wp} \times \xi_{\mathfrak{Z}}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}} \\
&= (2p+4q+2)\left(\frac{2\sqrt{2 \times 3}}{2+3}\right) + (2p+6q+6)\left(\frac{2\sqrt{3 \times 3}}{3+3}\right) + (4p+4q-4)\left(\frac{2\sqrt{3 \times 4}}{3+4}\right) \\
&\quad + (4p+8q+4)\left(\frac{2\sqrt{3 \times 5}}{3+5}\right) + (24pq+2p+6q-6)\left(\frac{2\sqrt{4 \times 4}}{4+4}\right) + (2p+4q+2)\left(\frac{2\sqrt{4 \times 5}}{4+5}\right) \\
&\quad + (12pq-6)\left(\frac{2\sqrt{4 \times 6}}{4+6}\right) \\
&= \left(24 + \frac{32\sqrt{6}}{5}\right)pq + \left(\frac{4\sqrt{6}}{5} + 4 + \frac{16\sqrt{3}}{7} + \sqrt{15} + \frac{8\sqrt{5}}{9}\right)p + \left(\frac{8\sqrt{6}}{5} + 12 + \frac{16\sqrt{3}}{7} + 2\sqrt{15} + \frac{16\sqrt{5}}{9}\right)q \\
&\quad - \frac{8\sqrt{6}}{5} - \frac{16\sqrt{3}}{7} + \sqrt{15} + \frac{8\sqrt{5}}{9} \\
&= 35.7576pq + 15.780p + 31.599q - 2.0177
\end{aligned} \tag{2.27}$$

By using the values of Table 1, the augmented Zagreb connection index calculated as:

$$\begin{aligned}
AZCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \left(\frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}} - 2}\right)^3 \\
&= (2p+4q+2)\left(\frac{2 \times 3}{2+3-2}\right)^3 + (2p+6q+6)\left(\frac{3 \times 3}{3+3-2}\right)^3 + (4p+4q-4)\left(\frac{3 \times 4}{3+4-2}\right)^3 \\
&\quad + (4p+8q+4)\left(\frac{3 \times 5}{3+5-2}\right)^3 + (24pq+2p+6q-6)\left(\frac{4 \times 4}{4+4-2}\right)^3 + (2p+4q+2)\left(\frac{4 \times 5}{4+5-2}\right)^3 \\
&\quad + (12pq-6)\left(\frac{4 \times 6}{4+6-2}\right)^3 \\
&= \frac{7984}{9}pq + \frac{8933175649}{37044000}p + \frac{6022267633}{12348000}q - \frac{1698872383}{12348000} \\
&= 779.1111pq + 241.15p + 487.71q - 137.58
\end{aligned} \tag{2.28}$$

By using the values of Table 1, the symmetric division degree connection index calculated as:

$$\begin{aligned}
SDDCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \left(\frac{\xi_{\wp}^2 + \xi_{\mathfrak{Z}}^2}{\xi_{\wp} \times \xi_{\mathfrak{Z}}}\right) \\
&= (2p+4q+2)\left(\frac{2^2+3^2}{2 \times 3}\right) + (2p+6q+6)\left(\frac{3^2+3^2}{3 \times 3}\right) + (4p+4q-4)\left(\frac{3^2+4^2}{3 \times 4}\right) \\
&\quad + (4p+8q+4)\left(\frac{3^2+5^2}{3 \times 5}\right) + (24pq+2p+6q-6)\left(\frac{4^2+4^2}{4 \times 4}\right) + (2p+4q+28)\left(\frac{4^2+5^2}{4 \times 5}\right) \\
&\quad + (12pq-6)\left(\frac{5^2+5^2}{4 \times 6}\right) \\
&= \frac{248}{3}pq + \frac{203}{6}p + \frac{202}{3}q - \frac{23}{6} = 74pq + 33.833p + 67.333q - 3.8333
\end{aligned} \tag{2.29}$$

By using the values of Table 1, the harmonic connection index calculated as:

$$\begin{aligned}
HCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \left(\frac{2}{\xi_{\wp} + \xi_{\mathfrak{Z}}}\right) \\
&= (2p+4q+2)\left(\frac{2}{2+3}\right) + (2p+6q+6)\left(\frac{2}{3+3}\right) + (4p+4q-4)\left(\frac{2}{3+4}\right) + (4p+8q+4)\left(\frac{2}{3+5}\right) \\
&\quad + (24pq+2p+6q-6)\left(\frac{2}{4+4}\right) + (2p+4q+2)\left(\frac{2}{4+5}\right) + (12pq-6)\left(\frac{2}{4+6}\right) \\
&= \frac{46}{5}pq + \frac{2869p}{630} + \frac{5753q}{630} + \frac{253}{630} = 8.4pq + 4.554p + 9.1317q + 0.40159
\end{aligned} \tag{2.30}$$

By using the values of Table 1, the inverse sum connection index calculated as:

$$\begin{aligned}
ISCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \sum_{\wp\mathfrak{Z} \in E(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \left(\frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}}\right) \\
&= (2p+4q+2)\left(\frac{2 \times 3}{2+3}\right) + (2p+6q+6)\left(\frac{3 \times 3}{3+3}\right) + (4p+4q-4)\left(\frac{3 \times 4}{3+4}\right) + (4p+8q+4)\left(\frac{3 \times 5}{3+5}\right) \\
&\quad + (24pq+2p+6q-6)\left(\frac{4 \times 4}{4+4}\right) + (2p+4q+2)\left(\frac{4 \times 5}{4+5}\right) + (12pq-6)\left(\frac{4 \times 6}{4+6}\right) \\
&= \frac{432}{5}pq + \frac{17767}{630}p + \frac{17812}{315}q - \frac{1249}{126} = 76.8pq + 28.202p + 56.546q - 9.9127
\end{aligned} \tag{2.31}$$

(p, q)	$FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$RC(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$SCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$ABCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$
(5, 5)	9500.0	19838.0	280.99	397.11	693.90
(6, 6)	13280.0	27862.0	387.80	550.23	962.57
(7, 7)	17684.0	37230.0	511.49	727.92	1274.6
(8, 8)	22712.0	47942.0	652.11	930.16	1629.6
(9, 9)	28364.0	59998.0	809.62	1157.0	2028.0
(10, 10)	34640.0	73398.0	984.03	1408.3	2469.7
(11, 11)	41540.0	88142.0	1175.3	1684.3	2954.6
(12, 12)	49064.0	104230.0	1383.5	1984.7	3482.7
(13, 13)	57212.0	121660.0	1608.5	2309.7	4054.1
(14, 14)	65984.0	140440.0	1850.7	2659.5	4668.7

**Table 2.** The numerical values of connection number-based TIs of  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$ .

(p, q)	$GACI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$AZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$SDDCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$HCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$	$ISCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})$
(5, 5)	1128.8	22985.0	2352.1	278.83	2333.8
(6, 6)	1569.6	32283.0	3267.2	384.91	3263.4
(7, 7)	2081.9	43141.0	4330.3	507.80	4346.5
(8, 8)	2665.5	55556.0	5541.6	647.48	5583.3
(9, 9)	3320.8	69529.0	6900.7	803.98	6973.6
(10, 10)	4047.6	85061.0	8407.8	977.26	8517.6
(11, 11)	4845.9	102150.0	10063.0	1167.4	10215.0
(12, 12)	5715.8	120790.0	11866.0	1374.2	12066.0
(13, 13)	6656.9	141000.0	13817.0	1597.9	14071.0
(14, 14)	7669.8	162780.0	15917.0	1838.4	16230.0

**Table 3.** The numerical values of connection number-based TIs of  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$ .

The numerical values of connection number-based of all above TIs for  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$  are shown in Tables 2 and 3 (Fig. 2).

Entropy measures

By putting the value of Eq. (2.22) in Eq. (1.3), we obtain the first Zagreb connection index entropy as:

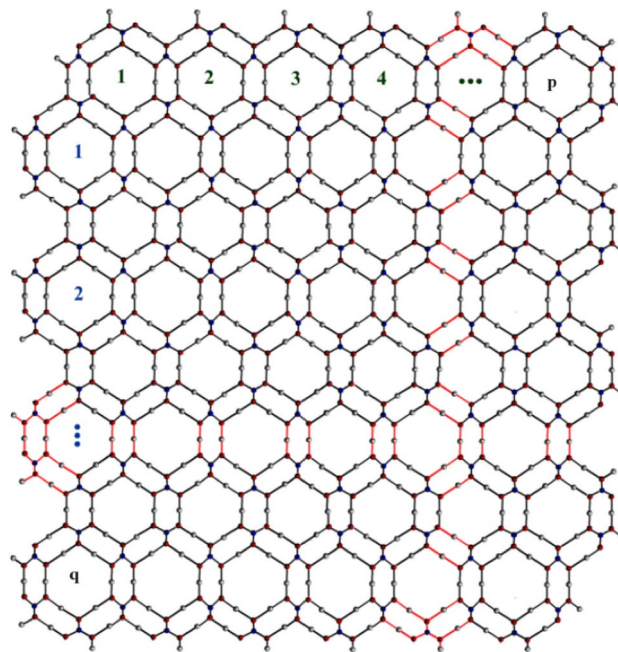
$$\begin{aligned} ENT_{FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} &= \log(FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})) - \frac{1}{FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} (\xi_{\wp} + \xi_{\mathfrak{Z}})^{(\xi_{\wp} + \xi_{\mathfrak{Z}})} \right\} \\ &= \log(312pq + 116p + 232q - 40) - \frac{1}{312pq + 116p + 232q - 40} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} (\xi_{\wp} + \xi_{\mathfrak{Z}})^{(\xi_{\wp} + \xi_{\mathfrak{Z}})} \right\} \\ &= \log(312pq + 116p + 232q - 40) - \frac{1}{312pq + 116p + 232q - 40} \log \left\{ 2^{73} 3^{24} 5^{15} 7^7 (p + 2q + 1)^3 \right. \\ &\quad \left. (p + 3q + 3)(p + q - 1)(12pq + p + 3q - 3)(8pq - 3) \right\} \end{aligned} \tag{2.32}$$

By putting the value of Eq. (2.23) in Eq. (1.5), we obtain the second Zagreb connection index entropy as:

$$\begin{aligned} ENT_{SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} &= \log(SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})) - \frac{1}{SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} (\xi_{\wp} \times \xi_{\mathfrak{Z}})^{(\xi_{\wp} \times \xi_{\mathfrak{Z}})} \right\} \\ &= \log(672pq + 210p + 422q - 122) - \frac{1}{672pq + 210p + 422q - 122} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} (\xi_{\wp} \times \xi_{\mathfrak{Z}})^{(\xi_{\wp} \times \xi_{\mathfrak{Z}})} \right\} \\ &= \log(672pq + 210p + 422q - 122) - \frac{1}{672pq + 210p + 422q - 122} \log \left\{ 2^{215} 3^{75} 5^{35} (p + 2q + 1)^3 \right. \\ &\quad \left. (p + 3q + 3)(p + q - 1)(12pq + p + 3q - 3)(8pq - 3) \right\} \end{aligned} \tag{2.33}$$

By putting the value of Eq. (2.24) in Eq. (1.7), we obtain the Randić connection index entropy as:





**Fig. 2.** Boric acid hydrogen-bonded 2D lattice sheets.

$$\begin{aligned}
 ENT_{RC}(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \log(RC(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})) - \frac{1}{RC(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \log \left\{ \prod_{\varphi \mathfrak{Z} \in E(G)} \left( \frac{1}{\sqrt{\xi_{\varphi} \times \xi_{\mathfrak{Z}}}} \right)^{\frac{1}{\sqrt{\xi_{\varphi} \times \xi_{\mathfrak{Z}}}}} \right\} \\
 &= \log(8.4495pq + 4.6179p + 9.2477q + 0.41702) \\
 &\quad - \frac{1}{8.4495pq + 4.6179p + 9.2477q + 0.41702} \log \left\{ \prod_{\varphi \mathfrak{Z} \in E(G)} \left( \frac{1}{\sqrt{\xi_{\varphi} \times \xi_{\mathfrak{Z}}}} \right)^{\frac{1}{\sqrt{\xi_{\varphi} \times \xi_{\mathfrak{Z}}}}} \right\} \quad (2.34) \\
 &= \log(8.4495pq + 4.6179p + 9.2477q + 0.41702) \\
 &\quad - \frac{1}{8.4495pq + 4.6179p + 9.2477q + 0.41702} \log \left\{ 44.352 (p + 2q + 1)^3 (p + 3q + 3) \right. \\
 &\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
 \end{aligned}$$

By putting the value of Eq. (2.25) in Eq. (1.9), we obtain the sum connectivity connection index entropy as:

$$\begin{aligned}
 ENT_{SCCI}(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \log(SCCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})) - \frac{1}{SCCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \log \left\{ \prod_{\varphi \mathfrak{Z} \in E(G)} \left( \frac{1}{\sqrt{\xi_{\varphi} + \xi_{\mathfrak{Z}}}} \right)^{\frac{1}{\sqrt{\xi_{\varphi} + \xi_{\mathfrak{Z}}}}} \right\} \\
 &= \log(12.280015pq + 6.0108p + 12.033q - 0.1058) \\
 &\quad - \frac{1}{12.280015pq + 6.0108p + 12.033q - 0.1058} \log \left\{ \prod_{\varphi \mathfrak{Z} \in E(G)} \left( \frac{1}{\sqrt{\xi_{\varphi} + \xi_{\mathfrak{Z}}}} \right)^{\frac{1}{\sqrt{\xi_{\varphi} + \xi_{\mathfrak{Z}}}}} \right\} \quad (2.35) \\
 &= \log(12.280015pq + 6.0108p + 12.033q - 0.1058) \\
 &\quad - \frac{1}{12.280015pq + 6.0108p + 12.033q - 0.1058} \log \left\{ 39.626752 (p + 2q + 1)^3 (p + 3q + 3) \right. \\
 &\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
 \end{aligned}$$

By putting the value of Eq. (2.26) in Eq. (1.11), we obtain the atom-bond connectivity connection index entropy as:

$$\begin{aligned}
ENT_{ABCCI}(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \log(ABCCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})) - \frac{1}{ABCCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \sqrt{\frac{\xi_\varphi + \xi_{\mathfrak{Z}} - 2}{\xi_\varphi \times \xi_{\mathfrak{Z}}}} \right)^{\sqrt{\frac{\xi_\varphi + \xi_{\mathfrak{Z}} - 2}{\xi_\varphi \times \xi_{\mathfrak{Z}}}}} \right\} \\
&= \log(21.6251pq + 10.267p + 20.510q - 0.5932) \\
&\quad - \frac{1}{21.6251pq + 10.267p + 20.510q - 0.5932} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \sqrt{\frac{\xi_\varphi + \xi_{\mathfrak{Z}} - 2}{\xi_\varphi \times \xi_{\mathfrak{Z}}}} \right)^{\sqrt{\frac{\xi_\varphi + \xi_{\mathfrak{Z}} - 2}{\xi_\varphi \times \xi_{\mathfrak{Z}}}}} \right\} \quad (2.36) \\
&= \log(21.6251pq + 10.267p + 20.510q - 0.5932) \\
&\quad - \frac{1}{21.6251pq + 10.267p + 20.510q - 0.5932} \log \left\{ 68.21376 (p + 2q + 1)^3 (p + 3q + 3) \right. \\
&\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
\end{aligned}$$

By putting the value of Eq. (2.27) in Eq. (1.13), we obtain the geometric-arithmetic connection index entropy as:

$$\begin{aligned}
ENT_{GACI}(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \log(GACI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})) - \frac{1}{GACI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \frac{2\sqrt{\xi_\varphi \times \xi_{\mathfrak{Z}}}}{\xi_\varphi + \xi_{\mathfrak{Z}}} \right)^{\frac{2\sqrt{\xi_\varphi \times \xi_{\mathfrak{Z}}}}{\xi_\varphi + \xi_{\mathfrak{Z}}}} \right\} \\
&= \log(35.7576pq + 15.780p + 31.599q - 2.0177) \\
&\quad - \frac{1}{35.7576pq + 15.780p + 31.599q - 2.0177} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \frac{2\sqrt{\xi_\varphi \times \xi_{\mathfrak{Z}}}}{\xi_\varphi + \xi_{\mathfrak{Z}}} \right)^{\frac{2\sqrt{\xi_\varphi \times \xi_{\mathfrak{Z}}}}{\xi_\varphi + \xi_{\mathfrak{Z}}}} \right\} \quad (2.37) \\
&= \log(35.7576pq + 15.780p + 31.599q - 2.0177) \\
&\quad - \frac{1}{35.7576pq + 15.780p + 31.599q - 2.0177} \log \left\{ 469.06368 (p + 2q + 1)^3 (p + 3q + 3) \right. \\
&\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
\end{aligned}$$

By putting the value of Eq. (2.28) in Eq. (1.15), we obtain the augmented Zagreb connection index entropy as:

$$\begin{aligned}
ENT_{AZCI}(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \log(AZCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})) - \frac{1}{AZCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \left( \frac{\xi_\varphi \times \xi_{\mathfrak{Z}}}{\xi_\varphi + \xi_{\mathfrak{Z}} - 2} \right)^3 \right)^{\left( \frac{\xi_\varphi \times \xi_{\mathfrak{Z}}}{\xi_\varphi + \xi_{\mathfrak{Z}} - 2} \right)^3} \right\} \\
&= \log(779.1111pq + 241.15p + 487.71q - 137.58) \\
&\quad - \frac{1}{779.1111pq + 241.15p + 487.71q - 137.58} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \left( \frac{\xi_\varphi \times \xi_{\mathfrak{Z}}}{\xi_\varphi + \xi_{\mathfrak{Z}} - 2} \right)^3 \right)^{\left( \frac{\xi_\varphi \times \xi_{\mathfrak{Z}}}{\xi_\varphi + \xi_{\mathfrak{Z}} - 2} \right)^3} \right\} \quad (2.38) \\
&= \log(779.1111pq + 241.15p + 487.71q - 137.58) \\
&\quad - \frac{1}{779.1111pq + 241.15p + 487.71q - 137.58} \log \left\{ 1.4856704 \times 10^{151} (p + 2q + 1)^3 (p + 3q + 3) \right. \\
&\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
\end{aligned}$$

By putting the value of Eq. (2.29) in Eq. (1.17), we obtain the symmetric division degree connection index entropy as:

$$\begin{aligned}
ENT_{SDDCI}(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q}) &= \log(SDDCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})) - \frac{1}{SDDCI(\mathfrak{B}\mathfrak{A}\mathfrak{H}_{p,q})} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \frac{\xi_\varphi^2 + \xi_{\mathfrak{Z}}^2}{\xi_\varphi \times \xi_{\mathfrak{Z}}} \right)^{\frac{\xi_\varphi^2 + \xi_{\mathfrak{Z}}^2}{\xi_\varphi \times \xi_{\mathfrak{Z}}}} \right\} \\
&= \log(74pq + 33.833p + 67.333q - 3.8333) \\
&\quad - \frac{1}{74pq + 33.833p + 67.333q - 3.8333} \log \left\{ \prod_{\varphi\mathfrak{Z} \in E(G)} \left( \frac{\xi_\varphi^2 + \xi_{\mathfrak{Z}}^2}{\xi_\varphi \times \xi_{\mathfrak{Z}}} \right)^{\frac{\xi_\varphi^2 + \xi_{\mathfrak{Z}}^2}{\xi_\varphi \times \xi_{\mathfrak{Z}}}} \right\} \quad (2.39) \\
&= \log(74pq + 33.833p + 67.333q - 3.8333) \\
&\quad - \frac{1}{74pq + 33.833p + 67.333q - 3.8333} \log \left\{ 3.000617106 \times 10^7 (p + 2q + 1)^3 (p + 3q + 3) \right. \\
&\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
\end{aligned}$$

By putting the value of Eq. (2.30) in Eq. (1.19), we obtain the harmonic connection index entropy as:

$$\begin{aligned}
ENT_{HCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} &= \log(HCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})) - \frac{1}{HCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} \left( \frac{2}{\xi_{\wp} + \xi_{\mathfrak{Z}}} \right)^{\frac{2}{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right\} \\
&= \log(8.4pq + 4.554p + 9.1317q + 0.40159) \\
&\quad - \frac{1}{8.4pq + 4.554p + 9.1317q + 0.40159} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} \left( \frac{2}{\xi_{\wp} + \xi_{\mathfrak{Z}}} \right)^{\frac{2}{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right\} \\
&= \log(8.4pq + 4.554p + 9.1317q + 0.40159) \\
&\quad - \frac{1}{8.4pq + 4.554p + 9.1317q + 0.40159} \log \left\{ 44.632064 (p + 2q + 1)^3 (p + 3q + 3) \right. \\
&\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
\end{aligned} \tag{2.40}$$

By putting the value of Eq. (2.31) in Eq. (1.21), we obtain the inverse sum connection index entropy as:

$$\begin{aligned}
ENT_{ISCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} &= \log(ISCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})) - \frac{1}{ISCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} \left( \frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}} \right)^{\frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right\} \\
&= \log(76.8pq + 28.202p + 56.546q - 9.9127) \\
&\quad - \frac{1}{76.8pq + 28.202p + 56.546q - 9.9127} \log \left\{ \prod_{\wp \mathfrak{Z} \in E(G)} \left( \frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}} \right)^{\frac{\xi_{\wp} \times \xi_{\mathfrak{Z}}}{\xi_{\wp} + \xi_{\mathfrak{Z}}}} \right\} \\
&= \log(76.8pq + 28.202p + 56.546q - 9.9127) \\
&\quad - \frac{1}{76.8pq + 28.202p + 56.546q - 9.9127} \log \left\{ 1.8484736 \times 10^6 (p + 2q + 1)^3 (p + 3q + 3) \right. \\
&\quad \left. (p + q - 1) (12pq + p + 3q - 3) (8pq - 3) \right\}
\end{aligned} \tag{2.41}$$

## Conclusion

The hydrogen-bonded 2D lattice sheets of boric acid play an important role in its thermodynamic and entropic properties, that have a broad range of applications in materials/data science, catalysis, energy storage etc. The active character of hydrogen bonds in these sheets, along with the correlated entropy changes, make boric acid an stimulating material for further research in both theoretical and particles. In this article, we studied some well-known connection number-based topological indices and determined their entropies. The numerical values of these connection number-based entropy measures for  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$  are shown in Tables 4 and 5. From Tables 2 and 3, we observe that

$$\begin{aligned}
RC(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) &< SCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) < ABCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) < FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) < SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) \\
HCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) &< GACI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) < SDDCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) < ISCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}) < AZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})
\end{aligned}$$

From Tables 4 and 5, we observe that

$$\begin{aligned}
ENT_{RC(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} &< ENT_{SCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} < ENT_{ABCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} < ENT_{FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} < ENT_{SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} \\
ENT_{HCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} &< ENT_{GACI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} < ENT_{SDDCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} < ENT_{ISCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})} < ENT_{AZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})}
\end{aligned}$$

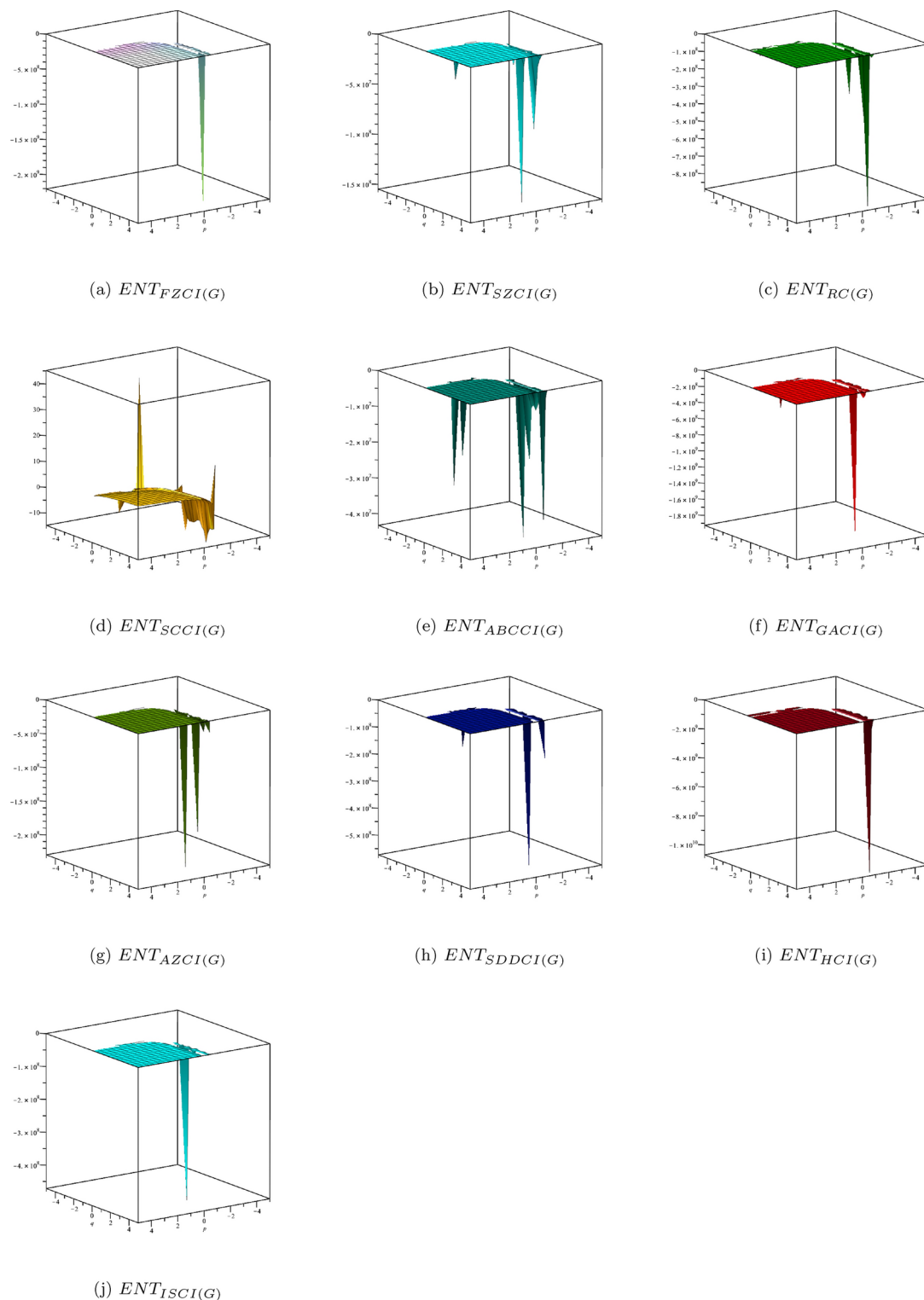
By Comparing the Tables 2, 3, 4 and 5, we can see that the greater the TIs, the entropy measure is greater. Also, the graphical representation of Entropy measures of the results are shown in Fig. 3.

(p, q)	$ENT_{FZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})}$	$ENT_{SZCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})}$	$ENT_{RC(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})}$	$ENT_{SCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})}$	$ENT_{ABCCI(\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q})}$
(5, 5)	9.1443	9.8796	5.5369	5.9208	6.5006
(6, 6)	9.4834	10.224	5.8829	6.2620	6.8379
(7, 7)	9.7723	10.517	6.1758	6.5520	7.1254
(8, 8)	10.025	10.771	6.4302	6.8044	7.3758
(9, 9)	10.248	10.997	6.6550	7.0279	7.5980
(10, 10)	10.449	11.200	6.8565	7.2284	7.7977
(11, 11)	10.630	11.383	7.0391	7.4105	7.9790
(12, 12)	10.798	11.551	7.2062	7.5771	8.1451
(13, 13)	10.952	11.706	7.3601	7.7308	8.2983
(14, 14)	11.095	11.851	7.5030	7.8734	8.4405

**Table 4.** The numerical values of connection number-based entropy measures of  $\mathfrak{B}\mathfrak{A}\mathfrak{S}_{p,q}$ .

$(p, q)$	$ENT_{GACI}(\mathfrak{B}\mathfrak{A}\mathfrak{N}_{p,q})$	$ENT_{AZCI}(\mathfrak{B}\mathfrak{A}\mathfrak{N}_{p,q})$	$ENT_{SDDCI}(\mathfrak{B}\mathfrak{A}\mathfrak{N}_{p,q})$	$ENT_{HCI}(\mathfrak{B}\mathfrak{A}\mathfrak{N}_{p,q})$	$ENT_{ISCI}(\mathfrak{B}\mathfrak{A}\mathfrak{N}_{p,q})$
(5, 5)	7.0016	10.027	7.7452	5.5284	7.7385
(6, 6)	7.3379	10.370	8.0784	5.8748	8.0780
(7, 7)	7.6248	10.663	8.3630	6.1682	8.3674
(8, 8)	7.8750	10.918	8.6117	6.4227	8.6198
(9, 9)	8.0972	11.145	8.8326	6.6477	8.8435
(10, 10)	8.2968	11.347	9.0312	6.8494	9.0446
(11, 11)	8.4781	11.530	9.2117	7.0320	9.2271
(12, 12)	8.6443	11.699	9.3772	7.1992	9.3942
(13, 13)	8.7975	11.854	9.5301	7.3533	9.5485
(14, 14)	8.9398	11.998	9.6719	7.4962	9.6916

**Table 5.** The numerical values of connection number-based entropy measures of  $\mathfrak{B}\mathfrak{A}\mathfrak{N}_{p,q}$ .



**Fig. 3.** Numerical values for different connection number based entropies, the data is taken from the Tables 2, 3, 4 and 5.

### Data availability

The datasets used and/or analysed during the current study available from the corresponding author on reasonable request.

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## References

- Azeem, M., Jamil, M. K. & Shang, Y. Notes on the localization of generalized hexagonal cellular networks. *Mathematics* **11**(4), article no. 844 (2023).
- Yasin, F. et al. Exploring physico-chemical properties of HIV/AIDS drugs using neighborhood topological indices of molecular graphs. *Discov. Appl. Sci.* **6**, 93. <https://doi.org/10.1007/s42452-024-05636-4> (2024).
- Al-Dayel, I., Nadeem, M. F. & Khan, M. A. Topological analysis of tetracyanobenzene metal-organic framework. *Sci. Rep.* **14**, 1789. <https://doi.org/10.1038/s41598-024-52194-1> (2024).
- Yu, G., Li, X. & He, D. Topological indices based on 2- or 3-eccentricity to predict anti-HIV activity. *Appl. Math. Comput.* **416**(1), 126748. <https://doi.org/10.1016/j.amc.2021.126748> (2022).
- Shanmukha, M. C., Basavarajappa, N. S., Shilpa, K. C. & Usha, A. Degree-based topological indices on anticancer drugs with QSPR analysis. *Heliyon* **6**(6), e04235. <https://doi.org/10.1016/j.heliyon.2020.e04235> (2020).
- Gutman, I. & Trinajstić, N. Graph theory and molecular orbitals: Total  $\pi$ -electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **17**(4), 535–538 (1972).
- Ullah, A., Jabeen, S., Zaman, S., Hamraz, A. & Meherban, S. Predictive potential of K-Banhatti and Zagreb type molecular descriptors in structure-property relationship analysis of some novel drug molecules. *J. Chin. Chem. Soc. [SPACE]* <https://doi.org/10.1002/jccs.202300450> (2023).
- Bertz, S. H. & Wright, W. F. The graph theory approach to synthetic analysis: Definition and application of molecular complexity and synthetic complexity. *Graph Theory Notes New York* **35**, 32–48 (1998).
- Meharban, S., Ullah, A., Zaman, S., Hamraz, A. & Razaq, A. Molecular structural modeling and physical characteristics of anti-breast cancer drugs via some novel topological descriptors and regression models. *Curr. Res. Struct. Biol.* **7**, 100134. <https://doi.org/10.1016/j.crstbi.2024.100134> (2024).
- Golbraikh, A., Bonchev, D. & Tropsha, A. Novel ZE-isomerism descriptors derived from molecular topology and their application to QSAR analysis. *J. Chem. Inf. Comput. Sci.* **42**(4), 769–787 (2002).
- Hayat, S. Distance-based graphical indices for predicting thermodynamic properties of benzenoid hydrocarbons with applications. *Comput. Mater. Sci.* **230**(25), 112492. <https://doi.org/10.1016/j.commatsci.2023.112492> (2023).
- Zaman, S., Yaqoob, H. S. A., Ullah, A. & Sheikh, M. QSPR analysis of some novel drugs used in blood cancer treatment via degree based topological indices and regression models. *Polycyclic Aromat. Compd. [SPACE]* <https://doi.org/10.1080/10406638.2023.2217990> (2023).
- Aslam, A., Saeed, S., Kanwal, S. & Tchier, F. Investigating hexagonal closed packed crystal lattice through QSPR modeling via linear regression analysis and Topsis. *Phys. Scr.* **99**(2), 025201. <https://doi.org/10.1088/1402-4896/ad1800> (2024).
- Estrada, E. Atom-bond connectivity and the energetic of branched alkanes. *Chem. Phys. Lett.* **463**(4), 422–425 (2008).
- Gutman, I., Tosovic, J., Radenkovic, S. & Markovic, S. On atom-bond connectivity index and its chemical applicability. *Indian J. Chem.* **51A**, 690–694 (2012).
- Aslam, A., Jamil, M. K., Gao, W. & Nazeer, W. Topological aspects of some dendrimer structures. *Nanotechnol. Rev.* **7**(2), 123–129 (2018).
- Zhang, G., Mushtaq, A., Aslam, A., Parveen, S. & Kanwal, S. Studying some networks using topological descriptors and multi-criterion decision making. *Mol. Phys.* **121**, 16. <https://doi.org/10.1080/00268976.2023.2222345> (2023).
- Khan, A. et al. Computational and topological properties of neural networks by means of graph-theoretic parameters. *Alex. Eng. J.* **66**(1), 957–977. <https://doi.org/10.1016/j.aej.2022.11.001> (2023).
- Govardhan, S. & Santiago, R. Degree-Sum based topological indices of supercoronene and triangle-shaped discotic graphene using NM-Polynomial. *Polycyclic Aromat. Compd.* **44**(1), 507–520. <https://doi.org/10.1080/10406638.2023.2177314> (2024).
- Tang, J.-H., Ali, U., Javaid, M. & Shabbir, K. Zagreb connection indices of subdivision and semi-total point operations on graphs. *J. Chem.* 2019(2019), Article ID 9846913.
- Ali, U., Javaid, M. & Kashif, A. Modified Zagreb connection indices of the T-Sum graphs. *Main Group Met. Chem.* **43**(1), 43–55 (2020).
- Cao, J., Ali, U., Javaid, M., & Huang, C. Zagreb connection indices of molecular graphs based on operations. *Complexity* **2020**(2020), Article ID 7385682.
- Ahmad, A., Koam, N. A., Masmali, I., Azeem, M. & Ghazwani, H. Connection number topological aspect for backbone DNA networks. *Eur. Phys. J. E* **46**, article no. 120 (2023).
- Liu, J.-B., Raza, Z. & Javaid, M. Zagreb connection numbers for cellular neural networks. *Discrete Dyn. Nat. Soc.* **2020**, Article ID 8038304 (2020).
- Javaid, M., Ali, U. & Siddiqui, K. Novel connection based Zagreb indices of several wheel-related graphs. *Comput. J. Comb. Math.* **1**, 1–28 (2021).
- Ullah, A., Shamsudin, Zaman, S. & Hamraz, A. Zagreb connection topological descriptors and structural property of the triangular chain structures. *Physica Scripta* **98**(2), 025009. <https://doi.org/10.1088/1402-4896/acb327> (2023).
- Koam, Ali N. A., Azeem, M., Ahmad, A. & Masmali, I. Connection number-based molecular descriptors of skin cancer drugs. *Ain Shams Eng. J.* article number 102750 (2024). <https://doi.org/10.1016/j.aej.2024.102750>.
- Sattar, A., Javaid, M. & Bonyah, E. On the studies of dendrimers via connection-based molecular descriptors. *Math. Probl. Eng.* **2022**, 1–13 (2022).
- Sattar, A., & Javaid, M. Topological aspects of metal-organic frameworks: Zinc silicate and oxide networks. *Comput. Theor. Chem.* **1222**, article no. 114056 (2023). <https://doi.org/10.1016/j.comptc.2023.114056>.
- Ali, U., Javaid, M. & Alanazi, A. M. Computing analysis of connection-based indices and coindices for product of molecular networks. *Symmetry* **12**(8), 12081320 (2020).
- Tan, Y. J. & Wu, J. Network structure entropy and its application to scale-free networks. *Syst. Eng. Theory Pract.* **6**, 1–3 (2004).
- Mowshowitz, A. & Dehmer, M. Entropy and the complexity of graphs revisited. *Entropy* **14**, 559–570 (2012).
- Morowitz, H. Some order-disorder considerations in living systems. *Bull. Math. Biophys.* **17**, 81–86 (1953).
- Manzoor, S., Siddiqui, M. K. & Ahmad, S. On entropy measures of molecular graphs using topological indices. *Arab. J. Chem.* **13**(8), 6285–6298. <https://doi.org/10.1016/j.arabj.2020.05.021> (2020).
- Zuo, X., Nadeem, M. F., Siddiqui, M. K. & Azeem, M. Edge weight based entropy of different topologies of carbon nanotubes. *IEEE Access* **9**, 102019–102029. <https://doi.org/10.1109/ACCESS.2021.3097905> (2021).
- Dehmer, M. Information processing in complex networks: Graph entropy and information functionals. *Appl. Math. Comput.* **201**, 82–94 (2008).
- Gao, W., Wu, H., Siddiqui, M. K. & Baig, A. Q. Study of biological networks using graph theory. *Saudi J. Biol. Sci.* **25**, 1212–1219 (2018).
- Chen, Z., Dehmer, M. & Shi, Y. A note on distance-based graph entropies. *Entropy* **16**, 5416–5427 (2014).
- Ishfaq, F., Nadeem, M. F. & El-Bahy, Z. M. On topological indices and entropies of diamond structure. *Int. J. Quant. Chem.* **123**, 21. <https://doi.org/10.1002/qua.27207> (2023).
- Jolly, W. L. *Modern Inorganic Chemistry* 2nd edn, 635 (McGraw-Hill, 1991).
- Housecroft, C. E. & Sharpe, A. G. *Inorganic Chemistry* 2nd edn, 905 (Pearson/Prentice Hall, 2005).
- Cohen, P. & Graves, H. W. Chemical shim control for power reactors. *Nucleonics* **22**(5), 75–82 (1964).
- Myerscough, P. B. *Nuclear Power Generation (Third ed.) Incorporating Modern Power System Practice* 1–110 (British Electricity International, 1992).

44. Hargraves, R. & Moir, R. Liquid fluoride thorium reactors: An old idea in nuclear power gets reexamined. *Am. Sci.* **98**(4), 304–313 (2010).
45. Jeyaraj, S. V. & Santiago, R. A study on efficient technique for generating vertex-based topological characterization of boric acid 2D structure. *ACS Omega* **8**, 23089–23097 (2023).

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## Declarations

## Competing interests

The authors declare no competing interests.

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