Baghdad Science Journal

Volume 22 | Issue 3 Article 22

3-26-2025

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How to Cite this Article

Yousef, Walid; Alameri, Abdu; Alsharafı, Mohammed; Al-Naggar, Noman; and Al-Fuhaid, Belal (2025) "Topological and Hyper Topological Coindices of Benzenoid Circumcoronene Series," *Baghdad Science Journal*: Vol. 22: Iss. 3, Article 22.
DOI: https://doi.org/10.21123/bsj.2024.10588

BAGHDAD SCIENCE JOURNAL 2025;22(3):966–978

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RESEARCH ARTICLE

Topological and Hyper Topological Coindices of Benzenoid Circumcoronene Series

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ABSTRACT

Numerous applications in chemistry are enabled by chemical graph theory, which is a branch of graph theory. Numerical quantities derived from the chemical graphs of a molecule, known as topological indices and co-indices, are used to model the chemical and physical properties of molecules in quantitative Structure-Property relationships (QSPR) and quantitative structure-activity relationships (QSAR) research. Fortunately, chemical-based experiments have found a strong connection between Topological descriptors (topological indices and co-indices) of molecular structures and their Physicochemical Properties, such as boiling point, and toxicity of drugs. Although several research reports have contributed to the computation of topological indices of the benzenoid circumcoronene series, studies on the calculation of topological co-indices are limited. This paper focuses on some topological co-indices. Several formulas of topological co-indices such as first Zagreb, second Zagreb, forgotten, and Yemen co-indices have been derived for the benzenoid circumcoronene series. In addition, the paper introduced new topological indices and their co-indices such as Gaza, Quds, and Palestine indices and co-indices and their mathematical formulas of the benzenoid circumcoronene series. Moreover, some algorithms have been built using Python programs to implement the mathematical formulas that are generally derived.

Keywords: Benzenoid circumcoronene series, Chemical graph theory, Molecular graphs, Topological co-indices, Topological indices

Introduction

Chemical graph theory is a branch of mathematical chemistry that applies graph theory to the study of chemical structure and properties. It is the process of visualizing molecules as graphs, with atoms serving as nodes(vertices) and atom-to-atom bonds as lines(edges). It is possible to describe the geometric structure of chemical compounds and estimate their physical characteristics, such as melting and boiling point temperatures, by using a variety of topological measures that are calculated using graph theory.[1] Chemical graph theory applies mathematical techniques from the field of graph theory and combinatorics to address chemical issues. It is related to several fields of graph theory.[2,3] It has become an integrative discipline that has a direct effect on maths and chemistry. It can be especially helpful in fields like structure description and isomer enumeration.[4] Discrete mathematics is used in chemical graph theory to represent the physical and biological characteristics of chemical substances. Compound features like melting and boiling points may be predicted using a variety of topological indices that come from the concept of graphs. These models can be used to anticipate a compound's physical

Received 3 January 2024; revised 19 February 2024; accepted 21 February 2024.
Available online 26 March 2025

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https://doi.org/10.21123/bsj.2024.10588

characteristics in the absence of experimental testimony.[5] Topological measures are numerical values that are computed from a molecule's chemical graph and are frequently associated with the molecule's chemical characteristics. These indices allow us to predict the properties of compounds without the need for complicated calculations.[6]

Topological indices and co-indices are powerful mathematical descriptors in chemical graph theory. These descriptors provide a quantitative method for defining the structural characteristics of chemical compounds, and they are built from the underlying molecular graph. Notably, there is a high link between several physicochemical features of molecules and topological indices. Examples of these indices that are often used are the Geometric-Arithmetic (GA) index and the Atom-Bond Connectivity (ABC) index, among others.[7] These topological indices have significance because of their foundational chemical relevance. They are remarkably good at predicting a number of important chemical compound attributes, such as stability, strain energy, boiling point, etc. Other topological indices that have been studied include the Zagreb indices, Forgotten index, Wiener index, Yemen index, Hyper-Zagreb and Hyper Forgotten indices, and Kirchhoff index.[8–11] These indices have been used to explore quantitative structure-property relationships and quantitative structure-activity relationships in cheminformatics.[12,13] They provide simple and easily computed chemical information with explicit mathematical formulas. The correlation between these topological indices and physicochemical properties of molecules has been examined.

A. Ashrafi et al. introduced Zagreb coindices and calculated exact formulae for the relationship between the first and second Zagreb indices and their coindices[14,15] such as:

$$\bar{M}_1(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} [\delta_\Gamma(\mu) + \delta_\Gamma(\nu)] \tag{1}$$

$$\bar{M}_2(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} [\delta_\Gamma(\mu)\,\delta_\Gamma(\nu)] \tag{2}$$

$$\bar{M}_1(\Gamma) = 2m(n-1) - M_1(\Gamma) \tag{3}$$

$$\bar{M}_2(\Gamma) = 2m^2 - \frac{1}{2}M_1(\Gamma) - M_2(\Gamma) \tag{4}$$

N. De et al.[16] introduced the F-coindex which is defined as follows.

$$\bar{F}(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} \left[\delta_\Gamma^2(\mu) + \delta_\Gamma^2(\nu)\right] \tag{5}$$

They also computed the relationship between F-index and F-coindex as:

$$\bar{F}(\Gamma) = (n-1)M_1(\Gamma) - F(\Gamma) \tag{6}$$

Alameri et al.[17] defined a new degree-based descriptor, denoted by the $(Y-coindex)$, and it is defined as:

$$\bar{Y}(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} \left[\delta_\Gamma^3(\mu) + \delta_\Gamma^3(\nu)\right], \tag{7}$$

In addition, in the same paper, $(Y-coindex)$ of a graph Γ was defined as:

$$\bar{Y}(\Gamma) = (n-1)F(\Gamma) - Y(\Gamma), \tag{8}$$

Sethumadhavan and Gokulathilagan[18] studied the S-index and S-coindex of some graph operations, and they defined as:

$$S(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} \left[\delta_\Gamma^4(\mu) + \delta_\Gamma^4(\nu)\right], \tag{9}$$

$$\bar{S}(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} \left[\delta_\Gamma^4(\mu) + \delta_\Gamma^4(\nu)\right]. \tag{10}$$

Veylaki, et al.[19] introduced Hyper-Zagreb coindex and it is defined as:

$$\overline{HM}(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} [\delta_\Gamma(\mu) + \delta_\Gamma{}^2(\nu)]^2, \tag{11}$$

Gutman I.[20] derived the formula for the Hyper-Zagreb coindex as follows:

$$\overline{HM}(\Gamma) = (n-2)M_1(\Gamma) + 4m^2 - HM(\Gamma), \tag{12}$$

Ayache et al.[21] defined the second Hyper-Zagreb coindex such as:

$$\overline{HM_2}(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} \delta_\Gamma{}^2(\mu)\,\delta_\Gamma{}^2(\nu) \tag{13}$$

Such that:

$$\overline{HM_2}(\Gamma) = \frac{1}{2}M_1^2(\Gamma) - \frac{1}{2}Y(\Gamma) - HM_2(\Gamma), \tag{14}$$

The benzenoid series includes compounds such as circumcoronene and ovalene. These compounds have been studied for their various properties and applications. For example, the topological indices of the double and strong double graphs of the Circumcoronene series of benzenoids have been calculated.[22] Additionally, Circumcoronene and Boron Nitride Circumcoronene have been explored as carriers for the anticancer drug floxuridine, showing

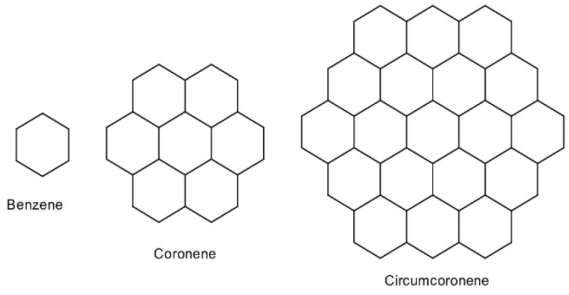

Fig. 1. The first three graphs from the Benzenoid Circumcoronene series.

promise as drug delivery systems.[23] The interactions of n-alkanes and n-per fluoroalkanes with Circumcoronene have also been investigated, revealing differences in their adsorption energies and steric repulsion.[24] Furthermore, the Multiplicative Zagreb Eccentricity index has been computed for the Circumcoronene series of benzenoid H_k.[25] The Sanskruti index has also been calculated for the Circumcoronene series of benzenoid.[26]

Let $(\Gamma = H_k : k \geq 1)$ be the Benzenoid Circumcoronene series Fig. 1, then

$$M_1(\Gamma) = 54k^2 - 30k, \tag{15}$$

$$M_2(\Gamma) = 81k^2 - 63k + 6, \tag{16}$$

$$F(H_k) = 162k^2 - 114k, \tag{17}$$

$$HM(H_k) = 324k^2 - 240k + 12. \tag{18}$$

Numerous studies have examined the computation of topological indices for Benzenoid Circumcoronene. Chemical descriptors, such as Randic, Zagreb, Harmonic, augmented Zagreb, atom-bond connectivity, and geometric-arithmetic indices, have been computed for Benzenoid networks theoretically.[27] Although numerous studies have examined the computation of topological indices for Benzenoid Circumcoronene, investigations into the calculation of topological coindices remain scarce. This paper highlights topological coindices of Benzenoid Circumcoronene. Specifically, mathematical formulas have been derived for the first Zagreb, second Zagreb, forgotten, hyper-first Zagreb, hyper-second Zagreb, and hyper-forgotten coindices of the Benzenoid Circumcoronene series. In addition, new topological coindices are introduced and their mathematical formulas are derived for the benzenoid coronene ocean series. Furthermore, some algorithms have been built using Python programs to calculate the mathematical formulas that are derived.

Preliminary results

In this section, the topological indices of the benzenoid circumcoronene series H_k are derived by us. $Y(H_k)$, $S(H_k)$ and $HM_2(H_k)$,

Lemma 1: *For $k \leq 1$, H_k is the benzene series (see Fig. 1). The number of vertices and edges of H_k*

- $n = |V(H_k)| = 6k^2$,
- $m = |E(H_k)| = 9k^2 - 3k$,
- $E_1(H_k) = \{e = \mu\nu \in E(\Gamma) : \delta(\mu) = \delta(\nu) = 2\}$,
- $E_2(H_k) = \{e = \mu\nu \in E(\Gamma) : \delta(\mu) = 2, \delta(\nu) = 3\}$,
- $E_3(H_k) = \{e = \mu\nu \in E(\Gamma) : \delta(\mu) = \delta(\nu) = 3\}$,

Proposition 1: The Y-index of benzenoid circumcoronene is given by:

$$Y(H_k) = 486k^2 - 390k.$$

Proof: By the definition of Y-index and (Lemma 1),

$$\begin{aligned} Y(H_k) &= \sum_{\mu\nu \in E(H_k)} \left[\delta^3(\mu) + \delta^3(\nu)\right] \\ &= \sum_{\mu\nu \in E_1} \left[\delta^3(\mu) + \delta^3(\nu)\right] \\ &\quad + \sum_{\mu\nu \in E_2} \left[\delta^3(\mu) + \delta^3(\nu)\right] \\ &\quad + \sum_{\mu\nu \in E_3} \left[\delta^3(\mu) + \delta^3(\nu)\right] \\ &= 16|E_1| + 35|E_2| + 54|E_3| \\ &= 16(6) + 35\left(12\left(k-1\right)\right) \\ &\quad + 54\left(9k^2 - 15k + 6\right) \\ &= 486k^2 - 390k. \end{aligned}$$

Proposition 2: The HM_2-index of benzenoid circumcoronene is given by:

$$HM_2(H_k) = 729k^2 - 783k + 150.$$

Proof: By the definition of HM_2-index and (Lemma 1),

$$\begin{aligned} HM_2(H_k) &= \sum_{\mu\nu \in E(H_k)} [\delta(\mu)\delta(\nu)]^2 = \sum_{\mu\nu \in E_1} [\delta(\mu)\delta(\nu)]^2 \\ &\quad + \sum_{\mu\nu \in E_2} [\delta(\mu)\delta(\nu)]^2 + \sum_{\mu\nu \in E_3} [\delta(\mu)\delta(\nu)]^2 \\ &= 16|E_1| + 36|E_2| + 81|E_3| \\ &= 16(6) + 36\left(12\left(k-1\right)\right) \end{aligned}$$

$$+ 81\left(9k^2 - 15k + 6\right)$$
$$= 729k^2 - 783k + 150.$$

Theorem 1: *The S-index of benzenoid circumcoronene is given by:*

$$S(H_k) = 1458k^2 - 1266k.$$

Proof: From Eq. (9),

$$\begin{aligned} S(H_k) &= \sum_{\mu\nu\in E(H_k)} [\delta^4(\mu) + \delta^4(\nu)] \\ &= \sum_{\mu\nu\in E_1} [\delta^4(\mu) + \delta^4(\nu)] \\ &\quad + \sum_{\mu\nu\in E_2} [\delta^4(\mu) + \delta^4(\nu)] \\ &\quad + \sum_{\mu\nu\in E_3} [\delta^4(\mu) + \delta^4(\nu)] \\ &= 32|E_1| + 97|E_2| + 162|E_3| \\ &= 32(6) + 97\left(12(k-1)\right) \\ &\quad + 162\left(9k^2 - 15k + 6\right) \\ &= 1458k^2 - 1266k. \end{aligned}$$

Results and discussion

A mathematical derivation of some old and new topological and Hyper topological coindices is being studied of the benzenoid circumcoronene series H_k and the mathematical formulas derived using the Python program will be supported.

Well-known topological coindices of benzenoid circumcoronene series

In this subsection, a mathematical derivation of topological coindices for the benzenoid circumcoronene series H_k is provided by including $\overline{M_1}(H_k)$, $\overline{M_2}(H_k)$, $\bar{F}(H_k)$, $\bar{Y}(H_k)$ and $\bar{S}(H_k)$.

Theorem 2: *The* M_1*-coindex of benzenoid circumcoronene is given by:*

$$\overline{M_1}(H_k) = 108k^4 - 36k^3 - 72k^2 + 36k$$

Proof: From (Lemma 1), and Eq. (15), $n = |V(H_k)| = 6k^2$, $m = |E(H_k)| = 9k^2 - 3k$, $M_1(\Gamma) = 54k^2 - 30k$, and $\bar{M}_1(\Gamma) = 2m(n-1) - M_1(\Gamma)$.

Thus,

$$\begin{aligned} \bar{M}_1(\Gamma) &= 2m(n-1) - M_1(\Gamma) \\ &= 2(9k^2 - 3k)[6k^2 - 1] + 54k^2 - 30k \\ &= 108k^4 - 36k^3 - 72k^2 + 36k \end{aligned}$$

Theorem 3: *The* M_2*-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\overline{M_2}(H_k) = 162k^4 - 108k^3 - 90k^2 + 78k - 6.$$

Proof: From (Lemma 1) and Eqs. (15) and (16), $n = |V(H_k)| = 6k^2$, $m = |E(H_k)| = 9k^2 - 3k$, $M_1(\Gamma) = 54k^2 - 30k$, $M_2(\Gamma) = 81k^2 - 63k + 6$, and since $\bar{M}_2(\Gamma) = 2m^2 - \frac{1}{2}M_1(\Gamma) - M_2(\Gamma)$.

Thus,

$$\begin{aligned} \bar{M}_2(\Gamma) &= 2m^2 - \frac{1}{2}M_1(\Gamma) - M_2(\Gamma) \\ &= 2(9k^2 - 3k)^2 - \frac{1}{2}[54k^2 - 30k] \\ &\quad - (81k^2 - 63k + 6) \\ &= 162k^4 - 108k^3 - 90k^2 + 78k - 6. \end{aligned}$$

Theorem 4: *The* F*-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\bar{F}(H_k) = 324k^4 - 180k^3 - 216k^2 + 144k.$$

Proof: From (Lemma 1), and Eqs. (15) and (17), $n = |V(H_k)| = 6k^2$, $m = |E(H_k)| = 9k^2 - 3k$, $M_1(\Gamma) = 54k^2 - 30k$, $F(H_k) = 162k^2 - 114k$, and since $\bar{F}(\Gamma) = (n-1)M_1(\Gamma) - F(\Gamma)$.

Thus,

$$\begin{aligned} \bar{F}(\Gamma) &= (n-1)M_1(\Gamma) - F(\Gamma) \\ &= (6k^2 - 1)(54k^2 - 30k) - (162k^2 - 114k) \\ &= 324k^4 - 180k^3 - 216k^2 + 144k. \end{aligned}$$

Theorem 5: *The* Y*-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\bar{Y}(H_k) = 972k^4 - 684k^3 - 648k^2 + 504k.$$

Proof: From (Lemma 1), Eq. (17), and (Proposition 2), $n = |V(H_k)| = 6k^2$, $F(H_k) = 162k^2 - 114k$, $Y(H_k) = 486k^2 - 390k$, and since $\bar{Y}(\Gamma) = (n-1)F(\Gamma) - Y(\Gamma)$,

Thus,

$$\begin{aligned} \bar{Y}(\Gamma) &= (n-1)F(\Gamma) - Y(\Gamma) \\ &= (6k^2 - 1)(162k^2 - 114k) - (486k^2 - 390k) \\ &= 972k^4 - 684k^3 - 648k^2 + 504k. \end{aligned}$$

Theorem 6: *The S-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\bar{S}(H_k) = 2916k^4 - 2376k^3 - 1944k^2 + 1656k.$$

Proof: The formula of the general first Zagreb coindex is given by:

$$\overline{M_1^{\alpha}}(\Gamma) = (n-1)M_1^{\alpha-1}(\Gamma) - M_1^{\alpha}(\Gamma), \tag{19}$$

Since $M_1^{\alpha} = \sum_{\mu\nu\in E}(\delta^{\alpha}(\mu) + \delta^{\alpha}(\nu))$

When

$$\alpha = 1 \quad M_1 = M_1^1 = \sum_{\mu\nu\in E}(\delta(\mu) + \delta(\nu))$$

$$\alpha = 2 \quad F = M_1^2 = \sum_{\mu\nu\in E}\left(\delta^2(\mu) + \delta^2(\nu)\right)$$

$$\alpha = 3 \quad Y = M_1^3 = \sum_{\mu\nu\in E}\left(\delta^3(\mu) + \delta^3(\nu)\right)$$

$$\alpha = 4 \quad S = M_1^4 = \sum_{\mu\nu\in E}(\delta^4(\mu) + \delta^4(\nu)).$$

Then,

$\overline{M_1^4}(\Gamma) = \bar{S}(\Gamma) = (n-1)Y(\Gamma) - S(\Gamma)$, and

$$n = |V(H_k)| = 6k^2,\ Y(H_k) = 486k^2 - 390k,$$
$$S(H_k) = 1458k^2 - 1266k.$$

Thun,

$$\begin{aligned}\bar{S}(H_k) &= (n-1)Y(H_k) - S(H_k)\\ &= \left(6k^2-1\right)\left(486k^2 - 390k\right)\\ &\quad - \left(1458k^2 - 1266k\right)\\ &= 2916k^4 - 2376k^3 - 1944k^2 + 1656k.\end{aligned}$$

New topological indices and their coindices of benzenoid circumcoronene

In this subsection, a mathematical derivation of new topological indices and their coindices of the benzenoid circumcoronene series H_k is provided, denoted Gaza index and Palestine index (in short G-index "$G(H_k)$" and P-index "$P(H_k)$") respectively. The topological coindices of these indices denoted as $\bar{G}(H_k)$ and $\bar{P}(H_k)$. G-index and P-index and their coindices are special cases of the first general Zagreb index and the first general coindex where $\alpha = 5$ and $\alpha = 6$ which define us:

$$G(\Gamma) = \sum_{\nu\in V(\Gamma)}[\delta_{\Gamma}^6\nu] = \sum_{\mu\nu\in E(\Gamma)}[\delta_{\Gamma}^5\mu + \delta_{\Gamma}^5\nu], \tag{20}$$

$$P(\Gamma) = \sum_{\nu\in V(\Gamma)}[\delta_{\Gamma}^7\nu] = \sum_{\mu\nu\in E(\Gamma)}[\delta_{\Gamma}^6\mu + \delta_{\Gamma}^6\nu], \tag{21}$$

Therefore,

$$\bar{G}(\Gamma) = (n-1)S(\Gamma) - G(\Gamma), \tag{22}$$

and

$$\bar{P}(\Gamma) = (n-1)G(\Gamma) - P(\Gamma) \tag{23}$$

Proposition 3: The G-index of benzenoid circumcoronene is given by:

$$G(H_k) = 4374k^2 - 3990k.$$

Proof: By the definition of G-index and (Lemma 1),

$$\begin{aligned}G(H_k) &= \sum_{\mu\nu\in E(H_k)}[\delta^5(\mu) + \delta^5(\nu)]\\ &= \sum_{\mu\nu\in E_1}[\delta^5(\mu) + \delta^5(\nu)]\\ &\quad + \sum_{\mu\nu\in E_2}[\delta^5(\mu) + \delta^5(\nu)]\\ &\quad + \sum_{\mu\nu\in E_3}[\delta^5(\mu) + \delta^5(\nu)]\\ &= 64|E_1| + 275|E_2| + 486|E_3|\\ &= 64(6) + 275\left(12(k-1)\right)\\ &\quad + 486\left(9k^2 - 15k + 6\right)\\ &= 4374k^2 - 3990k.\end{aligned}$$

Theorem 7: *The G-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\bar{G}(H_k) = 8748k^4 - 7596k^3 - 5832k^2 + 5256k.$$

Proof: We have $n = |V(H_k)| = 6k^2$, $S(H_k) = 1458k^2 - 1266k$, $G(H_k) = 4374k^2 - 3990k$, and since $\bar{G}(\Gamma) = (n-1)S(\Gamma) - G(\Gamma)$,

Thus,

$$\begin{aligned}\bar{G}(H_k) &= (n-1)S(H_k) - G(H_k)\\ &= \left(6k^2-1\right)\left(1458k^2-1266k\right) - \left(486k^2-390k\right)\\ &= 8748k^4 - 7596k^3 - 5832k^2 + 5256k.\end{aligned}$$

Proposition 4: The P-index of benzenoid circumcoronene is given by:

$$P(H_k) = 13122k^2 - 12354k.$$

Proof: By the definition of P-index and (Lemma 1),

$$\begin{aligned} P(H_k) &= \sum_{\mu\nu\in E(H_k)} [\delta^6(\mu)+\delta^6(\nu)] \\ &= \sum_{\mu\nu\in E_1} [\delta^6(\mu)+\delta^6(\nu)] \\ &\quad + \sum_{\mu\nu\in E_2} [\delta^6(\mu)+\delta^6(\nu)] \\ &\quad + \sum_{\mu\nu\in E_3} [\delta^6(\mu)+\delta^6(\nu)] \\ &= 64|E_1| + 275|E_2| + 486|E_3| \\ &= 13122k^2 - 12354k. \end{aligned}$$

Theorem 8: *The* P*-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\bar{P}(H_k) = 26244k^4 - 23940k^3 - 17496k^2 + 16344k.$$

Proof: We have $n = |V(H_k)| = 6k^2$, $G(H_k) = 4374k^2 - 3990k$, $P(H_k) = 13122k^2 - 12354k$, and since $\bar{P}(H_k) = (n-1)G(H_k) - P(H_k)$,

Thus,

$$\begin{aligned} \bar{P}(H_k) &= (n-1)G(H_k) - P(H_k) \\ &= \left(6k^2-1\right)\left(4374k^2 - 3990k\right) \\ &\quad - \left(13122k^2 - 12354k\right) \\ &= 26244k^4 - 23940k^3 - 17496k^2 + 16344k. \end{aligned}$$

Well-known hyper topological coindices of benzenoid circumcoronene

In this subsection, a mathematical derivation of hyper topological coindices of the benzenoid circumcoronene series H_k is provided such as $\overline{HM_1}(H_k)$, $\overline{HM_2}(H_k)$ and $\overline{HF}(H_k)$.

Theorem 9: *The* HM_1*-coindex of benzenoid circumcoronene is given by:*

$$\overline{HM_1}(H_k) = 648k^4 - 396k^3 - 396k^2 + 300k - 12.$$

Proof: From the definition of hyper Zagreb index,

$$\begin{aligned} HM_1(\Gamma) &= \sum_{\mu\nu\in E(\Gamma)} [\delta(\mu)+\delta(\nu)]^2 \\ &= \sum_{\mu\nu\in E(\Gamma)} [\delta^2(\mu)+\delta^2(\nu)+2\delta(\mu)\delta(\nu)] \\ &= \sum_{\mu\nu\in E(\Gamma)} \left[\delta^2(\mu)+\delta^2(\nu)\right] \\ &\quad + \sum_{\mu\nu\in E(\Gamma)} [2\delta(\mu)\delta(\nu)] \\ &= F(\Gamma) + 2M_2(\Gamma). \end{aligned}$$

Therefore,

$$\overline{HM_1}(\Gamma) = \bar{F}(\Gamma) + 2\overline{M_2}(\Gamma), \tag{24}$$

Applying (Theorems 3 and 4) in Eq. (24)

$$\begin{aligned} \overline{HM_1}(H_k) &= \bar{F}(H_k) + 2\overline{M_2}(H_k) \\ &= 648k^4 - 396k^3 - 396k^2 + 300k - 12. \end{aligned}$$

Theorem 10: *The* HM_2*-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\overline{HM_2}(H_k) = 1458k^4 - 1620k^3 - 522k^2 + 978k - 150.$$

Proof: By Eq. (15), and Propositions 1 and 2,

$$\begin{aligned} M_1(H_k) &= 54k^2 - 30k, \\ Y(H_k) &= 486k^2 - 390k, \\ HM_2(H_k) &= 3\left[243k^2 - 261k + 50\right], \end{aligned}$$

and by substitution on $\overline{HM_2}(H_k) = \frac{1}{2}M_1^2(H_k) - \frac{1}{2}Y(H_k) - HM_2(H_k)$, the required was obtained.

Theorem 11: *The* HF*-coindex of benzenoid circumcoronene is given by:*

$$\overline{HF}(H_k) = 5832k^4 - 5580k^3 - 2988k^2 + 3612k - 588.$$

Proof: From the definition of hyper F-index,

$$\begin{aligned} HF(\Gamma) &= \sum_{\mu\nu\in E(\Gamma)} [\delta(\mu)^2+\delta^2(\nu)]^2 \\ &= \sum_{\mu\nu\in E(\Gamma)} \left[\delta^4(\mu)+\delta^4(\nu)+2\delta^2(\mu)\delta^2(\nu)\right] \\ &= \sum_{\mu\nu\in E(\Gamma)} [\delta^4(\mu)+\delta^4(\nu)] \\ &\quad + 2\sum_{\mu\nu\in E(\Gamma)} [\delta^2(\mu)\delta^2(\nu)] \\ &= S(\Gamma) + 2HM_2(\Gamma). \end{aligned}$$

Therefore,

$$\overline{HF}(\Gamma) = \bar{S}(\Gamma) + 2\overline{HM_2}(\Gamma), \tag{25}$$

Applying (Theorems 6 and 10) in (Eq. (25)),

$$\begin{aligned} \overline{HF}(H_k) &= \bar{S}(H_k) + 2\overline{HM_2}(H_k) = 5832k^4 \\ &\quad - 5580k^3 - 2988k^2 + 3612k - 588. \end{aligned}$$

New hyper topological coindices of benzenoid circumcoronene series

In this subsection, a mathematical derivation of the new hyper topological index and their coindex of the benzenoid circumcoronene series H_k is provided, denoted hyper Yemen index (in short HY-index "$HY(H_k)$") which the hyper topological coindex of this index is $\overline{HY}(H_k)$. It is important here to introduce a new topological index for use in deriving the formula of the hyper topological index and their coindex, denoted Quds index (in short Q-index "$Q(H_k)$"). which the topological coindex of this index is $\bar{Q}(H_k)$.

The definitions of HY-index and Q-index are:

$$HY(\Gamma) = \sum_{\mu\nu \in E(\Gamma)} [\delta_\Gamma^3 \mu + \delta_\Gamma^3 \nu]^2, \tag{26}$$

$$Q(\Gamma) = \sum_{\mu\nu \in E(\Gamma)} [\delta_\Gamma^3 \mu \delta_\Gamma^3 \nu], \tag{27}$$

In addition, the definitions of HY-coindex and Q-coindex are as follows.

$$\overline{HY}(\Gamma) = \sum_{\mu\nu \notin E(\Gamma)} [\delta_\Gamma^3 \mu + \delta_\Gamma^3 \nu^2], \tag{28}$$

$$\bar{Q}(\Gamma) = \sum_{\mu\nu \notin E(\Gamma)} [\delta_\Gamma^3 \mu \delta_\Gamma^3 \nu], \tag{29}$$

It's easy to see that the M_2-index, the HM_2-index and the Q-index are special cases of the second general Zagreb indices where $\alpha = 1$, $\alpha = 2$, and $\alpha = 3$, respectively.

Lemma 2: *The* Q*-coindex of a graph* Γ *is given by:*

$$\bar{Q}(\Gamma) = \frac{1}{2}\left(F^2(\Gamma) - G(\Gamma)\right) - Q(\Gamma) \tag{30}$$

Proof: From the definitions of Q index and their coindex,

$$Q(\Gamma) + \bar{Q}(\Gamma) = \left(\sum_{\mu\nu \in E(\Gamma)} + \sum_{\mu\nu \notin E(\Gamma)}\right)\left(\delta^3(\mu)\delta^3(\nu)\right)$$

$$= \frac{1}{2}\left[\left(\sum_{\mu \in V(\Gamma)} \sum_{\nu \in V(\Gamma)}\right)\left(\delta^3(\mu)\delta^3(\nu)\right) - \sum_{(\mu=\nu)\in V(\Gamma)} \left(\delta^3(\mu)\delta^3(\nu)\right)\right]$$

$$= \frac{1}{2}\left[\sum_{\mu \in V(\Gamma)} \left(\delta^3(\mu)\right) \sum_{\nu \in V(\Gamma)} \left(\delta^3(\nu)\right) - \sum_{(\mu=\nu)\in V(\Gamma)} \left(\delta^6(\nu)\right)\right]$$

$$= \frac{1}{2}\left[F(\Gamma)F(\Gamma) - G(\Gamma)\right]$$

$$= \frac{1}{2}\left[F^2(\Gamma) - G(\Gamma)\right]$$

Proposition 4: The Q-index of benzenoid circumcoronene is given by:

$$Q(H_k) = 6561k^2 - 8343k + 2166$$

Proof: By the definition of Q-index and (Lemma 1),

$$Q(H_k) = \sum_{\mu\nu \in E(H_k)} [\delta(\mu)\delta(\nu)]^3 = \sum_{\mu\nu \in E_1} [\delta(\mu)\delta(\nu)]^3 + \sum_{\mu\nu \in E_2} [\delta(\mu)\delta(\nu)]^3 + \sum_{\mu\nu \in E_3} [\delta(\mu)\delta(\nu)]^3$$

$$= 64|E_1| + 216|E_2| + 729|E_3|$$

$$= 64(6) + 216\left(12(k-1)\right) + 729\left(9k^2 - 15k + 6\right)$$

$$= 6561k^2 - 8343k + 2166.$$

Theorem 12: *The* Q*-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\bar{Q}(H_k) = 13122k^4 - 18468k^3 - 2250k^2 + 10338k - 2166.$$

Proof: By Lemma 2,

$$F(H_k) = 162k^2 - 114k,\ G(H_k) = 4374k^2 - 3990k,$$

$$Q(H_k) = 6561k^2 - 8343k + 2166$$

and by substitution on $\overline{Q(\Gamma)} = \frac{1}{2}(F^2(\Gamma) - G(\Gamma)) - Q(\Gamma)$, the required was obtained.

Lemma 3: *The* HY*-index is a linear composition of the* P*-index and* Q*-index, in other words, we can write*

$$HY(\Gamma) = P(\Gamma) + 2Q(\Gamma) \tag{31}$$

Table 1. The edge set partition of the benzenoid circumcoronene series.

Edge	E_1	E_2	E_3
Cardinality	6	$12(k-1)$	$9k^2-15k+6$

Proof: From the definition of $HY(\Gamma)$,

$$\begin{aligned} HY(\Gamma) &= \sum_{\mu\nu\in E(\Gamma)} [\delta_\Gamma^3\mu + \delta_\Gamma^3\nu]^2 \\ &= \sum_{\mu\nu\in E(\Gamma)} [\delta_\Gamma^6\mu + \delta_\Gamma^6\nu] + 2\sum_{\mu\nu\in E(\Gamma)} \delta_\Gamma^3(\mu)\delta_\Gamma^3(\nu) \\ &= P(\Gamma) + 2Q(\Gamma). \end{aligned}$$

Proposition 5: The HY-index of benzenoidcircumcoronene is given by:

$$HY(H_k) = 26244k^2 - 29040k + 4332$$

Proof: By Lemma 3,

$$P(H_k) = 13122k^2 - 12354k,$$
$$Q(H_k) = 6561k^2 - 8343k + 2166,$$

and by substitution on $HY(H_k) = P(H_k) + 2Q(H_k)$, we get the required.

Theorem 13: *The* HY*-coindex of benzenoid circumcoronene* (H_k) *is given by:*

$$\begin{aligned} \overline{HY}(H_k) &= 52488k^4 - 60876k^3 - 21996k^2 \\ &\quad + 37020k - 4332. \end{aligned}$$

Proof: By Lemmas 2 and 3,

$$\bar{P}(H_k) = 26244k^4 - 23940k^3 - 17496k^2 + 16344k,$$
$$\begin{aligned} \bar{Q}(H_k) &= 13122k^4 - 18468k^3 - 2250k^2 \\ &\quad + 10338k - 2166, \end{aligned}$$

and by substitution on $\overline{HY}(H_k) = \overline{P(H_k)} + 2\overline{Q(H_k)}$, the required was obtained.

Discuss 1: In the previous part, we derived mathematical formulas for some of the topological descriptors of the benzenoid circumcoronene series by taking advantage of the properties of the compound listed in Table 1. In the next part, we will calculate these formulas in general via the Python program. Also, we will address these formulas as groups in special cases, and each group will be discussed independently.

An algorithm to calculate topological and hyper-topological indices and their coindices

This section presents a program to implement an algorithm for calculating topological and Hyper-topological indices and their coindices of benzenoid circumcoronene series using Python (see Figs. 2 to 5).

Some special cases of these topological indices will be computed (specifically when the parameter $k = 1, 2, \ldots, 8$) and then study the relationship between these indicators by analyzing these data.

Discuss 2: Table 2 presented quantitatively examines eight benzenoid circumcoronene structures of increasing size as denoted by the parameter k, ranging from 1 to 8. It compares the values of several commonly used topological indices in this series to assess their trends concerning molecular size growth. The values of the indices increase with increasing k, indicating that the molecules become more complex as the number of rings in the circumcoronene series benzenoid H_k increases. Specifically, the First and Second Zagreb indices (M_1 and M_2, respectively), which are calculated based on vertex degrees, both predictably increase stepwise with each additional k-value. Similarly, the Forgotten, Yemen, S, G, Q, and P indices, which are also based on vertex degrees, in their formulation, also increase more quickly and monotonically from k = 1 to k = 8, albeit at varying rates due to their distinct mathematical definitions.

Discuss 3: Table 3 presents the values of four hyper-topological indices (HTIs) for the benzenoid circumcoronene series H_k, k = 1, 2, . . . , 8. Specifically, it monitors the Hyper-first Zagreb index (HM_1), Hyper-second Zagreb index (HM_2), Hyper-Forgotten index (HF), and Hyper Yemen index (HY). All

Table 2. Topological indices (TI) for benzenoid circumcoronene series H_k, k = 1, 2, . . . , 8.

TI&*k*	1	2	3	4	5	6	7	8
*M*1	24	156	396	744	1200	1764	2436	3216
*M*2	24	204	546	1050	1716	2544	3534	4686
F	48	420	1116	2136	3480	5148	7140	9456
Y	96	1164	3204	6216	10200	15156	21084	27984
S	192	3300	9324	18264	30120	44892	62580	83184
G	384	9516	27396	54024	89400	133524	186396	248016
Q	384	11724	36186	73770	124476	188304	265254	355326
P	768	27780	81036	160536	266280	398268	556500	740976

Table 3. Hyper topological indices (HTI) for benzenoid circumcoronene series H_k, $k = 1, 2, \ldots, 8$.

HTI&k	1	2	3	4	5	6	7	8
*HM*1	96	828	2208	4236	6912	10236	14208	18828
*HM*2	96	1500	4362	8682	14460	21696	30390	40542
HF	384	6300	18048	35628	59040	88284	123360	164268
HY	1536	51228	153408	308076	515232	774876	1087008	1451628

Table 4. Topological coindices (TC) for benzenoid circumcoronene series H_k, $k = 1, 2, \ldots, 8$.

TC&k	1	2	3	4	5	6	7	8
*M*1*c*	36	1224	7236	24336	61380	129816	243684	419616
*M*2*c*	36	1518	9624	33426	85884	183846	348048	603114
Fc	72	3168	19872	68544	175320	374112	706608	1222272
Yc	144	8496	55944	196704	508320	1091664	2070936	3593664
Sc	252	23184	159516	569952	1485180	3205872	6102684	10616256
Gc	576	66384	466776	1681056	4398480	9518256	18149544	31611456
Qc	576	71718	572844	2180466	5886024	12995886	25131348	44228634
Pc	1152	191088	1370952	4971744	13054320	28309392	54057528	94249152

```
k = int(input("k = "))

M1=54*k**2-30*k
M2=81*k**2-63*k+6
F =162*k**2 -114*k
Y =486*k**2  - 390*k
S =1458*k**2 - 1266*k
G =4374*k**2 -  3990*k
Q =6561*k**2-8343*k+2166
P = 13122*k**2  - 12354*k

print("M1-index    :{}".format(M1))
print("M2-index    :{}".format(M2))
print("F-index     :{}".format(F))
print("Y-index     :{}".format(Y))
print("S-index     :{}".format(S))
print("G-index     :{}".format(G))
print("Q-index     :{}".format(Q))
print("P-index     :{}".format(P))
```

Fig. 2. Topological indices of the Benzenoid Circumcoronene series using PYTHON.

indices presented in the table are generalized hyper-topological descriptors that account for higher-order interactions between vertices, and edges in molecular graphs. As with traditional topological indices, monotonic increasing trends are observed concerning the size parameter k for each index type. For instance, HY exhibits the steepest rises relative to HM_1, HM_2, and HF due to its inclusion of longer-range topological features in its definition.

Discuss 4: Table 4 presents the values of various topological coindices for an increasingly large series of benzenoid circumcoronene structures, denoted as H_k where $k = 1, 2, \ldots, 8$ represents the size of the structure. Specifically, it reports the First Zagreb coindex ($M_1{}^c$), Second Zagreb coindex ($M_2{}^c$), Forgotten coindex (F^c), Yemen coindex (Y^c), S-coindex (S^c), G-coindex (G^c), Q-coindex (Q^c), and P-coindex (P^c) for each value of k. The coindices generally increase consistently with larger k values, as would be expected as the size and complexity of the circumcoronene structures grow with each additional ring. M1c displays the lowest values while P^c exhibits the highest values across all k. Some coindices like $M_1{}^c$, $M_2{}^c$, and F^c show relatively linear increases, while others like Y^c, S^c, G^c, Q^c,

```
k = int(input("k = "))

HM1 = 324*k**2  -240*k +12
HM2 = 729*k**2 -783*k  +150
HF = 2916*k**2 -2832*k +300
HY = 26244*k**2 -29040*k +4332

print("HM1-index   :{}".format(HM1))
print("HM2-index   :{}".format(HM2))
print("HF-index    :{}".format(HF))
print("HY-index    :{}".format(HY))
```

Fig. 3. Hyper Topological indices of the Benzenoid Circumcoronene series using PYTHON.

```
k = int(input("k = "))

M1c=108*k**4 -36*k**3 -72*k**2 +36*k
M2c=162*k**4-108*k**3-90*k**2 +78*k-6
Fc=324*k**4 -180*k**3 -216*k**2 +144*k
Yc=972*k**4 -684*k**3 -648*k**2 +504*k
Sc=2916*k**4 -2376*k**3 -1944*k**2 +1656*k
Gc=8748*k**4 -7596*k**3 -5832*k**2 +5256*k
Qc=13122*k**4-18468*k**3-2250*k**2+10338*k-2166
Pc= 26244*k**4 -23940*k**3 -17496*k**2 + 16344*k

print("M1-coindex   :{}".format(M1c))
print("M2-coindex   :{}".format(M2c))
print("F-coindex    :{}".format(Fc))
print("Y-coindex    :{}".format(Yc))
print("S-coindex    :{}".format(Sc))
print("G-coindex    :{}".format(Gc))
print("Q-coindex    :{}".format(Qc))
print("P-coindex    :{}".format(Pc))
```

Fig. 4. Topological coindices of the Benzenoid Circumcoronene series using PYTHON.

```
k = int(input("k = "))

HM1c=648*k**4 -396*k**3 -396*k**2 +300*k -12
HM2c=1458*k**4 -1620*k**3 -522*k**2 +978*k -150
HFc=5832*k**4 -5580*k**3 -2988*k**2 +3612*k -588
HYc=52488*k**4-60876*k**3-21996*k**2+37020*k-4332

print("HM1-coindex :{}".format(HM1c))
print("HM2-coindex :{}".format(HM2c))
print("HF-coindex  :{}".format(HFc))
print("HY-coindex  :{}".format(HYc))
```

Fig. 5. Hyper topological coindices of the Benzenoid Circumcoronene series using PYTHON.

Table 5. Hyper topological coindices (HTC) for benzenoid circumcoronene series H_k, $k = 1, 2, \ldots, 8$.

HTC&k	1	2	3	4	5	6	7	8
HM1c	144	6204	39120	135396	347088	741804	1402704	2428500
HM2c	144	10086	72444	264978	700440	1526574	2926116	5116794
HFc	288	43356	305088	1101924	2890272	6266508	11966976	20867988
HYc	2304	334524	2516640	9332676	24826368	54301164	104320224	182706420

and P^c rise more sharply suggesting they are more strongly influenced by the rapid topological changes occurring in these structures as they expand in size.

Discuss 5: Table 5 presents data on the first Hyper Zagreb coindex, second Hyper Zagreb coindex, Hyper-Forgotten coindex, and Hyper Yemen coindex for benzenoid circumcoronene series H_k of increasing order (k) from 1 to 8. The values of each coindex increase substantially with increasing k, demonstrating a higher topological complexity for benzenoid graphs of larger size according to these metrics. It is noteworthy that the second Hyper Zagreb coindex yields consistently higher values than the first Hyper Zagreb coindex, while the Hyper-Forgotten coindex and Hyper Yemen coindex present much larger figures overall, indicating greater sensitivity to graph order for these coindices. This analysis of quantitative topological properties aids in characterizing the structural evolution of benzenoid circumcoronene molecular graphs.

Conclusion

This study contributes to advancing the quantitative structure-topology analysis of benzenoid circumcoronenes by calculating various topological coindices. Although previous work has computed indices for this important class of polycyclic aromatic hydrocarbons, investigations into coindex properties were limited. The present research addresses this gap by deriving mathematical expressions for key coindices describing the circumcoronene topology, including Zagreb, forgotten, Yemen, S, hyper-Zagreb, and hyper-forgotten coindices. The trends in these coindices as a function of molecular size were then systematically analyzed. Moreover, new topological indices and their coindices are introduced, and mathematical derivations of the benzenoid circumcoronene series are studied. All derived formulas are supported by algorithms using the Python program. The results show that the topological coindices increase steadily with the parameter *k*, validly encoding and increasing connective complexity. Notably, hyper-topological descriptors more strongly accentuate escalating superstructural characteristics. Overall, this computational analysis enhances understanding of the intricate architectural principles that govern the composition and properties of circumcoronene from a quantitative graph theory perspective. The growth formulas of the topological coindices provide a framework supporting future modeling of the behavior of circumcoronenes and the design of novel structural analogs.

Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any Figures and images, that are not ours, have been included with the necessary permission for republication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at University of Science and Technology, Sana'a, Yemen.

Authors' contribution statement

W. S. conceived of the idea, wrote the manuscript, and proofread it. A. A. designed the research, performed the computations, and acquired data. M. A. implemented the research, analyzed, interpreted, and drafted the results. N. A. verified the methods, reviewed the results, and supervised this work. B. A. reviewed the work, designed the program, and linguistic checking. All authors discussed the results and contributed to the final manuscript.

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التطابقات التبولوجية والتبولوجية المفرطة لسلسلة بنزينويد سيركوم كورونين

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[3]قسم علوم الحاسوب، كلية الحاسبات وتكنولوجيا المعلومات، جامعة العلوم والتكنولوجيا، صنعاء، اليمن.

الخلاصة

يتم تمكين العديد من التطبيقات في الكيمياء من خلال نظرية الرسم البياني الكيميائي، وهو فرع من نظرية الرسم البياني. تُستخدم الكميات العددية المشتقة من الرسوم البيانية الكيميائية للجزيء، والمعروفة باسم المؤشرات التبولوجية والمؤشرات التبولوجية المشتركة، لنمذجة الخواص الكيميائية والفيزيائية للجزيئات في أبحاث العلاقات الكمية بين البنية والملكية (QSPR) والعلاقات الكمية بين البنية والنشاط (QSAR). لحسن الحظ، وجدت التجارب القائمة على المواد الكيميائية علاقة قوية بين الواصفات التبولوجية (المؤشرات التبولوجية والمؤشرات التبولوجية المشتركة) للهياكل الجزيئية وخصائصها الفيزيائية والكيميائية، مثل نقطة الغليان، وسمية الأدوية. على الرغم من أن العديد من التقارير البحثية قد ساهمت في حساب المؤشرات التبولوجية لسلسلة البنزينويد سيركوم كورونين، إلا أن الدراسات حول حساب المؤشرات التبولوجية المشتركة محدودة. تركز هذه الورقة على بعض المؤشرات التبولوجية المشتركة. تم اشتقاق العديد من صيغ المؤشرات التبولوجية المشتركة مثل المؤشر المشترك لزغرب الأول والمؤشر المشترك لزغرب الثاني والمؤشر المشترك المنسي والمؤشر اليمني المشترك لسلسلة البنزينويد سيركوم كورونين. بالإضافة إلى ذلك، قدم البحث مؤشرات تبولوجية ومؤشرات تبولوجية مشتركة جديدة مثل مؤشر غزة ومؤشر القدس ومؤشر فلسطين ومؤشراتها المشتركة وصيغها الرياضية لسلسلة البنزينويد سيركوم كورونين. علاوة على ذلك، تم بناء بعض الخوارزميات باستخدام برامج البايثون لتنفيذ الصيغ الرياضية المشتقة بشكل عام.

الكلمات المفتاحية: سلسلة البنزينويد سيركوم كورونين، نظرية الرسم البياني الكيميائي، الرسوم البيانية الجزيئية، المؤشرات التبولوجية المشتركة، المؤشرات التبوبولوجية.