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Geometric Approach to Degree-Based Topological Indices: Cosine-Rule Generalized Sombor Indices

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Abstract

Motivated by the classical cosine rule from the trigonometric geometry, a novel generalization of the Sombor index is proposed. The Cosine-Rule Generalized Sombor index $CoRSO_\theta$ is defined via the expression $\sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}$ where $d(u)$ and $d(v)$ denote the degrees of adjacent vertices, and $\cos\theta$ is the cosine modulator of the degree interaction. The recently proposed variable Euler-Sombor topological index $EU(\lambda, G)$ defined via the expression $\sqrt{d(u)^2 + d(v)^2 + \lambda d(u)d(v)}$ with restricted parameter $\lambda \in [-2, 2]$ is derived from the new index. The functional generalization of the Sombor index is proposed. Mathematical properties of $CoRSO_\theta$ index are established and its chemical applicability is demonstrated.

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1 Introduction

This paper is concerned with simple graphs (i.e undirected, unweighted, and no multiple edges or loops). Let $G = (V(G), E(G))$ be a simple graph with n vertices and m edges, where $V(G) = \{v_1, v_2, \ldots, v_n\}$ is the vertex-set and $E(G)$ is the edge-set. The degree of the vertex u is denoted by $d(u)$. The edge connecting the adjacency vertices u and v is denoted by uv.

Chemical graph theory utilizes topological indices and the principles of graph theory to model molecular structures and predict their physico-chemical properties and biological activities [5, 18]. The IUPAC defines a *topological index* as a numerical value associated with the chemical constitution, used to correlate molecular structure with various physical properties, chemical reactivity or biological activity [28].

A degree-based topological index of a (molecular) graph G denoted by $TI(G)$ is generally defined as

$$TI(G) = \sum_{uv \in E(G)} f(d(u), d(v)) \tag{1}$$

where $f(x, y) \geq 0$ (non-negative and real-valued) such that $f(x, y) = f(y, x)$ (symmetric).

The classical and modern degree-based topological indices along with certain generalizations, have proven highly effective in QSPR and QSAR studies. Examples of these indices include Zagreb indices (M_1 and M_2), Albertson *Alb*, geometric-arithmetic *GA*, atom-bond connectivity *ABC*, sum-connectivity *SCI*, Randić *R*, Sombor *SO*, Elliptic-Sombor *ESO*, Euler-Sombor *EU*, the Diminished Sombor (DSO), and the hyperbolic Sombor *HSO* indices, among others. Despite extensive research on topological indices of (chemical) graphs, there remains a critical need to develop novel generalized indices with enhanced predictive potential.

Recently, in 2021, Ivan Gutman proposed a novel geometric approach for developing degree-based topological indices [12]. Based on an Euclidean geometric perspective he developed a novel degree-based topological index called Sombor index, defined as follows:

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}$$

After his work, a lot of articles that use the geometric approach to develop topological indices have been published, refer to [4, 13, 16, 27] as illustrative examples. Geometric approach attracted many researchers because it provides a base for derivation of the functions $f(x, y)$ used in constructing topological indices. More recently, [14] proposed a variable Euler-Sombor index $EU(\lambda, G)$ defined as follows:

$$EU(\lambda, G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 + \lambda d(u)d(v)}$$

The variable index $EU(\lambda, G)$ constitutes a generalization of recently introduced Euler–Sombor index [27]. This paper presents the geometric derivation of the variable Euler-Sombor index via the cosine rule. Several generalized topological indices involve parametric generalization, see Table 2. This paper introduces a novel functional generalization framework using simple bounded bivariate functions. In summary, this work makes four key contributions:

1. The development of a novel cosine-rule generalization of the Sombor index [12]. The reduced, normalized, diminished, and two-parameter variants are proposed. Mathematical properties of the cosine-rule generalized Sombor index are rigorously established.

2. The paper serves as the base for geometric derivation of the recently introduced variable Euler-Sombor index [14], with parameter λ restricted to the compact interval $[-2, 2]$.

3. The proposal of a novel functional generalization framework based on a bounded function ϕ with range restricted to the interval $[-1, 1]$.

4. Chemical applicability of the novel index is demonstrated. The closed forms of $CoRSO_\theta$ index of certain carbon compounds are derived.

Table 1 contains a not necessarily complete list of functions $f(d(u), d(v))$ used to define the classical and recently introduced degree-based topological indices. The functions are the inputs in the equation (1).

Name of the index	**Year**	$f\left(d(u), d(v)\right)$
First Zagreb [11]	1972	$d(u) + d(v)$
Second Zagreb [11]	1972	$d(u)d(v)$
Randić [23]	1975	$\frac{1}{\sqrt{d(u)d(v)}}$
Albertson [1]	1997	$\lvert d(u) - d(v)\rvert$
Atom-Bond Connectivity [8]	1998	$\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$
Geometric-Arithmetic [29]	2009	$\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$
Sum-Connectivity [30]	2009	$\frac{1}{\sqrt{d(u)+d(v)}}$
Forgotten [10]	2015	$d(u)^2 + d(v)^2$
Sombor [12]	2021	$\sqrt{d(u)^2 + d(v)^2}$
Diminished Sombor [22]	2021	$\frac{\sqrt{d(u)^2+d(v)^2}}{d(u)+d(v)}$
Nirmala [17]	2021	$\sqrt{d(u) + d(v)}$
Atom-Bond-Sum [2, 32]	2022	$\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$
Harmonic-Arithmetic [7]	2023	$\frac{4d(u)d(v)}{\left(d(u)+d(v)\right)^2}$
Euler-Sombor [27]	2024	$\sqrt{d(u)^2 + d(v)^2 + d(u)d(v)}$
Elliptic Sombor [13]	2024	$\left(d(u)+d(v)\right)\sqrt{d(u)^2 + d(v)^2}$
Hyperbolic Sombor [4]	2025	$\frac{\sqrt{d(u)^2+d(v)^2}}{d(u)}$

Table 1. Function forms of certain classical and recently proposed degree-based topological indices

Generalization of topological indices involves defining the indices using the parametric functions $f(x, y; \alpha, \beta, \gamma, \lambda, \dots)$. Table 2 contains a not necessarily complete list of parametric functions $f(d(u), d(v); \alpha, \beta, \gamma, \lambda, \dots)$ used to define the classical and recently introduced generalized degree-based topological indices.

Generalized index	**Year**	$f(d(u), d(v); \alpha, \beta, \gamma, \lambda, \dots)$
Generalized Randić [3]	1998	$(d(u)d(v))^{\alpha}$
Generalized M_1 [20]	2004	$d(u)^{2\lambda}$
Generalized M_2 [20]	2004	$d(u)^{\lambda}d(v)^{\lambda}$
Generalized χ [31]	2010	$(d(u)+d(v))^{\alpha}$
Generalized ISI [6]	2020	$(d(u)d(v))^{\alpha}(d(u)+d(v))^{\beta}$
Generalized ISI [15]	2020	$\dfrac{(d(u)d(v))^{\alpha}}{(d(u)+d(v))^{\beta}}$
Generalized Sombor [24]	2021	$(d(u)^p+d(v)^p)^{\frac{1}{p}}$
Generalized Sombor [19]	2024	$\left(d(u)^2+d(v)^2\right)^{\alpha}$
Generalized EU [14]	2025	$\sqrt{d(u)^2+d(v)^2+\lambda d(u)d(v)}$

Table 2. Parametric function forms used to define certain classical and novel degree-based generalized topological indices

In this paper we present an extension of the recently introduced Sombor and Euler-Sombor degree-based topological indices of (molecular) graphs via the trigonometric-geometric perspective.

2 Generalization of the Sombor index via the cosine rule (the law of cosines)

According to the law of cosines, the sides a, b, and c of any triangle ABC satisfy the three equations:

$$\begin{aligned} a^2 &= b^2 + c^2 - 2bc\cos\alpha \\ b^2 &= a^2 + c^2 - 2ac\cos\gamma \\ c^2 &= a^2 + b^2 - 2ab\cos\theta \end{aligned}$$

where α, γ, and θ denote the angles between the sides AB and AC, BC and AB, and AC and BC, respectively. In the Figure 1, we consider a triangle OAB where O is the origin and $\angle AOB = \theta$.The line segment OA makes angle β with the positive X-axis. Thus, the line segment OB makes an angle $\beta - \theta$ with the positive X-axis. The coordinates of the vertices A and B are given in terms of the sides a and b and angles θ and β.

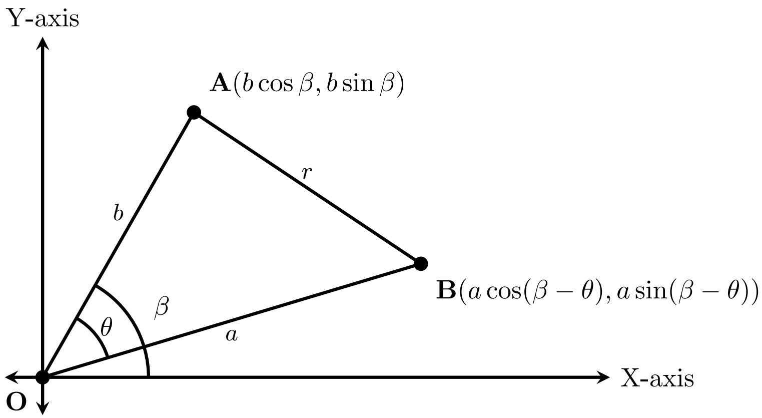

Figure 1. Illustration of the Cosine Rule

We derive the Euclidean distance from vertex A to B as follows:

$$\begin{aligned} r =& \sqrt{(b\cos\beta - a\cos(\beta-\theta))^2 + (b\sin\beta - a\sin(\beta-\theta))^2} \\ =& \sqrt{a^2 + b^2 - 2ab\left[\cos\beta\cos(\beta-\theta) + \sin\beta\sin(\beta-\theta)\right]} \\ =& \sqrt{a^2 + b^2 - 2ab\cos\left[\beta - (\beta-\theta)\right]} \\ \implies r =& \sqrt{a^2 + b^2 - 2ab\cos\theta} \end{aligned}$$

where $\theta \in [0, \pi]$. The expression for r can also be written as an Euclidean norm of the point $(a - b\cos\theta, b\sin\theta)$ as follows:

$$r = \|(a - b\cos\theta, b\sin\theta)\|_2 = \sqrt{a^2 + b^2 - 2ab\cos\theta}$$

Construction of the novel index uses the following parametric function:

$$f_\theta(x, y) = \sqrt{x^2 + y^2 - 2xy\cos\theta} \tag{2}$$

Let $x = d(u)$ and $y = d(v)$ be the degrees of adjacent vertices u and v, respectively. Motivated by the variable Euler-Sombor index recently introduced in [14] and the parametric function (2), we formally define a novel generalized Sombor index, which we refer to it as the *Cosine-Rule Generalized Sombor Index* $CoRSO_\theta$ of a graph G as

$$CoRSO_\theta(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \tag{3}$$

where $\theta \in [0, \pi]$, and consequently $\cos\theta \in [-1, 1]$. The cosine function $\cos\theta$ modulates (or scales) the interaction between the degrees, and accordingly, we refer to it as the cosine modulator. This is the cosine-rule generalization of the Sombor index. Let $(d(u), d(v))$ be the raw degree point of an edge $uv \in E(G)$, the corresponding cosine-rule degree point is given by $(d(u) - d(v)\cos\theta, d(v)\sin\theta)$. Thus, the $CoRSO_\theta$ index (3) can alternatively be interpreted in a sense of the original Sombor index SO by considering the Euclidean norm of the cosine-rule degree point. The Table 3 shows the novel variants of the $CoRSO_\theta$ index for the given standard angles θ.

θ	**Novel Sombor Variant**
$\frac{\pi}{6}$	$CoRSO_{\frac{\pi}{6}}(\mathrm{G}) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 - \sqrt{3}d(u)d(v)}$
$\frac{\pi}{4}$	$CoRSO_{\frac{\pi}{4}}(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 - \sqrt{2}d(u)d(v)}$
$\frac{\pi}{3}$	$CoRSO_{\frac{\pi}{3}}(\mathrm{G}) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 - d(u)d(v)}$
$\frac{3\pi}{4}$	$CoRSO_{\frac{3\pi}{4}}(\mathrm{G}) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 + \sqrt{2}d(u)d(v)}$
$\frac{5\pi}{6}$	$CoRSO_{\frac{5\pi}{6}}(\mathrm{G}) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 + \sqrt{3}d(u)d(v)}$

Table 3. The resultant novel Cosine-Rule Sombor indices for the given standard angles

The Cosine-Rule Sombor indices $CoRSO_0$, $CoRSO_{\frac{\pi}{2}}$, $CoRSO_{\frac{2\pi}{3}}$, and

$CoRSO_\pi$ correspond to the Albertson, Sombor, ordinary Euler-Sombor and first Zagreb indices, respectively.

Considering the superior predictive performance of the reduced Sombor index over the original Sombor index [25], we propose the reduced version of $CoRSO_\theta$ index, defined as:

$$RCoRSO_\theta(G) = \sum_{uv \in E(G)} \sqrt{d_r(u)^2 + d_r(v)^2 - 2\, d_r(u)\, d_r(v) \cos\theta} \tag{4}$$

where $d_r(v) = d(v) - 1$ denote the reduced degree of a vertex v.

By letting $\lambda = -2\cos\theta \in [-2, 2]$ our framework provides a geometric derivation of a variable Euler-Sombor index introduced by [14]. In the same notation, we write a parametric generalization of the Sombor index and Euler-Sombor index as follows:

$$CoRSO_\lambda(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 + \lambda d(u)d(v)} \tag{5}$$

The values $\lambda = 2, -2, 0, 1$ recover the first Zagreb, Albertson, Sombor and, the ordinary Euler-Sombor indices, respectively [14]. Interestingly, the index (5) naturally conforms to the approximation results of $EU(\lambda, G)$ in [14] where

$$\mathrm{EU}(\lambda, G) \approx \frac{\lambda^2}{8}\left(\mathrm{M}_1 + \mathrm{Alb} - 2\mathrm{SO}\right) + \frac{\lambda}{4}\left(\mathrm{M}_1 - \mathrm{Alb}\right) + \mathrm{SO} \tag{6}$$

is best suited for $\lambda \in [-2, 2]$.

We also propose a functional generalization of the Sombor index defined as follows:

$$CoRSO_\phi(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\phi(d(u), d(v))} \tag{7}$$

where $\phi : \mathbb{N} \times \mathbb{N} \to [-1, 1]$ is a bounded bivariate function, that is $-1 \leq \phi(d(u), d(v)) \leq 1$ and $0 < d(u) \leq d(v)$. We give some examples of suitable functions $\phi(d(u), d(v))$ and their range $\subseteq [-1, 1]$ for defining new indices based on the functional generalization $f(d(u), d(v))$ of the $CoRSO_\phi$ index. The kernel functions of the Geometric–Arithmetic (GA) and Harmonic–Arithmetic (HA) indices are bounded within the interval $(0,1]$. That is $\phi_{GA}(x,y) = \frac{2\sqrt{xy}}{x+y} \in (0,1]$ and $\phi_{HA}(x,y) = \frac{4xy}{(x+y)^2} \in (0,1]$. The two functions are simple and therefore can be used to develop a new expression for defining new index using the general index (7). The sigmoid activation function $\sigma(z)$ defined as

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

is a well-known function in the field of machine learning and deep learning. It is a simple function which maps the values of z in the interval $(\frac{1}{2}, 1) \subseteq [-1,1]$ for $z > 0$. We adapt this function and define simple bounded functions of x and y obtained by substituting $z_p = xy$ and $z_s = x+y$. The Sigmoid-Product and Sigmoid-Sum functions are defined as $\phi_{sp}(x,y) = \frac{1}{1+e^{-xy}}$ and $\phi_{ss}(x,y) = \frac{1}{1+e^{-(x+y)}}$, respectively. Table 4 shows some relevant examples of the bounded functions $\phi(d(u), d(v))$ and their corresponding new kernels $f(d(u), d(v))$.

$\phi(d(u), d(v))$	Range	$f(d(u), d(v)), 0 < d(u) \leq d(v)$
$\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$	$(0,1]$	$\sqrt{d(u)^2 + d(v)^2 - \frac{4(d(u)d(v))^{\frac{3}{2}}}{d(u)+d(v)}}$
$\frac{4d(u)d(v)}{(d(u)+d(v))^2}$	$(0,1]$	$\sqrt{d(u)^2 + d(v)^2 - 8\left(\frac{d(u)d(v)}{d(u)+d(v)}\right)^2}$
$\frac{1}{1+e^{-d(u)d(v)}}$	$\left(\frac{1}{2}, 1\right)$	$\sqrt{d(u)^2 + d(v)^2 - \frac{2d(u)d(v)}{1+e^{-d(u)d(v)}}}$
$\frac{1}{1+e^{-(d(u)+d(v))}}$	$\left(\frac{1}{2}, 1\right)$	$\sqrt{d(u)^2 + d(v)^2 - \frac{2d(u)d(v)}{1+e^{-(d(u)+d(v))}}}$

Table 4. Examples of bounded functions $\phi(d(u), d(v))$ and their resultant function forms $f(d(u), d(v))$

Motivated by recent study [4], we also propose a normalized $CoRSO_\theta$

index *NCoRSO(G)*, defined as

$$NCoRSO_\theta(G) = \sum_{uv\in E(G)} \frac{\sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}}{d(u)} \tag{8}$$

where $0 < d(u) \leq d(v)$. The angle $\theta = \frac{\pi}{2}$ recovers the original Hyperbolic Sombor index. Motivated by [22] we also define a Diminished Cosine-Rule Generalized Sombor $DCoRSO_\theta$ index as follows:

$$DCoRSO_\theta(G) = \sum_{uv\in E(G)} \frac{\sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}}{d(u)+d(v)} \tag{9}$$

where $0 < d(u) \leq d(v)$. It is evident that $DCoRSO_{\frac{\pi}{2}}(G) = DSO(G)$ and $DCoRSO_\pi(G) = |E(G)|$. Motivated by the diminished $CoRSO_\theta$ index in eq. (9), we proposed a two-parameter cosine-rule index $CoRSO_{\alpha,\theta}$ as follows:

$$CoRSO_{\alpha,\theta}(G) = \sum_{uv\in E(G)} (d(u)+d(v))^\alpha \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \tag{10}$$

Table 5 presents some special cases of $CoRSO_{\alpha,\theta}$ index.

Topological index	$\boldsymbol{CoRSO_{\alpha,\theta}}$ **index**
Albertson index, $Alb(G)$	$CoRSO_{0,0}(G)$
First Zagreb index, $M_1(G)$	$CoRSO_{0,\pi}(G)$
Sombor index, $SO(G)$	$CoRSO_{0,\frac{\pi}{2}}(G)$
Diminished Sombor index, $DSO(G)$	$CoRSO_{-1,\frac{\pi}{2}}(G)$
Euler-Sombor index, $EU(G)$	$CoRSO_{0,\frac{2\pi}{3}}(G)$
Elliptic Sombor index, $ESO(G)$	$CoRSO_{1,\frac{\pi}{2}}(G)$
First hyper-Zagreb index, $HM_1(G)$	$CoRSO_{1,\pi}(G)$
Variable Euler-Sombor index, $EU(\lambda, G)$	$CoRSO_{0,\theta}(G)$

Table 5. The relationship between $CoRSO_{\alpha,\theta}$ index and other topological indices

3 Mathematical properties of the CoRSO index

In this section, some basic mathematical properties of the CoRSO_θ index are established.

Proposition 1. *Let θ be an angle such that $0 \le \theta \le \pi$, $\theta = \cos^{-1}\left(-\frac{\lambda}{2}\right)$, and $\lambda \in [-2, 2]$ and let CoRSO_θ be the corresponding Cosine–Rule Generalized Sombor index. Then*

$$\mathrm{CoRSO}_\theta(G) = EU(\lambda, G), \tag{11}$$

$$\mathrm{CoRSO}_0(G) = Alb(G), \tag{12}$$

$$\mathrm{CoRSO}_{\frac{\pi}{2}}(G) = SO(G), \tag{13}$$

$$\mathrm{CoRSO}_{\frac{2\pi}{3}}(G) = EU(G), \tag{14}$$

$$\mathrm{CoRSO}_\pi(G) = M_1(G), \tag{15}$$

The equations(11)–(15) *hold for any simple and connected graph G.*

The relations stated in Proposition 1 provides the basic mathematical properties of the novel cosine-rule generalized Sombor index $CoRSO_\theta(G)$.

Proposition 2. *Let P_n, C_n, S_n, and K_n denote the path, cycle, star, and complete graphs on n vertices, respectively. Consider $n \ge 2$ for P_n, $n \ge 3$ for C_n and S_n, and $n \ge 1$ for K_n, then:*

$$\mathrm{CoRSO}_\theta(P_n) = 2\sqrt{5 - 4\cos\theta} + 4(n-3)\sin\left(\frac{\theta}{2}\right)$$

$$\mathrm{CoRSO}_\theta(C_n) = 4n\sin\left(\frac{\theta}{2}\right)$$

$$\mathrm{CoRSO}_\theta(S_n) = (n-1)\sqrt{(n-2)^2 + 4(n-1)\sin^2\left(\frac{\theta}{2}\right)}$$

$$\mathrm{CoRSO}_\theta(K_n) = n(n-1)^2\sin\left(\frac{\theta}{2}\right)$$

Proof. Given a path P_n, $|V(P_n)| = n$ and $|E(P_n)| = n - 1$. The path P_n

has the degree sequence $(1, 2, 2, 2, \ldots, 2, 1)$. So, there are exactly two types of edges $E_{1,2}$ and $E_{2,2}$ such that $|E_{1,2}(P_n)| = 2$ and $|E_{2,2}(P_n)| = n - 3$. Therefore

$$\begin{aligned}
\mathrm{CoRSO}_\theta(P_n) = &\sum_{uv \in E(P_n)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \\
=&2\sqrt{1^2 + 2^2 - 2(1)(2)\cos\theta} + (n-3)\sqrt{2^2 + 2^2 - 2^3\cos\theta} \\
=&2\sqrt{5 - 4\cos\theta} + 2\sqrt{2}(n-3)\sqrt{1 - \cos\theta} \\
=&2\sqrt{5 - 4\cos\theta} + 4(n-3)\sin\left(\frac{\theta}{2}\right)
\end{aligned}$$

Also, given a cycle C_n, $|V(C_n)| = |E(C_n)| = n$. Every vertex of C_n has degree 2. Thus

$$\begin{aligned}
\mathrm{CoRSO}_\theta(C_n) = &\sum_{uv \in E(C_n)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \\
=&n\sqrt{2^2 + 2^2 - 2^3\cos\theta} = 2n\sqrt{2 - 2\cos\theta} = 4n\sin\left(\frac{\theta}{2}\right)
\end{aligned}$$

Similarly, for a star graph S_n, $|V(S_n)| = n$ and $|E(S_n)| = n - 1$. There is only one type of edge $E_{1,n-1}$. Thus

$$\begin{aligned}
\mathrm{CoRSO}_\theta(S_n) = &\sum_{uv \in E(S_n)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \\
=&(n-1)\sqrt{1^2 + (n-1)^2 - 2(n-1)\cos\theta} \\
=&(n-1)\sqrt{1 + (n-1)^2 - 2(n-1)\cos\theta}
\end{aligned}$$

Substituting $\cos\theta = 1 - 2\sin^2\left(\frac{\theta}{2}\right)$, we have

$$\begin{aligned}
\mathrm{CoRSO}_\theta(S_n) =&(n-1)\sqrt{1 + (n-1)^2 - 2(n-1)\left[1 - 2\sin^2\left(\frac{\theta}{2}\right)\right]} \\
=&(n-1)\sqrt{(n-2)^2 - 4(n-1)\sin^2\left(\frac{\theta}{2}\right)}
\end{aligned}$$

In a complete graph K_n, every vertex has degree $d(u) = d(v) = n - 1$.

Then,

$$\begin{aligned}
\mathrm{CoRSO}_\theta(K_n) &= \sum_{uv\in E(K_n)} \sqrt{d(u)^2+d(v)^2-2d(u)d(v)\cos\theta} \\
&= \sum_{uv\in E(K_n)} \sqrt{(n-1)^2+(n-1)^2-2(n-1)^2\cos\theta} \\
&= \sum_{uv\in E(K_n)} \sqrt{2(n-1)^2(1-\cos\theta)} \\
&= \sum_{uv\in E(K_n)} (n-1)\sqrt{2(1-\cos\theta)}
\end{aligned}$$

Substitute $1-\cos\theta = 2\sin^2\left(\frac{\theta}{2}\right)$

$$\begin{aligned}
\mathrm{CoRSO}_\theta(K_n) &= \sum_{uv\in E(K_n)} (n-1)\sqrt{2(1-\cos\theta)} \\
&= \sum_{uv\in E(K_n)} (n-1)\sqrt{4\sin^2\left(\frac{\theta}{2}\right)} \\
&= \sum_{uv\in E(K_n)} 2(n-1)\sin\left(\frac{\theta}{2}\right)
\end{aligned}$$

Since, the compete graph K_n has $m = \binom{n}{2} = \frac{n(n-1)}{2}$ edges, then

$$\begin{aligned}
\mathrm{CoRSO}_\theta(K_n) =& \frac{n(n-1)}{2}\cdot 2(n-1)\sin\left(\frac{\theta}{2}\right) \\
\implies \mathrm{CoRSO}_\theta(K_n) =& n(n-1)^2\sin\left(\frac{\theta}{2}\right)
\end{aligned}$$

■

Theorem 1. *Let G be a simple and connected graph having m edges. Then, for a fixed angle $\theta \in (0,\pi]$, we have:*

$$\mathrm{CoRSO}_\theta(G) \geq 2m\,\sin\left(\frac{\theta}{2}\right)$$

with equality if and only if $G \cong K_2$*. Moreover, the equality*

$$\mathrm{CoRSO}_\theta(G) = 2mr\,\sin\left(\frac{\theta}{2}\right)$$

holds if and only if G *is an* r*-regular graph.*

Proof. For $x, y > 0$ and $\theta \in (0, \pi]$ we have

$$\begin{aligned}
x^2 + y^2 - 2xy\cos\theta =& (x-y)^2 + 2xy(1-\cos\theta)\\
\implies x^2 + y^2 - 2xy\cos\theta \geq& 2xy(1-\cos\theta)\\
\sqrt{x^2 + y^2 - 2xy\cos\theta} \geq& \sqrt{2xy(1-\cos\theta)}\\
\sqrt{x^2 + y^2 - 2xy\cos\theta} \geq& 2\sin\left(\frac{\theta}{2}\right)\sqrt{xy}
\end{aligned}$$

By letting $x = d(u)$ and $y = d(v)$, we get

$$\begin{aligned}
\sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \geq& 2\sin\left(\frac{\theta}{2}\right)\sqrt{d(u)d(v)}\\
\sum_{uv\in E(G)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \geq& 2\sin\left(\frac{\theta}{2}\right)\sum_{uv\in E(G)} \sqrt{d(u)d(v)}
\end{aligned}$$

Since $1 \leq d(u), d(v) \leq 4$, in a simple and connected (molecular) graph, each term $\sqrt{d(u)d(v)} \geq 1$. Thus,

$$\begin{aligned}
\sum_{uv\in E(G)} \sqrt{d(u)d(v)} \geq& m\\
\implies \mathrm{CoRSO}_\theta(G) \geq& 2\sin\left(\frac{\theta}{2}\right)\sum_{uv\in E(G)} \sqrt{d(u)d(v)} \geq 2m\sin\left(\frac{\theta}{2}\right)
\end{aligned}$$

Hence, for any simple and connected graph G of size m, we have

$$\mathrm{CoRSO}_\theta(G) \geq 2m\sin\left(\frac{\theta}{2}\right)$$

If $G \cong K_2$, both vertices have degree $d(u) = d(v) = 1$ and

$$\begin{aligned} \sum_{uv \in E(G)} \sqrt{d(u)d(v)} &= \sum_{uv \in E(G)} 1 = m = 1 \\ \implies \text{CoRSO}_\theta(G) =& 2m \sin\left(\frac{\theta}{2}\right) = 2\sin\left(\frac{\theta}{2}\right) \end{aligned}$$

If G is an r-regular graph, both vertices have degree $d(u) = d(v) = r$. Then

$$\begin{aligned} \sum_{uv \in E(G)} \sqrt{d(u)d(v)} = \sum_{uv \in E(G)} \sqrt{r \cdot r} = \sum_{uv \in E(G)} r = mr \\ \text{CoRSO}_\theta(G) =& 2\sin\left(\frac{\theta}{2}\right) \sum_{uv \in E(G)} \sqrt{d(u)d(v)} = 2mr \sin\left(\frac{\theta}{2}\right) \\ \implies \text{CoRSO}_\theta(G) =& 2mr \sin\left(\frac{\theta}{2}\right) \end{aligned}$$

■

Theorem 2. *Let G be a simple connected graph and $\theta \in \left[\frac{\pi}{2}, \pi\right]$ be a fixed angle. Then,*

$$\sin\left(\frac{\theta}{2}\right) \text{M}_1(G) \leq \text{CoRSO}_\theta(G) \leq \text{M}_1(G)$$

with equality if and only if G is a complete graph.

Proof. For $x, y \geq 0$ and $\theta \in \left[\frac{\pi}{2}, \pi\right]$, we have

$$\begin{aligned} x^2 + y^2 - 2xy \cos\theta =& (x - y)^2 + 2xy(1 - cos\theta) \\ x^2 + y^2 - 2xy \cos\theta =& x^2 + y^2 - 2xy \cos\theta \end{aligned}$$

By AM-GM inequality

$$\frac{a + b}{2} \geq \sqrt{ab}$$

By letting $a = x^2$ and $b = y^2$, we have

$$\begin{aligned} \frac{x^2 + y^2}{2} \geq& xy \implies x^2 + y^2 \geq 2xy \\ \implies x^2 + y^2 - 2xy \cos\theta \geq& x^2 + y^2 - (x^2 + y^2) \cos\theta \end{aligned}$$

$$x^2 + y^2 - 2xy\cos\theta \geq \left(x^2 + y^2\right)(1 - \cos\theta)$$
$$2\sin^2\left(\frac{\theta}{2}\right)\left(x^2 + y^2\right) \leq x^2 + y^2 - 2xy\cos\theta$$
$$\sqrt{2}\sin\left(\frac{\theta}{2}\right)\sqrt{x^2 + y^2} \leq \sqrt{x^2 + y^2 - 2xy\cos\theta}$$

Consider the RMS-AM inequality

$$\sqrt{\frac{x^2 + y^2}{2}} \geq \frac{x + y}{2} \implies \frac{x + y}{\sqrt{2}} \leq \sqrt{x^2 + y^2}$$
$$\implies \sqrt{2}\sin\left(\frac{\theta}{2}\right)\left(\frac{x + y}{\sqrt{2}}\right) \leq \sqrt{x^2 + y^2 - 2xy\cos\theta}$$
$$\sin\left(\frac{\theta}{2}\right)(x + y) \leq \sqrt{x^2 + y^2 - 2xy\cos\theta}$$
$$\sin\left(\frac{\theta}{2}\right)(x + y) \leq \sqrt{x^2 + y^2 - 2xy\cos\theta} \leq x + y$$

By letting $x = d(u)$ and $y = d(v)$ and taking summation over $uv \in E(G)$, we get

$$\sin\left(\frac{\theta}{2}\right)\sum_{uv\in E(G)}(d(u) + d(v)) \leq \sum_{uv\in E(G)}\sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}$$
$$\leq \sum_{uv\in E(G)} d(u) + d(v)$$
$$\implies \sin\left(\frac{\theta}{2}\right)\mathrm{M}_1(G) \leq \mathrm{CoRSO}_\theta(G) \leq \mathrm{M}_1(G) \qquad \blacksquare$$

Theorem 3. *Let G be a simple connected graph and $\theta \in \left[\frac{\pi}{2}, \pi\right]$ be a fixed angle. Then,*

$$\sqrt{2}\sin\left(\frac{\theta}{2}\right)\mathrm{SO}(G) \leq \mathrm{CoRSO}_\theta(G) \leq \mathrm{SO}(G)$$

with equality if and only if G is a complete graph.

Proof. Consider

$$x^2 + y^2 - 2xy\cos\theta = x^2 + y^2 - 2xy\cos\theta$$

By AM-GM inequality of x^2 and y^2, we have

$$\begin{aligned} x^2 + y^2 \geq& 2xy \\ \implies x^2 + y^2 - 2xy\cos\theta \geq& \left(x^2 + y^2\right) - \left(x^2 + y^2\right)\cos\theta \\ x^2 + y^2 - 2xy\cos\theta \geq& \left(x^2 + y^2\right)(1 - \cos\theta) \\ 2\sin^2\left(\frac{\theta}{2}\right)\left(x^2 + y^2\right) \leq& x^2 + y^2 - 2xy\cos\theta \\ \sqrt{2}\sin\left(\frac{\theta}{2}\right)\sqrt{x^2 + y^2} \leq& \sqrt{x^2 + y^2 - 2xy\cos\theta} \end{aligned}$$

$$\implies \sqrt{2}\sin\left(\frac{\theta}{2}\right)\sqrt{x^2 + y^2} \leq \sqrt{x^2 + y^2 - 2xy\cos\theta} \leq \sqrt{x^2 + y^2}$$

By letting $x = d(u)$ and $y = d(v)$ and by taking the summation over all $uv \in E(G)$, we obtain

$$\sqrt{2}\sin\left(\frac{\theta}{2}\right)\mathrm{SO}(G) \leq \mathrm{CoRSO}_\theta(G) \leq \mathrm{SO}(G)$$ ■

Theorem 4. *Let G be a simple connected graph and $\theta \in [0, \pi]$ be a fixed angle. Then*

$$\mathrm{Alb}(G) \leq \mathrm{CoRSO}_\theta(G) \leq \mathrm{M}_1(G)$$

Proof. For $x, y > 0$:

$$\begin{aligned} (x - y)^2 \leq& (x - y)^2 + 2xy(1 - \cos\theta) = x^2 + y^2 - 2xy\cos\theta \\ (x - y)^2 \leq& x^2 + y^2 - 2xy\cos\theta \\ |x - y| \leq& \sqrt{x^2 + y^2 - 2xy\cos\theta} \end{aligned}$$

By letting $x = d(u)$ and $y = d(v)$, we get

$$|d(u) - d(v)| \leq \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}$$

$$\sum_{uv\in E(G)} |d(u)-d(v)| \leq \sum_{uv\in E(G)} \sqrt{d(u)^2+d(v)^2-2d(u)d(v)\cos\theta}$$
$$\implies Alb(G) \leq CoRSO_\theta(G)$$

On the other hand

$$\begin{aligned}(x+y)^2 &\geq (x+y)^2 - 2xy(1+\cos\theta) = x^2+y^2-2xy\cos\theta \\ (x+y)^2 &\geq x^2+y^2-2xy\cos\theta \\ x+y &\geq \sqrt{x^2+y^2-2xy\cos\theta}\end{aligned}$$

By letting $x = d(u)$ and $y = d(v)$, we get

$$\begin{aligned} d(u)+d(v) &\geq \sqrt{d(u)^2+d(v)^2-2d(u)d(v)\cos\theta} \\ \sum_{uv\in E(G)} d(u)+d(v) &\geq \sum_{uv\in E(G)} \sqrt{d(u)^2+d(v)^2-2d(u)d(v)\cos\theta} \\ \implies M_1(G) &\geq CoRSO_\theta(G)\end{aligned}$$

Hence

$$Alb(G) \leq CoRSO_\theta(G) \leq M_1(G) \qquad \blacksquare$$

Theorem 5. *Let G be a simple connected graph and $\theta \in [0,\pi]$ be a fixed angle. Then*

$$\mathrm{CoRSO}_\theta(G) \begin{cases} \leq EU(G) & \textit{if} \quad 0 \leq \theta \leq \frac{2\pi}{3} \\ \geq EU(G) & \textit{if} \quad \frac{2\pi}{3} \leq \theta \leq \pi \end{cases} \tag{16}$$

Proof. For $0 \leq \theta \leq \frac{2\pi}{3}$ $\left(\text{i.e} \quad 1 \leq \cos\theta \leq -\frac{1}{2}\right)$, we have

$$\begin{aligned} x^2+y^2-2xy\cos\theta &\leq x^2+y^2+xy \\ \sqrt{x^2+y^2-2xy\cos\theta} &\leq \sqrt{x^2+y^2+xy}\end{aligned}$$

By letting $x = d(u)$ and $y = d(v)$, and by taking the summation over all $uv \in E(G)$, we obtain

$$CoRSO_\theta(G) \leq EU(G)$$

On the other hand, for $-\frac{1}{2} \le \cos\theta \le -1$ i.e $\frac{2\pi}{3} \le \theta \le \pi$

$$x^2 + y^2 - 2xy\cos\theta \ge x^2 + y^2 + xy$$
$$\sqrt{x^2 + y^2 - 2xy\cos\theta} \ge \sqrt{x^2 + y^2 + xy}$$

By letting $x = d(u)$ and $y = d(v)$, and by taking the summation over all $uv \in E(G)$, we obtain

$$CoRSO_\theta(G) \ge EU(G)$$

Hence

$$CoRSO_\theta(G) \begin{cases} \le \text{EU}(G) & \text{if} \quad 0 \le \theta \le \frac{2\pi}{3} \\ \ge \text{EU}(G) & \text{if} \quad \frac{2\pi}{3} \le \theta \le \pi \end{cases} \qquad \blacksquare$$

Theorem 6. *Let G be a simple graph and $\theta \in [0, \frac{\pi}{2}]$ be a fixed angle. Then*

$$Alb(G) \le CoRSO_\theta(G) \le SO(G)$$

Proof. For $0 \le \theta \le \frac{\pi}{2}$ (i.e $0 \le \cos\theta \le 1$)

$$x^2 + y^2 - 2xy\cos\theta \ge x^2 + y^2 - 2xy = (x-y)^2$$
$$|x - y| \le \sqrt{x^2 + y^2 - 2xy\cos\theta}$$

By letting $x = d(u)$ and $y = d(v)$, we get

$$|d(u) - d(v)| \le \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}$$
$$\sum_{uv \in E(G)} |d(u) - d(v)| \le \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}$$
$$\implies Alb(G) \le CoRSO_\theta(G)$$

On the other hand, for $0 \le \theta \le \frac{\pi}{2}$ (i.e $0 \le \cos\theta \le 1$)

$$x^2 + y^2 - 2xy\cos\theta \le x^2 + y^2$$
$$\sqrt{x^2 + y^2 - 2xy\cos\theta} \le \sqrt{x^2 + y^2}$$

By letting $x = d(u)$ and $y = d(v)$, we have

$$\sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \leq \sqrt{d(u)^2 + d(v)^2}$$

$$\sum_{uv\in E(G)} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta} \leq \sum_{uv\in E(G)} \sqrt{d(u)^2 + d(v)^2}$$

$$\implies CoRSO_\theta(G) \leq SO(G)$$

Hence

$$Alb(G) \leq CoRSO_\theta(G) \leq SO(G) \qquad \blacksquare$$

4 Chemical applicability of the Cosine-Rule Generalized Sombor index

One of the key contributions of this study is the geometric derivation of the variable Euler-Sombor index $EU(\lambda, G)$ with $\lambda \in [-2, 2]$ recently introduced in [27]. To demonstrate the chemical applicability of the variable Euler-Sombor index, [27] considered the standard entropy S^0 of the octane isomers. In light of Eq. (6), the model $EU(\lambda, G)+0.5EU(-\lambda, G)$ gives the best performance under the following unique combination of topological indices:

$$S^0 = 70.179375M_1(G) - 0.004375Alb(G) + 1.315250SO(G)$$

In addition, the chemical applications of the $CoRSO_\theta$ index discussed in this paper focus on derivation of closed forms of $CoRSO_\theta$ index of three carbon allotropes namely graphene G, carbon graphite CG, and crystal cubic structure of carbon CCC. This application is motivated by the computation of some topological indices for certain chemical structures, see for example [6, 17, 26].

Graphene is a single layer of carbon atoms arranged in a hexagonal honeycomb lattice. It is recognized as the world's two dimensional organic material. The stack of multiple graphene layers is known as graphite. Graphene and graphite have many real life applications. For example, graphene are useful in production of high-speed transistors, flexible electronic circuits, transparent conductive film, and sensors. Graphene is also used to make photodetectors and touchcreens of smart phones and optical devices. Graphite is useful in producing electrodes, batteries, strong fibers, gas absorbers, pencils (lead) and coatings. It is also used as a moderator and reflector in nuclear reactors. The crystal cubic structure of carbon is a three-dimensional carbon allotrope consisting of carbon atoms arranged in a periodic cubic lattice with t levels. The vertex degrees of the $CCC[t]$ molecular graph are either 3 or 4 depending on the stomic position. In real life, CCC is used to produce superhard coatings, semiconductors, energy storage, and thermal devices.

The number of vertices and edges of graphene are, respectively, given by

$$|V(G(m,n))| = 2mn + 2m + 2n$$
$$|E(G(m,n))| = 3mn + 2m + 2n - 1$$

The degree of adjacent vertices of molecular graph of graphene with m rows and n benzene ring per row can be partitioned into three parts as follows:

$$E_{22}(G(m,n)) = \{uv \in E(G(m,n)) : d(u) = 2 \text{ and } d(v) = 2\},$$
$$E_{23}(G(m,n)) = \{uv \in E(G(m,n)) : d(u) = 2 \text{ and } d(v) = 3\},$$
$$E_{33}(G(m,n)) = \{uv \in E(G(m,n)) : d(u) = 3 \text{ and } d(v) = 3\}.$$

The cardinality of the edge partitions are given as follows:

$$|E_{22}(G(m,n))| = m + 4,$$
$$|E_{23}(G(m,n))| = 4n + 2m - 4,$$
$$|E_{33}(G(m,n))| = 3mn - 2n - m - 1.$$

In the following theorem, we derive the $CoRSO_\theta$ index for the molecular graph of graphene.

Theorem 7. *The* CoRSO_θ *index of graphene G with m rows and n ben-*

zene rings in each row is given by

$$\mathrm{CoRSO}_\theta(G(m,n)) = 2\sin\left(\frac{\theta}{2}\right) f(m,n) + \left(2\sqrt{13-12\cos\theta}\right) g(m,n)$$

where

$$\begin{aligned} f(m,n) =& 9mn - 6n - m + 5 \\ g(m,n) =& 2n + m - 2 \end{aligned}$$

Proof. By definition:

$$\mathrm{CoRSO}_\theta(G(m,n)) = \sum_{uv\in E(G(m,n))} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}$$

By substituting the degrees $d(u)$ and $d(v)$ of $G(m,n)$, we have:

$$\begin{aligned} \mathrm{CoRSO}_\theta(G(m,n)) =& \sum_{uv\in E_{22}(G(m,n))} \sqrt{2^2+2^2-2^3\cos\theta} \\ &+ \sum_{uv\in E_{2,3}(G(m,n))} \sqrt{2^2+3^2-4\cdot 3\cos\theta} \\ &+ \sum_{uv\in E_{33}(G(m,n))} \sqrt{3^2+3^2-2\cdot 3^2\cos\theta} \\ =& \sum_{uv\in E_{22}(G(m,n))} \sqrt{8-8\cos\theta} \\ &+ \sum_{uv\in E_{2,3}(G(m,n))} \sqrt{13-12\cos\theta} \\ &+ \sum_{uv\in E_{33}(G(m,n))} \sqrt{18-18\cos\theta} \\ =& \sum_{uv\in E_{22}(G(m,n))} 2\sqrt{2-2\cos\theta} \\ &+ \sum_{uv\in E_{23}(G(m,n))} \sqrt{13-12\cos\theta} \\ &+ \sum_{uv\in E_{33}(G(m,n))} 3\sqrt{2-2\cos\theta} \\ =& \left(2\left|E_{22}(G(m,n))\right| + 3\left|E_{33}(G(m,n))\right|\right)\sqrt{2-2\cos\theta} \end{aligned}$$

$$
\begin{aligned}
&+ |E_{23}(G(m,n))| \sqrt{13-12\cos\theta} \\
&= (2(m+4) + 3(3mn-2n-m-1)) \sqrt{2-2\cos\theta} \\
&+ (4n+2m-4)\sqrt{13-12\cos\theta} \\
&=(9mn-6n-m+5)\sqrt{2-2\cos\theta} \\
&+ (4n+2m-4)\sqrt{13-12\cos\theta}
\end{aligned}
$$

Substituting $\sqrt{2-2\cos\theta} = 2\sin\left(\frac{\theta}{2}\right)$, we obtain

$$
\begin{aligned}
\mathrm{CoRSO}_\theta(G(m,n)) =&(9mn-6n-m+5)\cdot 2\sin\left(\frac{\theta}{2}\right) \\
&+ (2n+m-2)\left(2\sqrt{13-12\cos\theta}\right)
\end{aligned}
$$

Hence

$$
\mathrm{CoRSO}_\theta(G(m,n)) =2\sin\left(\frac{\theta}{2}\right) f(m,n) + \left(2\sqrt{13-12\cos\theta}\right) g(m,n)
$$

where

$$
\begin{aligned}
f(m,n) =&9mn-6n-m+5 \\
g(m,n) =&2n+m-2
\end{aligned}
$$

■

The degrees of adjacent vertices of carbon graphite's molecular graph provide six edge-types defined as:

$$E_{22}(CG[r,s]) = \{\, uv \in E(CG[r,s]) : d(u) = 2 \text{ and } d(v) = 2 \,\},$$

$$E_{23}(CG[r,s]) = \{\, uv \in E(CG[r,s]) : d(u) = 2 \text{ and } d(v) = 3 \,\},$$

$$E_{24}(CG[r,s]) = \{\, uv \in E(CG[r,s]) : d(u) = 2 \text{ and } d(v) = 4 \,\},$$

$$E_{33}(CG[r,s]) = \{\, uv \in E(CG[r,s]) : d(u) = 3 \text{ and } d(v) = 3 \,\},$$

$$E_{34}(CG[r,s]) = \{\, uv \in E(CG[r,s]) : d(u) = 3 \text{ and } d(v) = 4 \,\},$$

$$E_{44}(CG[r,s]) = \{\, uv \in E(CG[r,s]) : d(u) = 4 \text{ and } d(v) = 4 \,\}.$$

The cardinalities of the edge partitions of $CG([r,s])$ are given by,

$$|E_{22}(CG[r,s])| = 4,$$

$$|E_{23}(CG[r,s])| = 4(s+t-1),$$

$$|E_{24}(CG[r,s])| = 4(st+r-s-t),$$

$$|E_{33}(CG[r,s])| = 4r+4t-10,$$

$$|E_{34}(CG[r,s])| = 6rs+6rt-14r-4s-6t+12,$$

$$|E_{44}(CG[r,s])| = (4rs-3r-2s+1)t-7rs+5r+4s-2.$$

In the following theorem, we derive the $CoRSO_\theta$ index for the molecular graph of carbon graphite.

Theorem 8. *The $CoRSO_\theta$ index of carbon graphite CG with r rows of benzene rings, s benzene rings per row, and t levels is given by*

$$\begin{aligned}\mathrm{CoRSO}_\theta(CG[r,s]) =& 2\sin\left(\frac{\theta}{2}\right)A(r,s,t) + \left(\sqrt{13-12\cos\theta}\right)B(r,s,t) + \\ & \left(\sqrt{5-4\cos\theta}\right)C(r,s,t) + \left(\sqrt{25-24\cos\theta}\right)D(r,s,t)\end{aligned}$$

where

$$A(r,s,t) = 2\big(8rst-6rt-4st-14rs+16r+8s+8t-15\big),$$

$$B(r,s,t) = 4(s+t-1),$$

$$C(r,s,t) = 8(st+r-s-t),$$

$$D(r,s,t) = 2(3rs+3rt-7r-2s-3t+6)$$

Proof.

$$\begin{aligned}\mathrm{CoRSO}_\theta(CG[r,s]) = & \sum_{uv\in E_{22}}\sqrt{2^2+2^2-2{\cdot}2{\cdot}2\cos\theta} + \sum_{uv\in E_{23}}\sqrt{2^2+3^2-2{\cdot}2{\cdot}3\cos\theta} \\ & + \sum_{uv\in E_{24}}\sqrt{2^2+4^2-2{\cdot}2{\cdot}4\cos\theta} + \sum_{uv\in E_{33}}\sqrt{3^2+3^2-2{\cdot}3{\cdot}3\cos\theta} \\ & + \sum_{uv\in E_{34}}\sqrt{3^2+4^2-2{\cdot}3{\cdot}4\cos\theta} + \sum_{uv\in E_{44}}\sqrt{4^2+4^2-2{\cdot}4{\cdot}4\cos\theta}.\end{aligned}$$

Substituting $\sqrt{2-2\cos\theta} = 2\sin\left(\frac{\theta}{2}\right)$, we get

$$\sqrt{2\cdot 2^2 - 8\cos\theta} = 4\sin\left(\frac{\theta}{2}\right),$$
$$\sqrt{2\cdot 3^2 - 18\cos\theta} = 6\sin\left(\frac{\theta}{2}\right),$$
$$\sqrt{2\cdot 4^2 - 32\cos\theta} = 8\sin\left(\frac{\theta}{2}\right).$$

and other radicals simplify to

$$\sqrt{2^2+3^2-12\cos\theta} = \sqrt{13-12\cos\theta},$$
$$\sqrt{2^2+4^2-16\cos\theta} = 2\sqrt{5-4\cos\theta},$$
$$\sqrt{3^2+4^2-24\cos\theta} = \sqrt{25-24\cos\theta}.$$

Hence

$$\begin{aligned}\mathrm{CoRSO}_\theta(CG[r,s]) = \sin\left(\frac{\theta}{2}\right)&(4\,|E_{22}| + 6\,|E_{33}| + 8\,|E_{44}|)\\ &+ \sqrt{13-12\cos\theta}\,|E_{23}| + 2\sqrt{5-4\cos\theta}\,|E_{24}|\\ &+ \sqrt{25-24\cos\theta}\,|E_{34}|.\end{aligned}$$

Substituting the cardinalities of edge partitions, we get

$$\begin{aligned}\mathrm{CoRSO}_\theta(CG[r,s]) =& 2\sin\left(\frac{\theta}{2}\right)A(r,s,t) + \left(\sqrt{13-12\cos\theta}\right)B(r,s,t) +\\ &\left(\sqrt{5-4\cos\theta}\right)C(r,s,t) + \left(\sqrt{25-24\cos\theta}\right)D(r,s,t)\end{aligned}$$

where

$$A(r,s,t) = 2\big(8rst - 6rt - 4st - 14rs + 16r + 8s + 8t - 15\big),$$

$$B(r,s,t) = 4(s+t-1),$$

$$C(r,s,t) = 8(st + r - s - t),$$

$$D(r,s,t) = 2(3rs + 3rt - 7r - 2s - 3t + 6)$$

■

The number of vertices $n = |V(CCC[t])|$ and edges $m = |E(CCC[t])|$ in the molecular graph of crystal cubic structure of carbon for $t \geq 3$ layers are respectively given by:

$$n = 2\left\{24\sum_{r=3}^{t}\left(2^3-1\right)^{r-3} + 31\left(2^3-1\right)^{t-2} + 2\sum_{r=0}^{t-2}\left(2^3-1\right)^{r} + 3\right\},$$

and

$$m = 4\left\{24\sum_{r=3}^{t}\left(2^3-1\right)^{r-3} + 24\left(2^3-1\right)^{t-2} + 2\sum_{r=0}^{t-2}\left(2^3-1\right)^{r} + 3\right\}.$$

The degree of the adjacent vertices of the molecular graph of crystal cubic structure of carbon gives the following edge-types:

$$E_{33}(CCC[t]) = \{\, uv \in E(CCC[t]) : d(u) = 3 \text{ and } d(v) = 3\,\},$$

$$E_{34}(CCC[t]) = \{\, uv \in E(CCC[t]) : d(u) = 3 \text{ and } d(v) = 4\,\},$$

$$E_{44}(CCC[t]) = \{\, uv \in E(CCC[t]) : d(u) = 4 \text{ and } d(v) = 4\,\}.$$

where the cardinality of these edge sets are given as follows:

$$|E_{33}(CCC[t])| = 72(2^3-1)^{t-2},$$

$$|E_{34}(CCC[t])| = 24(2^3-1)^{t-2},$$

$$|E_{44}(CCC[t])| = 12\left(1 + \sum_{i=3}^{t} 2^3(2^3-1)^{i-3}\right) + 8\sum_{i=0}^{t-2}(2^3-1)^{i}.$$

In the following theorem, we derive the $CoRSO_\theta$ index for the molecular graph of crystal cubic structure of carbon.

Theorem 9. *The* CoRSO_θ *index of crystal cubic structure of carbon CCC* *with t levels is given by*

$$\mathrm{CoRSO}_\theta\big(\mathrm{CCC}[t]\big) = 7^{\,t-2}\left(\frac{1904}{3}\,\sigma + 24\sqrt{1+48\sigma^2}\right) - \frac{128}{3}\,\sigma.$$

where $\sigma = \sin\big(\frac{\theta}{2}\big)$.

Proof. By definition, we have

$$\mathrm{CoRSO}_\theta(CCC[t]) = \sum_{uv\in E(CCC[t])} \sqrt{d(u)^2 + d(v)^2 - 2d(u)d(v)\cos\theta}.$$

Using the identity $\sqrt{2-2\cos\theta} = 2\sin\left(\frac{\theta}{2}\right)$, we have

$$\sqrt{3^2+3^2-2\cdot 3\cdot 3\cos\theta} = 6\sin\left(\frac{\theta}{2}\right),$$

$$\sqrt{4^2+4^2-2\cdot 4\cdot 4\cos\theta} = 8\sin\left(\frac{\theta}{2}\right),$$

and

$$\sqrt{3^2+4^2-2\cdot 3\cdot 4\cos\theta} = \sqrt{1+48\sin^2\left(\frac{\theta}{2}\right)}.$$

Hence, by letting $\sigma = \sin\left(\frac{\theta}{2}\right)$, we have

$$\mathrm{CoRSO}_\theta\big(\mathrm{CCC}[t]\big) = 6\sigma|E_{33}| + 8\sigma|E_{44}| + |E_{34}|\sqrt{1+48\sigma^2}.$$

Using geometric-series sums, we simplify $|E_{44}|$ as follows:

$$\sum_{i=3}^{t} 2^3 7^{i-3} = 8\sum_{k=0}^{t-3} 7^k = 8\cdot\frac{7^{\,t-2}-1}{7-1} = \frac{4}{3}\big(7^{t-2}-1\big),$$

$$\sum_{i=0}^{t-2} 7^i = \frac{7^{t-1}-1}{7-1} = \frac{7^{t-1}-1}{6}.$$

Then,

$$|E_{44}| = 12\left(1+\frac{4}{3}(7^{t-2}-1)\right) + 8\cdot\frac{7^{t-1}-1}{6} = \frac{76}{3}7^{t-2} - \frac{16}{3}.$$

Substituting the number of edges, we get

$$\operatorname{CoRSO}_\theta(CCC[t]) = 6\sigma\big(72 \cdot 7^{\,t-2}\big) + \sqrt{1+48\sigma^2}\big(24 \cdot 7^{t-2}\big) + 8\sigma\left(\frac{76}{3}\,7^{\,t-2} - \frac{16}{3}\right).$$

Factoring 7^{t-2}, we get

$$\operatorname{CoRSO}_\theta\big(\mathrm{CCC}[t]\big) = 7^{\,t-2}\left(\frac{1904}{3}\,\sigma + 24\sqrt{1+48\sigma^2}\right) - \frac{128}{3}\,\sigma. \qquad \blacksquare$$

5 Conclusion

In this paper, we introduced the Cosine-Rule Generalized Sombor index ($CoRSO_\theta$), whose formulation is motivated by the cosine law from the trigonometric geometry. The reduced, normalized, diminished, and two-parameter generalized $CoRSO_\theta$ variants are proposed. This paper presents a geometric derivation of the variable Euler–Sombor index. The novel functional generalization framework is proposed. Graph-theoretic properties of the $CoRSO_\theta$ index are rigorously established. In addition, the analytical expressions of the $CoRSO_\theta$ index of graphene, carbon graphite, and crystal cubic structures of carbon are derived. All topological indices and analytical formulas presented in this article could emerge as promising alternatives for QSPR analysis.

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