Research Article

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On topological descriptors of ceria oxide and their applications

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Abstract: A topological descriptor is a mathematical illustration of a molecular construction that relates particular physicochemical properties of primary molecular structure as well its mathematical depiction. Topological co-indices are usually applied for quantitative structure actions relationships (QSAR) and quantitative structures property relationships (QSPR). Topological co-indices are topological descriptors which are considered the noncontiguous vertex set. We study the accompanying some renowned topological co-indices: first and second Zagreb co-indices, first and second multiplicative Zagreb co-indices and the F-coindex, and some other degree-based indices of the co-indices of ceria oxide.

Keywords: topological co-indices, cuprite, Zagreb types co-index, atom-bond connectivity co-index, ceria oxide

1 Introduction

In graph theory, a vertex describes an atom and edges bonds between atoms. A topological descriptor is a mathematical entity which is handled methodically on the atomic structure. Which is linked with copied composition displaying for relationships among the substances of the structure through several physical, chemical characteristics. Topological descriptors of some nanostar dendrimers studied and plotted in Imran et al. (2016) and Siddiqui et al. (2016)."

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Topological index is a mathematical parameter of a structure which depict the topology and generally structure invariants. In QSAR/QSPR research, physicochemical characteristics, and topological co-indices such as Randic, atom bond connectivity and geometric arithmetic coindices are utilized to forecast bio activity of molecular structure. Graph theory has observed a substantial usage in this part of study."

Many molecular compounds are vital for the existence of alive things. Many molecular structures are important for the existence of alive thing. Such as carbon, oxygen, hydrogen, and nitrogen help in construction of living cells. Carbon is a vital element for alive cells. Carbon is valuable in creation of protein, carbohydrate, and nucleic acid. It is vibrant for development of plant in forms of carbon dioxide. The carbon atom link composed in numerous states, named allotrope of carbons. The renowned form is graphite and diamonds. Lately, numerous innovative forms have been revealed together with nanotubes, buck minster fullerenes, and sheet, crystals cubic structures."

Let G be a chemical graph, this graph is simple connected with set of atoms $V(G)$ and set of bonds $E(G)$. Degree $\Xi(v)$ of an atom $v \in V(G)$ is the amount of neighboring atoms to v . A simple connected structure is called r regular, if each atom of G has exactly r -neighbour. Complement of a structure G that is represented as $\bar{G}$ is a structure with the same set of atoms $V(G)$, and any two atoms $uv \in E(G)$ if and only if $uv \notin E(G)$.

Zagreb and Randic indices are amongst the eldest and utmost completely researched structure-based topological descriptor along with various application. The first Zagreb $\bar{M}_1$ index and second $\bar{M}_2$ Zagreb index was defined by Gutman and Trinajstic (Doslic, 2008) and give a relation with the total π -electron energy (ϵ) of a structure, in which estimated formulations of the total π -electron energy (ϵ). These co-indices deliver a quantity of the separating of the carbon-atoms skeletons. These indices are defined as follows:

$$\bar{M}_1(G) = \sum_{uv \in \bar{E}(G)} (\S(u) + \S(v)) \quad (1)$$

$$\bar{M}_2(G) = \sum_{uv \in \bar{E}(G)} (\S(u) \times \S(v)) \quad (2)$$

Recently, multiplicative Zagreb co-indices are studied by Xu et al. (2013), these indices are counted as the multiplicative version of Zagreb co-indices and studied few characteristics and upper bound and lower bound of a structure, and defined as:

$$\bar{\Pi}_1(G) = \prod_{uv \in \bar{E}(G)} (\S(u) + \S(v)) \quad (3)$$

$$\bar{\Pi}_2(G) = \prod_{uv \in \bar{E}(G)} (\S(u) \times \S(v)) \quad (4)$$

De et al. (2016) presented the F-co-index of a structure, symbolized by $\bar{F}$; later attesting that correlation coefficient amongst the logarithm of octanol-water divider number ($\log(P)$) and the equivalent F-co-index value of octane isomer is learnt to be approximately 0.996 that show F-co-index can also forecast the $\log(P)$ value with great precision. F co-index is formulated as:

$$\bar{F}(G) = \sum_{uv \in \bar{E}(G)} (\S(u)^2 + \S(v)^2) \quad (5)$$

Atom bond connective index is renowned connectivity topological descriptor defined by Estrada et al. (1998):

$$\overline{ABC}(G) = \sum_{uv \in \bar{E}(G)} \sqrt{\frac{(\S(u) + \S(v)) - 2}{\S(u)\S(v)}} \quad (6)$$

Second very important topological index is geometric arithmetic, defined by Vukicevic and Furtula (2009):

$$\overline{GA}(G) = \sum_{uv \in \bar{E}(G)} \frac{2\sqrt{\S(u) \times \S(v)}}{\S(u) + \S(v)} \quad (7)$$

We will use Lemma 1 to calculate the equations below.

For $i = j = 4$;

$$\begin{aligned} \bar{m}_{44} &= |\bar{E}_{44}| = \frac{n_4(n_4 - 1)}{2} - m_{44} \\ &= \frac{1}{2}((8pqt + 2pq + 2pt + 2qt + p + q + t + 5)(8pqt + 2pq + 2pt + 2qt + p + q + t + 5 - 1)) \\ &\quad - (16pqt + 4pq + 4pt + 4qt + 2p + 2q + 2t + 10) \end{aligned}$$

First topological index constructed on degree of a structure is Randic index (Randic, 1975) presented by Milan Randic. The general Randic co-index was defined as:

$$\bar{R}_\alpha(G) = \sum_{uv \in \bar{E}(G)} (\S(u) \times \S(v))^\alpha; \quad \alpha = 1, -1, \frac{1}{2}, -\frac{1}{2} \quad (8)$$

Lemma 1

For a simple graph G order n with where n_i are amount vertices with degrees i and m_{ij} are the amount of edges joining the vertex of degree i with the vertex of degree j (Berhe and Wang, 2019). Then, for:

$$\begin{aligned} \bar{E}_{ij} &= \{uv \in \bar{E}(G) | \S(u) = i, \text{ and } \S(v) = j\} \\ \bar{m}_{ij} &= |\bar{E}_{ij}| = \begin{cases} \frac{n_i(n_i - 1)}{2} - m_{ii}, & i = j \\ n_i n_j - m_{ij}, & i < j \end{cases} \end{aligned}$$

In this paper, we study the result for ceria oxide CeO_2 and computed analytically close results of first, second Zagreb and multiplicative Zagreb, forgotten, atom bond connectivity, geometric-arithmetic, and general Randic co-indices for different values of α , for result for ceria oxide CeO_2 .

2 Result for ceria oxide CeO_2

Let $G \cong \text{CeO}_2[p, q, r]$ be the structure of CeO_2 with $p \times q$ unit cell and t layers. We create the structure by choosing first $p \times q$ units in the pq -plane after that joining them up in t layers see Figure 1. The cardinality of vertex and edge set of $\text{CeO}_2[p, q, t]$ are $12pqt + 2pq + 2pt + 2qt + p + q + t + 1$ and $22pqt + 4pq + 4pt + 4qt + 2p + 2q + 2t + 4$, respectively. As, three types of vertices are in $\text{CeO}_2[p, q, t]$ namely, the vertices of degree 4, 6, and 8. The partitions of the vertex set of $\text{CeO}_2[p, q, t]$ are given in Table 1. Also, the edge partitions of $\text{CeO}_2[p, q, t]$ constructed on degree of end vertices of edges are given in Table 2.

$$\begin{aligned}\bar{m}_{44} = & 32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + 12p^2qt + \\ & 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \frac{1}{2}t^2 + 2p^2q^2 + \\ & 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \frac{5}{2}t.\end{aligned}$$

Figure 1: (a) CeO₂ crystal unit is shown in cubic fluorite lattice; (b) constructions of Ce and O atoms by joining the unit cells of CeO₂ in the x, y, and z axis in 3-orthonormal sides (c) supercells of cubical CNP of ~1 nm for relaxation calculations; (d) zoomed picture of the solid collection of atoms (c) to illustrate the crystal construction of {001} - terminat CNPs. Yellow nodes represent Ce atom, purple nodes represent O atom, and blue nodes represents probable cover of O grid which can be partly or completely filled by either distinct O atom or OH.

Table 1: Vertex partition of CeO₂ [p, q, t] based on degree of vertex

(S(u))	Frequency	Set of vertices
4	$8pqt + 2pq + 2pt + 2qt + p + q + t + 5$	n_4
6	$2pqt - pq - pt - qt + p + q + t - 2$	n_6
8	$2pqt + pq + pt + qt - p - q - t - 2$	n_8

Table 2: Edge partition of CeO₂ [p, q, t] based on degrees of end vertices

(S(u), S(v))	Frequency	Set of edges
(4,4)	$16pqt + 4pq + 4pt + 4qt + 2p + 2q + 2t + 10$	m_{44}
(4,6)	$2pqt + 2pq + 2pt + 2qt - p - q - t - 5$	m_{46}
(4,8)	$2pqt - pq - pt - qt + 1$	m_{48}
(6,6)	$2pqt - pq - pt - qt + p + q + t - 2$	m_{66}

For $i = 4, j = 6$;

$$\begin{aligned}\bar{m}_{46} &= |\bar{E}_{46}| = n_4 n_6 - m_{46} \\ &= (8pqt + 2pq + 2pt + 2qt + p + q + t + 5)(2pqt - pq - pt - qt + p + q + t - 2) \\ &\quad - (2pqt + 2pq + 2pt + 2qt - p - q - t - 5) \\ \bar{m}_{46} &= 16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - 2p^2t^2 + p^2t + \\ &\quad p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + pt^2 - 9pt + 4p - \\ &\quad 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5.\end{aligned}$$

For $i = 4, j = 8$;

$$\begin{aligned}\bar{m}_{48} &= |\bar{E}_{48}| = n_4 n_8 - m_{48} \\ &= (8pqt + 2pq + 2pt + 2qt + p + q + t + 5)(2pqt + pq + pt + qt - p - q - t - 2) \\ &\quad - (2pqt - pq - pt - qt + 1) \\ \bar{m}_{48} &= 16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + 2p^2t^2 - \\ &\quad 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\ &\quad pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11.\end{aligned}$$

For $i = j = 6$;

$$\begin{aligned}\bar{m}_{66} &= |\bar{E}_{66}| = \frac{n_6(n_6-1)}{2} - m_{66} \\ &= \frac{1}{2}(2pqt - pq - pt - qt + p + q + t - 2)(2pqt - pq - pt - qt + p + \\ &\quad q + t - 2 - 1) - (2pqt - pq - pt - qt + p + q + t - 2) \\ \bar{m}_{66} &= 5 - p^2t - pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \\ &\quad \frac{1}{2}p^2 + \frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - \\ &\quad 2pq^2t^2 - 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t.\end{aligned}$$

2.1 First Zagreb co-index of CeO_2 [p, q, t]

$$\begin{aligned}\bar{M}_1(G) &= \sum_{uv \in \bar{E}(G)} (\S(u) + \S(v)) \\ &= (4 + 4)\bar{m}_{44} + (4 + 6)\bar{m}_{46} + (4 + 8)\bar{m}_{48} + (6 + 6)\bar{m}_{66} \\ &= (4 + 4)\bar{m}_{44} + (4 + 6)\bar{m}_{46} + (4 + 8)\bar{m}_{48} + (6 + 6)\bar{m}_{66} \\ &= 8 \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\ &\quad 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\ &\quad \left. \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \right. \\ &\quad \left. \frac{5}{2}t \right) + 10 \left(16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \right. \\ &\quad 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\ &\quad pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\ &\quad 12(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt\end{aligned}$$

$$\begin{aligned}
& + 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
& pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + 12(5 - p^2t - \\
& pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \\
& \frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
& 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t)
\end{aligned}$$

$$\begin{aligned}
\bar{M}_1(G) &= 632p^2q^2t^2 + 208p^2q^2t + 26p^2q^2 + 208p^2qt^2 + 168p^2qt + 2p^2q + \\
& 26p^2t^2 + 2p^2t + 8p^2 + 208pq^2t^2 + 168pq^2t + 2pq^2 + 168pqt^2 - \\
& 94pqt + 12pq + 2pt^2 + 12pt - 66p + 26q^2t^2 + 2q^2t + 8q^2 + \\
& 2qt^2 + 12qt - 66q + 8t^2 - 66t - 122.
\end{aligned}$$

2.2 Second Zagreb co-index of CeO_2 [p, q, t]

$$\begin{aligned}
\bar{M}_2(G) &= \sum_{uv \in E(G)} (\S(u) \times \S(v)) \\
&= (4 \times 4) \bar{m}_{44} + (4 \times 6) \bar{m}_{46} + (4 \times 8) \bar{m}_{48} + (6 \times 6) \bar{m}_{66} \\
&= 16 \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
& 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
& \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
& \left. \frac{5}{2}t \right) + 24(16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
& 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
& pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
& 32(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
& 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
& pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + 36(5 - p^2t - \\
& pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \\
& \frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
& 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t)
\end{aligned}$$

$$\begin{aligned}
\bar{M}_2(G) &= 1480p^2q^2t^2 + 472p^2q^2t + 66p^2q^2 + 472p^2qt^2 + 380p^2qt - \\
& 12p^2q + 66p^2t^2 - 12p^2t + 18p^2 + 472pq^2t^2 + 380pq^2t - 12pq^2 + \\
& 380pqt^2 - 416pqt + 42pq - 12pt^2 + 42pt - 214p + 66q^2t^2 - \\
& 12q^2t + 18q^2 - 12qt^2 + 42qt - 214q + 18t^2 - 214t - 292.
\end{aligned}$$

2.3 First multiplicative Zagreb co-index of CeO_2 [p, q, t]

$$\begin{aligned}
 \bar{\Pi}_1(G) &= \prod_{uv \in \bar{E}(G)} (\S(u) + \S(v)) \\
 &= (4 + 4) \bar{m}_{44} \times (4 + 6) \bar{m}_{46} \times (4 + 8) \bar{m}_{48} \times (6 + 6) \bar{m}_{66} \\
 &= 8 \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
 &\quad 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
 &\quad \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
 &\quad \left. \frac{5}{2}t \right) \times 10(16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
 &\quad 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
 &\quad pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) \times \\
 &\quad 12(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
 &\quad 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
 &\quad pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) \times 12(5 - p^2t - \\
 &\quad pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \\
 &\quad \frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
 &\quad 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t)
 \end{aligned}$$

$$\begin{aligned}
 \bar{\Pi}_1(G) &= 2880(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - \\
 &\quad 2p^2qt + 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - \\
 &\quad 11pqt - pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - \\
 &\quad 11)(64p^2q^2t^2 + 32p^2q^2t + 32p^2qt^2 + 32pq^2t^2 + 4p^2q^2 + 24p^2qt + \\
 &\quad 4p^2t^2 + 24pq^2t + 24pqt^2 + 4q^2t^2 + 4p^2q + 4p^2t + 4pq^2 + \\
 &\quad 52pqt + 4pt^2 + 4q^2t + 4qt^2 + p^2 + 12pq + 12pt + q^2 + 12qt + \\
 &\quad t^2 + 5p + 5q + 5t)(4p^2q^2t^2 - 4p^2q^2t - 4p^2qt^2 - 4pq^2t^2 + p^2q^2 + \\
 &\quad 6p^2qt + p^2t^2 + 6pq^2t + 6pqt^2 + q^2t^2 - 2p^2q - 2p^2t - 2pq^2 - \\
 &\quad 20pqt - 2pt^2 - 2q^2t - 2qt^2 + p^2 + 9pq + 9pt + q^2 + 9qt + t^2 - \\
 &\quad 7p - 7q - 7t + 10)(16p^2q^2t^2 - 4p^2q^2t - 4p^2qt^2 - 4pq^2t^2 - \\
 &\quad 2p^2q^2 + 6p^2qt - 2p^2t^2 + 6pq^2t + 6pqt^2 - 2q^2t^2 + p^2q + p^2t + \\
 &\quad pq^2 - 5pqt + pt^2 + q^2t + qt^2 + p^2 - 9pq - 9pt + q^2 - 9qt + \\
 &\quad t^2 + 4p + 4q + 4t - 5).
 \end{aligned}$$

2.4 Second multiplicative Zagreb co-index of CeO_2 [p, q, t]

$$\begin{aligned}
 \bar{\Pi}_2(G) &= \prod_{uv \in \bar{E}(G)} (\S(u) \times \S(v)) \\
 &= (4 \times 4) \bar{m}_{44} \times (4 \times 6) \bar{m}_{46} \times (4 \times 8) \bar{m}_{48} \times (6 \times 6) \bar{m}_{66}
 \end{aligned}$$

$$\begin{aligned}
&= 16 \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
&12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
&\frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
&\left. \frac{5}{2}t \right) \times 24(16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
&2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
&pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) \times \\
&32(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
&2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
&pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) \times 36(5 - p^2t - \\
&pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \\
&\frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
&10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t)
\end{aligned}$$

$$\begin{aligned}
\bar{\Pi}_2(G) &= (110592(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - \\
&2p^2qt + 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - \\
&11pqt - pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - \\
&11))(64p^2q^2t^2 + 32p^2q^2t + 32p^2qt^2 + 32pq^2t^2 + 4p^2q^2 + 24p^2qt + \\
&4p^2t^2 + 24pq^2t + 24pqt^2 + 4q^2t^2 + 4p^2q + 4p^2t + 4pq^2 + 52pqt + \\
&4pt^2 + 4q^2t + 4qt^2 + p^2 + 12pq + 12pt + q^2 + 12qt + t^2 + 5p + \\
&5q + 5t)(4p^2q^2t^2 - 4p^2q^2t - 4p^2qt^2 - 4pq^2t^2 + p^2q^2 + 6p^2qt + \\
&p^2t^2 + 6pq^2t + 6pqt^2 + q^2t^2 - 2p^2q - 2p^2t - 2pq^2 - 20pqt - \\
&2pt^2 - 2q^2t - 2qt^2 + p^2 + 9pq + 9pt + q^2 + 9qt + t^2 - 7p - 7q - \\
&7t + 10)(16p^2q^2t^2 - 4p^2q^2t - 4p^2qt^2 - 4pq^2t^2 - 2p^2q^2 + 6p^2qt - \\
&2p^2t^2 + 6pq^2t + 6pqt^2 - 2q^2t^2 + p^2q + p^2t + pq^2 - 5pqt + pt^2 + \\
&q^2t + qt^2 + p^2 - 9pq - 9pt + q^2 - 9qt + t^2 + 4p + 4q + 4t - 5).
\end{aligned}$$

2.5 Forgotten topological co-index of CeO_2 $[p, q, t]$

$$\begin{aligned}
\bar{F}(G) &= \sum_{uv \in E(G)} (\S(u)^2 + \S(v)^2) \\
&= (4^2 + 4^2) \bar{m}_{44} + (4^2 + 6^2) \bar{m}_{46} + (4^2 + 8^2) \bar{m}_{48} + (6^2 + 6^2) \bar{m}_{66} \\
&= 32 \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
&12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
&\frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
&\left. \frac{5}{2}t \right) + 52(16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q -
\end{aligned}$$

$$\begin{aligned}
& 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
& pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
& 80(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
& 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
& pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + 72(5 - p^2t - \\
& pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \\
& \frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
& 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t)
\end{aligned}$$

$$\begin{aligned}
\bar{F}(G) &= 3280p^2q^2t^2 + 1120p^2q^2t + 156p^2q^2 + 1120p^2qt^2 + 752p^2qt - \\
& 36p^2q + 156p^2t^2 - 36p^2t + 24p^2 + 1120pq^2t^2 + 752pq^2t - 36pq^2 + \\
& 752pqt^2 - 1028pqt + 48pq - 36pt^2 + 48pt - 524p + 156q^2t^2 - \\
& 36q^2t + 24q^2 - 36qt^2 + 48qt - 524q + 24t^2 - 524t - 780.
\end{aligned}$$

2.6 Atom-bond connectivity topological co-index of CeO_2 [p, q, t]

$$\begin{aligned}
\overline{ABC}(G) &= \sum_{uv \in E(G)} \sqrt{\frac{(\S(u) + \S(v)) - 2}{\S(u)\S(v)}} \\
&= \sqrt{\frac{4+4-2}{4.4}} \bar{m}_{44} + \sqrt{\frac{4+6-2}{4.6}} \bar{m}_{46} + \sqrt{\frac{4+8-2}{4.8}} \bar{m}_{48} + \sqrt{\frac{6+6-2}{6.6}} \bar{m}_{66} \\
\overline{ABC}(G) &= \sqrt{\frac{3}{8}} (32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \\
& 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
& \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
& \frac{5}{2}t) + \sqrt{\frac{1}{3}} (16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
& 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
& pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
& \sqrt{\frac{5}{16}} (16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
& 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
& pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + \sqrt{\frac{5}{18}} (5 - p^2t - \\
& pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \\
& \frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
& 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t).
\end{aligned}$$

2.7 Geometric arithmetic topological co-index of CeO_2 [p, q, t]

$$\begin{aligned}
 \overline{GA}(G) &= \sum_{uv \in \overline{E}(G)} \frac{2\sqrt{\S(u) \times \S(v)}}{\S(u) + \S(v)} \\
 &= \frac{2\sqrt{4.4}}{4+4} \overline{m}_{44} + \frac{2\sqrt{4.6}}{4+6} \overline{m}_{46} + \frac{2\sqrt{4.8}}{4+8} \overline{m}_{48} + \frac{2\sqrt{6.6}}{6+6} \overline{m}_{66} \\
 &= \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
 &\quad 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
 &\quad \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
 &\quad \left. \frac{5}{2}t \right) + \frac{24}{5} (16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
 &\quad 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
 &\quad pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
 &\quad \frac{16}{3} (16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
 &\quad 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
 &\quad pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + (5 - p^2t - pt^2 - \\
 &\quad q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \frac{1}{2}q^2 + \\
 &\quad 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
 &\quad 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t) \\
 \overline{GA}(G) &= \frac{2942p^2q^2t^2}{15} + \frac{294p^2q^2t}{5} + \frac{107p^2q^2}{30} + \frac{294p^2qt^2}{5} + \frac{497p^2qt}{15} + \frac{7p^2q}{15} + \frac{107p^2t^2}{30} + \\
 &\quad \frac{7p^2t}{15} + \frac{7p^2}{15} + \frac{294pq^2t^2}{5} + \frac{497pq^2t}{15} + \frac{7pq^2}{15} + \frac{497pqt^2}{15} - \frac{200pqt}{3} - \frac{327pq}{10} + \frac{7pt^2}{15} - \\
 &\quad \frac{327pt}{10} - \frac{287p}{15} + \frac{107q^2t^2}{30} + \frac{7q^2t}{15} + \frac{7q^2}{15} + \frac{7qt^2}{15} - \frac{327qt}{10} - \frac{287q}{15} + \frac{7t^2}{15} - \frac{287t}{15} - \frac{233}{3}.
 \end{aligned}$$

2.8 The general Randic co-index of CeO_2 [p, q, t]

$$\overline{R}_\alpha(G) = \sum_{uv \in \overline{E}(G)} (\S(u) \times \S(v))^\alpha; \quad \alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$$

2.8.1 For $\alpha = 1$

$$\begin{aligned}
 \overline{R}_1(G) &= \sum_{uv \in \overline{E}(G)} (\S(u) \times \S(v))^1 \\
 &= (4 \times 4)^1 \overline{m}_{44} + (4 \times 6)^1 \overline{m}_{46} + (4 \times 8)^1 \overline{m}_{48} + (6 \times 6)^1 \overline{m}_{66} \\
 &= 16 \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
 &\quad 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
 &\quad \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
 &\quad \left. \frac{5}{2}t \right) + 24 (16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
 &\quad 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
 &\quad pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5)
 \end{aligned}$$

$$\begin{aligned}
& 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
& pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
& 32(16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
& 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
& pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + 36(5 - p^2t - \\
& pt^2 - q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \\
& \frac{1}{2}q^2 + 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
& 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t) \\
\bar{R}_1(G) &= 1480p^2q^2t^2 + 472p^2q^2t + 66p^2q^2 + 472p^2qt^2 + 380p^2qt - \\
& 12p^2q + 66p^2t^2 - 12p^2t + 18p^2 + 472pq^2t^2 + 380pq^2t - 12pq^2 + \\
& 380pqt^2 - 416pqt + 42pq - 12pt^2 + 42pt - 214p + 66q^2t^2 - \\
& 12q^2t + 18q^2 - 12qt^2 + 42qt - 214q + 18t^2 - 214t - 292.
\end{aligned}$$

2.8.2 For $\alpha = -1$

$$\begin{aligned}
\bar{R}_{-1}(G) &= \sum_{uv \in E(G)} (\S(u) \times \S(v))^{-1} \\
&= (4 \times 4)^{-1} \bar{m}_{44} + (4 \times 6)^{-1} \bar{m}_{46} + (4 \times 8)^{-1} \bar{m}_{48} + (6 \times 6)^{-1} \bar{m}_{66} \\
&= \frac{1}{16} \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
& 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
& \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
& \left. \frac{5}{2}t \right) + \frac{1}{24} (16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
& 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
& pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
& \frac{1}{32} (16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
& 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
& pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + \frac{1}{36} (5 - p^2t - pt^2 - \\
& q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \frac{1}{2}q^2 + \\
& 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
& 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t) \\
\bar{R}_{-1}(G) &= \frac{29p^2q^2t^2}{9} + \frac{83p^2q^2t}{72} + \frac{17p^2q^2}{144} + \frac{83p^2qt^2}{72} + \frac{49p^2qt}{48} + \frac{31p^2q}{288} + \frac{17p^2t^2}{144} + \frac{31p^2t}{288} + \frac{p^2}{18} + \\
& \frac{83pq^2t^2}{72} + \frac{49pq^2t}{48} + \frac{31pq^2}{288} + \frac{49pqt^2}{48} + \frac{229pqt}{288} + \frac{pq}{8} + \frac{31pt^2}{288} + \frac{pt}{8} + \frac{p}{144} + \frac{17q^2t^2}{144} + \\
& \frac{31q^2t}{288} + \frac{q^2}{18} + \frac{31qt^2}{288} + \frac{qt}{8} + \frac{q}{144} + \frac{t^2}{18} + \frac{t}{144} - \frac{119}{288}.
\end{aligned}$$

2.8.3 For $\alpha = \frac{1}{2}$

$$\begin{aligned}
 \bar{R}_{\frac{1}{2}}(G) &= \sum_{uv \in E(G)} (\S(u) \times \S(v))^{\frac{1}{2}} \\
 &= (4 \times 4)^{\frac{1}{2}} \bar{m}_{44} + (4 \times 6)^{\frac{1}{2}} \bar{m}_{46} + (4 \times 8)^{\frac{1}{2}} \bar{m}_{48} + (6 \times 6)^{\frac{1}{2}} \bar{m}_{66} \\
 &= 4 \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
 &\quad 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
 &\quad \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + 15p^2q + \frac{5}{2}p + \\
 &\quad \left. \frac{5}{2}t \right) + 2\sqrt{6} (16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
 &\quad 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
 &\quad pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
 &\quad 4\sqrt{2} (16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
 &\quad 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
 &\quad pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + 6(5 - p^2t - pt^2 - \\
 &\quad q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \frac{1}{2}q^2 + \\
 &\quad 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
 &\quad 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t) \\
 \bar{R}_{\frac{1}{2}}(G) &= 11p^2t^2 - 11q - 11t - 11p + 11q^2t^2 - 28\left(\frac{1}{2^{\frac{1}{2}}}\right)p + 8\left(\frac{1}{6^{\frac{1}{2}}}\right)p - \\
 &\quad 28\left(\frac{1}{2^{\frac{1}{2}}}\right)q + 8\left(\frac{1}{6^{\frac{1}{2}}}\right)q - 28\left(\frac{1}{2^{\frac{1}{2}}}\right)t + 8\left(\frac{1}{6^{\frac{1}{2}}}\right)t + 51pq + 51pt + 51qt - \\
 &\quad 44\left(\frac{1}{2^{\frac{1}{2}}}\right) - 10\left(\frac{1}{6^{\frac{1}{2}}}\right) - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2 + 2\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2 - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)q^2 + 2\left(\frac{1}{6^{\frac{1}{2}}}\right)q^2 - \\
 &\quad 4\left(\frac{1}{2^{\frac{1}{2}}}\right)t^2 + 2\left(\frac{1}{6^{\frac{1}{2}}}\right)t^2 + 2pq^2 + 2p^2q + 2pt^2 + 2p^2t + 2qt^2 + 2q^2t + \\
 &\quad 5p^2 + 5q^2 + 5t^2 + 11p^2q^2 - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)pt^2 - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2t + 2\left(\frac{1}{6^{\frac{1}{2}}}\right)pt^2 + \\
 &\quad 2\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2t - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)qt^2 - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)q^2t + 2\left(\frac{1}{6^{\frac{1}{2}}}\right)qt^2 + 2\left(\frac{1}{6^{\frac{1}{2}}}\right)q^2t + \\
 &\quad 66pqt^2 + 66pq^2t + 66p^2qt + 8\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2q^2 - 4(612)p^2q^2 + \\
 &\quad 8\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2t^2 - 4\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2t^2 + 8\left(\frac{1}{2^{\frac{1}{2}}}\right)q^2t^2 - 4\left(\frac{1}{6^{\frac{1}{2}}}\right)q^2t^2 + 52pq^2t^2 + \\
 &\quad 52p^2qt^2 + 52p^2q^2t - 18\left(\frac{1}{6^{\frac{1}{2}}}\right)pq - 18\left(\frac{1}{6^{\frac{1}{2}}}\right)pt - 18\left(\frac{1}{6^{\frac{1}{2}}}\right)qt + \\
 &\quad 44pqt + 140p^2q^2t^2 - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)pq^2 - 4\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2q + 2\left(\frac{1}{6^{\frac{1}{2}}}\right)pq^2 + \\
 &\quad 2\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2q - 44\left(\frac{1}{2^{\frac{1}{2}}}\right)pqt - 10\left(\frac{1}{6^{\frac{1}{2}}}\right)pqt + 64\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2q^2t^2 + \\
 &\quad 32\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2q^2t^2 - 8\left(\frac{1}{2^{\frac{1}{2}}}\right)pqt^2 - 8\left(\frac{1}{2^{\frac{1}{2}}}\right)pq^2t - 8\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2qt + \\
 &\quad 12\left(\frac{1}{6^{\frac{1}{2}}}\right)pqt^2 + 12\left(\frac{1}{6^{\frac{1}{2}}}\right)pq^2t + 12\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2qt + 48\left(\frac{1}{2^{\frac{1}{2}}}\right)pq^2t^2 + \\
 &\quad 48\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2qt^2 + 48\left(\frac{1}{2^{\frac{1}{2}}}\right)p^2q^2t - 8\left(\frac{1}{6^{\frac{1}{2}}}\right)pq^2t^2 - 8\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2qt^2 - \\
 &\quad 8\left(\frac{1}{6^{\frac{1}{2}}}\right)p^2q^2t + 30.
 \end{aligned}$$

2.8.4 For $\alpha = -\frac{1}{2}$

$$\begin{aligned}
\bar{R}_{-\frac{1}{2}}(G) &= \sum_{uv \in \bar{E}(G)} (\S(u) \times \S(v))^{-\frac{1}{2}} \\
&= (4 \times 4)^{-\frac{1}{2}} \bar{m}_{44} + (4 \times 6)^{-\frac{1}{2}} \bar{m}_{46} + (4 \times 8)^{-\frac{1}{2}} \bar{m}_{48} + (6 \times 6)^{-\frac{1}{2}} \bar{m}_{66} \\
&= \frac{1}{4} \left(32p^2q^2t^2 + 12pqt^2 + 16p^2t^2q + 16q^2t^2p + 16p^2q^2t + 12pq^2t + \right. \\
&\quad 12p^2qt + 2p^2q + 2p^2t + \frac{1}{2}p^2 + 2pq^2 + 2q^2t + \frac{1}{2}q^2 + 2pt^2 + 2qt^2 + \\
&\quad \frac{1}{2}t^2 + 2p^2q^2 + 2p^2t^2 + 2q^2t^2 + 6pq + 6pt + 6qt + 26pqt + \frac{5}{2}q + \frac{5}{2}p + \\
&\quad \left. \frac{5}{2}t \right) + \frac{1}{2\sqrt{6}} (16p^2q^2t^2 - 4p^2q^2t - 2p^2q^2 - 4p^2qt^2 + 6p^2qt + p^2q - \\
&\quad 2p^2t^2 + p^2t + p^2 - 4pq^2t^2 + 6pq^2t + pq^2 + 6pqt^2 - 5pqt - 9pq + \\
&\quad pt^2 - 9pt + 4p - 2q^2t^2 + q^2t + q^2 + qt^2 - 9qt + 4q + t^2 + 4t - 5) + \\
&\quad \frac{1}{4\sqrt{2}} (16p^2q^2t^2 + 12p^2q^2t + 12p^2qt^2 + 12pq^2t^2 + 2p^2q^2 - 2p^2qt + \\
&\quad 2p^2t^2 - 2pq^2t - 2pqt^2 + 2q^2t^2 - p^2q - p^2t - pq^2 - 11pqt - \\
&\quad pt^2 - q^2t - qt^2 - p^2 - q^2 - t^2 - 7p - 7q - 7t - 11) + \frac{1}{6} (5 - p^2t - pt^2 - \\
&\quad q^2t - qt^2 + \frac{1}{2}p^2q^2 - p^2q - pq^2 + \frac{1}{2}p^2t^2 + \frac{1}{2}q^2t^2 + \frac{1}{2}t^2 + \frac{1}{2}p^2 + \frac{1}{2}q^2 + \\
&\quad 3p^2qt + 3pq^2t + 3pqt^2 - 2p^2q^2t + 2p^2q^2t^2 - 2p^2qt^2 - 2pq^2t^2 - \\
&\quad 10pqt - \frac{7}{2}q - \frac{7}{2}p + \frac{9}{2}qt + \frac{9}{2}pq + \frac{9}{2}pt - \frac{7}{2}t)
\end{aligned}$$

$$\begin{aligned}
\bar{R}_{-\frac{1}{2}}(G) &= \frac{p}{24} + \frac{q}{24} + \frac{t}{24} + \frac{7p^2t^2}{12} + \frac{7q^2t^2}{12} - \frac{7\sqrt{2}p}{4} + 2\sqrt{6}p - \frac{7\sqrt{2}q}{4} + 2\sqrt{6}q - \frac{7\sqrt{2}t}{4} + \\
&\quad 2\sqrt{6}t + \frac{9pq}{4} + \frac{9pt}{4} + \frac{9qt}{4} - \frac{11\sqrt{2}}{4} - \frac{5\sqrt{6}}{2} - \frac{\sqrt{2}p^2}{4} + \frac{\sqrt{6}p^2}{2} - \frac{\sqrt{2}q^2}{4} + \frac{\sqrt{6}q^2}{2} - \sqrt{2}\frac{t^2}{4} + \\
&\quad \frac{\sqrt{6}t^2}{2} + \frac{pq^2}{3} + \frac{p^2q}{3} + \frac{pt^2}{3} + \frac{p^2t}{3} + \frac{qt^2}{3} + \frac{q^2t}{3} + \frac{5p^2}{24} + \frac{5q^2}{24} + \frac{5t^2}{24} + \frac{7p^2q^2}{12} - \frac{\sqrt{2}pt^2}{4} - \\
&\quad \frac{\sqrt{2}p^2t}{4} + \frac{\sqrt{6}pt^2}{2} + \frac{\sqrt{6}p^2t}{2} - \frac{\sqrt{2}qt^2}{4} - \frac{\sqrt{2}q^2t}{4} + \frac{\sqrt{6}qt^2}{2} + \frac{\sqrt{6}q^2t}{2} + \frac{7pqt^2}{2} + \frac{7pq^2t}{2} + \frac{7p^2qt}{2} + \\
&\quad \frac{\sqrt{2}p^2q^2}{2} - \sqrt{6}p^2q^2 + \frac{\sqrt{6}p^2t^2}{2} - \sqrt{6}p^2t^2 + \frac{\sqrt{2}q^2t^2}{2} - \sqrt{6}q^2t^2 + \frac{11pq^2t^2}{3} + \frac{11p^2qt^2}{3} + \\
&\quad \frac{11p^2q^2t}{3} - \frac{9\sqrt{6}pq}{2} - \frac{9\sqrt{6}pt}{2} - \frac{9\sqrt{6}qt}{2} + \frac{29pqt}{6} + \frac{25p^2q^2t^2}{3} - \frac{\sqrt{2}pq^2}{4} - \frac{\sqrt{2}p^2q}{4} + \frac{\sqrt{6}pq^2}{2} + \\
&\quad \frac{\sqrt{6}p^2q}{2} - \frac{11\sqrt{2}pqt}{4} - \frac{5\sqrt{6}pqt}{2} + 4\sqrt{2}p^2q^2t^2 + 8\sqrt{6}p^2q^2t^2 - \frac{\sqrt{2}pqt^2}{2} - \frac{\sqrt{2}p^2qt^2}{2} - \\
&\quad \frac{\sqrt{2}p^2qt}{2} + 3\sqrt{6}pqt^2 + 3\sqrt{6}pq^2t + 3\sqrt{6}p^2qt + 3\sqrt{2}pq^2t^2 + 3\sqrt{2}p^2qt^2 + \\
&\quad 3\sqrt{2}p^2q^2t - 2\sqrt{6}pq^2t^2 - 2\sqrt{6}p^2qt^2 - 2\sqrt{6}p^2q^2t + \frac{5}{6}.
\end{aligned}$$

3 Numerical and graphical comparison

The numerical representations of the computed calculations are shown in Tables 3-5 and graphs of the comparisons are shown in Figures 2-4.

Table 3: Numerical comparison of $\bar{M}_1(G)$, $\bar{M}_2(G)$, $\bar{\Pi}_1(G)$, and $\bar{\Pi}_2(G)$ for CeO_2 $[p, q, t]$

$[p, q, t]$	$\bar{M}_1(G)$	$\bar{M}_2(G)$	$\bar{\Pi}_1(G)$	$\bar{\Pi}_2(G)$
[1,1,1]	1496	2992	0	0
[2,2,2]	68794	156680	1.6155	6.2035
[3,3,3]	657112	1517612	4.5657	1.7532
[4,4,4]	3371438	7823380	4.9544	1.9025
[5,5,5]	12178888	28326248	1.0798	4.1465
[6,6,6]	35076226	81692672	8.7006	3.3410
[7,7,7]	86212424	200968420	3.5444	1.3610
[8,8,8]	188466262	439609292	8.7781	3.3707
[9,9,9]	376478968	878577440	1.4874	5.7117
[10,10,10]	700141898	1634503288	1.8689	7.1767

Table 4: Numerical comparison of $\bar{F}(G)$, $\overline{ABC}(G)$, and $\overline{GA}(G)$ for CeO_2 $[p, q, t]$

$[p, q, t]$	$\bar{F}(G)$	$\overline{ABC}(G)$	$\overline{GA}(G)$
[1,1,1]	5984	1.14513	1.8699
[2,2,2]	348012	4.40448	1.8868
[3,3,3]	3391104	4.1156	1.9191
[4,4,4]	17489636	2.09622	1.0062
[5,5,5]	63293760	7.5463	3.6738
[6,6,6]	182418204	2.16920	1.0647
[7,7,7]	448472672	5.3250	2.6276
[8,8,8]	980453844	1.16311	5.7606
[9,9,9]	999868798	2.32201	1.1531
[10,10,10]	9.8×10^9	4.3162	2.1480

Table 5: Numerical comparison of $\bar{R}_1(G)$, $\bar{R}_{-1}(G)$, $\bar{R}_{\frac{1}{2}}(G)$, and $\bar{R}_{-\frac{1}{2}}(G)$ for CeO_2 $[p, q, t]$

$[p, q, t]$	$\bar{R}_1(G)$	$\bar{R}_{-1}(G)$	$\bar{R}_{\frac{1}{2}}(G)$	$\bar{R}_{-\frac{1}{2}}(G)$
[1,1,1]	2992	11.6875	7.4800	46.7500
[2,2,2]	156680	3.8487	3.3642	2.7993
[3,3,3]	1517612	3.5095	3.2077	2.8722
[4,4,4]	7823380	1.7714	1.6453	1.5349
[5,5,5]	28326248	6.34832	5.9436	5.6955
[6,6,6]	81692672	1.8198	1.7119	1.6717
[7,7,7]	200968420	4.4593	4.2082	4.1674
[8,8,8]	439609292	9.7277	9.2003	9.2103
[9,9,9]	878577440	1.9401	1.8380	1.8558
[10,10,10]	1.6345	3.6037	3.4184	3.4758

Figure 2: Comparison of: (a) $\bar{M}_1(G)$ and $\bar{M}_2(G)$, (b) $\bar{\Pi}_1(G)$ and $\bar{\Pi}_2(G)$.

Figure 3: Comparison of $\bar{F}(G)$, $\overline{ABC}(G)$, and $\overline{GA}(G)$.

Figure 4: Comparison of: (a) $\bar{R}_\alpha(G)$ for $\alpha = 1, -1$, (b) $\bar{R}_\alpha(G)$ for $\alpha = 1/2, -1/2$.

4 Conclusion

In this study, we computed the degree based topological coindices such as first, second Zagreb, and multiplicative Zagreb coindices, forgotten atom-bond connectivity (ABC), geometric arithmetic, and general Randic coindices of silicate network and triangular chain cactus graphs

for different values of α , and shown their numerical comparisons.”

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