Cut method and algorithmic approaches to Szeged-type indices of non-partial cube zeolite frameworks

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Abstract

Szeged index is an additive edge function-based invariant associated with the closeness sets of each edge's end vertices. The computation of Szeged-type indices includes computer algorithms, numerical interpolations, and cut method, among which the latter method is highly preferred due to the computational complexity compared to other techniques. Szeged-type indices of zeolite frameworks which are partial cubes have been already computed using the cut method. Due to the complex three dimensional molecular framework of BCT (body-centered tetragonal tectosilicate), the application of the standard or the strength-weighted cut method is not sufficient for the computation of its Szeged-type indices. This paper introduces a hybrid methodology that integrates the cut method with algorithmic techniques by classifying the edges of the graph into Θ-classes as well as Θ^*-classes to compute Szeged-type indices of non-partial cube zeolites. For edges belonging to Θ-classes, the standard cut method is employed. In contrast, for edges associated with Θ^*-classes, a novel algorithmic approach is developed to generalize the corresponding closeness measures, and the corresponding algorithm is explicitly presented in the paper. The results obtained from both approaches are then systematically integrated to compute the Szeged-type indices of the zeolite BCT framework.

Keywords: Szeged-type indices; cut method; algorithmic approach; zeolite framework; body-centered tetragonal tectosilicate.

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1 Introduction

Topological indices are numerical quantities that are associated with the underlying structure of the molecular framework [1–3]. Graph theoretical techniques have a predominant role in computing these structural invariants of chemical compounds [4, 5]. Wiener's contribution in predicting the boiling points of paraffins using graph theoretical path number paved the way for the development of chemical graph theory [6]. Following the success of the Wiener index, a large set of indices have been introduced over the years which are associated with the degree, distance, and spectrum of the molecular graphs [7–9]. Those topological indices are found to have a high correlation with various physical, chemical, and electrostatic properties [10–12].

Initially, Gutman introduced the vertex variant of Szeged index by considering the vertex closeness of each edge's end vertices [13]. Further, researchers started introducing various variants of Szeged index by manipulating the edge function with different operations [14–16]. Szeged-type indices are distance-based indices that are modeled to compute the physicochemical properties such as the boiling point, proton-ligand formation constants, the vapor pressure, the molecular volume, the molar volume, the van der Waals volume, etc., for various drugs and chemical compounds [17, 18]. Algorithmic and programming based techniques can be incorporated to compute the Szeged-type indices for drugs and chemical compounds. In contrast, these techniques are tedious for large molecular systems due to their high time complexity [19, 20]. Deriving generalized algebraic expressions for these indices is a challenging problem and has potential insights into computational and theoretical chemistry [21]. The cut method is an extremely fruitful technique in the case of partial cubes. For graphs more general than partial cubes, the strength weighted cut method can be incorporated depending on size of the quotient graphs [22]. Certain cases, such as the melem ring frameworks, require additional techniques to compute Szeged type indices [23].

The BCT framework crystallizes in the tetragonal crystal system and is characterized by a framework density of 19.0 T/1000 Å^3, and essential 4 and 8-membered rings, which influence its transport and adsorption behavior. Computational investigations have identified BCT as one of the most promising pure-silica zeolite frameworks for the cryogenic separation of hydrogen isotopes, exhibiting exceptionally high selectivities for D_2/H_2 and T_2/H_2 mixtures through quantum sieving effects [24]. Furthermore, BCT-type tetrahedral networks have been realized in nitridoaluminate and nitridosilicate compounds such as $Li_2Sr_4Al_2Ta_2N_8O$, $LiCa_4Si_4N_8F$, and $LiSr_4Si_4N_8F$, demonstrating the versatility and robustness of the BCT framework across a broad range of inorganic materials [25, 26]. These structural characteristics and multifunctional applications make the BCT zeolite framework an attractive subject for theoretical investigations. Topological entropy characterizations of BCT using

degree-based descriptors are performed by researchers to investigate the structural properties of the framework [27].

The present study employs a variant of the cut method to derive generalized expressions that attain Szeged-type indices of zeolite BCT framework. The molecular framework of BCT is bipartite but more a partial cube, hence computing Szeged-type indices for this framework via strength weighted cut method is a complex procedure. Therefore, a hybrid computational framework has been developed by integrating the classical cut method with a tailored algorithmic technique that evaluates the closeness measures of each edge in a graph, enabling the effective evaluation of Szeged-type indices. Computing structural invariants of crystalline aluminosilicate materials have been an important study in QSAPR research [28, 29], these topological measures exhibit a strong correlation with the potential energies of the framework [12], and combining the measures with information theory provides insights into the framework's stability [30].

For investigating the structural properties of a molecular graph, we define G as the simple connected molecular graph, where the collection of atoms and bonds are denoted by $V(G)$ and $E(G)$, which represent the vertex and the edge set of G. The total number of atoms and bonds in the graph is represented by $|V(G)|$ and $|E(G)|$ respectively. The valency of an atom v is defined as $d(v)$, which denotes the degree of d. For $u, v \in V(G)$, the notation $d_G(u, v)$ denotes the distance in G between u and v, that is, the length of a shortest u, v-path in the molecular graph G. The distance in G between the edges $e = xy$ and $f = wz$ is $d_G(e, f) = \min\{d_G(x, w), d_G(x, z), d_G(y, w), d_G(y, z)\}$. For an edge $e = xy \in E(G)$, we define the following:

$$\begin{aligned}
N_x(e|G) &= |\{u \in V(G) : \ d_G(x, u) < d_G(y, u)\}|, \\
M_x(e|G) &= |\{g \in E(G) : \ d_G(x, g) < d_G(y, g)\}|, \\
N_y(e|G) &= |\{u \in V(G) : \ d_G(y, u) < d_G(x, u)\}|, \\
M_y(e|G) &= |\{g \in E(G) : \ d_G(y, g) < d_G(x, g)\}|.
\end{aligned}$$

It should be noted that the notations listed above are not standardized in the literature. For example, W_{xy} and W_{yx} are often used instead of $N_x(e|G)$ and $N_x(e|G)$, respectively.

Further, we define weighted edge functions $w^+(e) = d(x) + d(y)$ and $w^\times(e) = d(x) \times d(y)$. With the aid of defined notations we present the formulas of Szeged-type indices [13–15, 31–33].

Szeged-type indices:

$$SZ_v(G) = \sum_{e=xy \in E(G)} N_x(e|G) N_y(e|G) \ \ \text{(vertex Szeged)},$$

$$SZ_e(G) = \sum_{e=xy\in E(G)} M_x(e|G)M_y(e|G) \quad \text{(edge Szeged)},$$
$$SZ_{ve}(G) = \frac{1}{2}\sum_{e=xy\in E(G)} \big[N_x(e|G)M_y(e|G) + N_y(e|G)M_x(e|G)\big] \quad \text{(vertex-edge Szeged)},$$
$$PI_v(G) = \sum_{e=xy\in E(G)} \big[N_x(e|G) + N_y(e|G)\big] \quad \text{(vertex Padmakar–Ivan)},$$
$$PI_e(G) = \sum_{e=xy\in E(G)} \big[M_x(e|G) + M_y(e|G)\big] \quad \text{(edge Padmakar–Ivan)}.$$

Weighted Szeged-type indices: for $\# \in \{+, \times\}$, let

$$w^{\#}SZ_v(G) = \sum_{e=xy\in E(G)} w^{\#}(e)N_x(e|G)N_y(e|G) \quad \text{(weighted Szeged)},$$
$$w^{\#}SZ_e(G) = \sum_{e=xy\in E(G)} w^{\#}(e)M_x(e|G)M_y(e|G) \quad \text{(weighted edge Szeged)},$$
$$w^{\#}PI_v(G) = \sum_{e=xy\in E(G)} w^{\#}(e)\big(N_x(e|G) + N_y(e|G)\big) \quad \text{(weighted vertex Padmakar–Ivan)},$$
$$w^{\#}PI_e(G) = \sum_{e=xy\in E(G)} w^{\#}(e)\big(M_x(e|G) + M_y(e|G)\big) \quad \text{(weighted edge Padmakar–Ivan)}.$$

The generalized expression for computing Szeged-type indices can be then given as

$$X(G) = \sum_{e\in E(G)} w^{\#}(e)\phi(e), \tag{1}$$

where X represents various Szeged-type indices, $\phi(e)$ is the edge function depending on parameters such as $N_x(e|G)$, $N_y(e|G)$, $M_x(e|G)$, $M_y(e|G)$, and $w^{\#}(e)$ is an edge function of $w^{+}(e)$ or $w^{\times}(e)$. In the following section, we briefly explain the cut method which plays a major part in computing these indices for the zeolite BCT framework.

2 Graph theoretical cut method

The cut method is one of the classical techniques used in the computation of distance-based topological indices of chemical graphs. The method relies on the following Djoković-Winkler relation Θ. Edges $e = xy$ and $f = wz$ of a (molecular) graph G are in relation Θ, i.e., $e\Theta f$, if $d_G(x, w) + d_G(y, z) \neq d_G(x, z) + d_G(y, w)$ [34, 35]. The relation Θ is reflexive, symmetric and transitive for partial cubes. In fact, partial cubes, which are defined as the graphs isometrically embeddable into hypercubes, can be characterized as those connected bipartite graphs in which the relation Θ is transitive. In general, however, Θ is not transitive. Let Θ^* denote the transitive closure of Θ. The relation Θ^* is

an equivalence relation on the edge set of an arbitrary connected graph. From what we said above, the relation Θ is an equivalence relation on partial cubes, and in this case the Θ^*-equivalence classes coincide with the Θ-equivalence classes. Moreover, if F is such a class of partial cube G, then $G - F$ consists of exactly two components. On the other hand, if F' is an equivalence class of an arbitrary connected graph H, then $H - F'$ can contain an arbitrary number of connected components.

In order to deal with the above described general situation, we partition the edge set of G as $E(G) = \cup_i E_{1i} \bigcup \cup_j E_{2j}$, where $E_{11}, \ldots, E_{1k}$ are the Θ^*-equivalence classes such that $G - E_{1i}$ consists of two connected components, while $E_{21}, \ldots, , E_{2l}$ are the Θ^*-equivalence classes such that $G - E_{2j}$ consists of more than two connected components. Equation (1) can now be written as

$$\begin{aligned} X(G) &= \sum_{e \in \cup_i E_{1i}} w^{\#}(e)\phi(e) + \sum_{e \in \cup_j E_{2j}} w^{\#}(e)\phi(e) \\ &= X(\Phi_1) + X(\Phi_2), \end{aligned} \tag{2}$$

where $X(\Phi_1)$ and $X(\Phi_2)$ represent the sum of the Szeged-type index values of $e \in \cup_i E_{1i}$ and $e \in \cup_j E_{2j}$, respectively. For the defined Szeged-type indices, $X(\Phi_1)$ of Equation (2) can be computed using the following results [36–38].

For each E_{1i}, the quotient graph G/E_{1i} is the P_2 graph whose vertices represents the 2 components A_{1i} and A_{2i}, $1 \leq i \leq k$. We define $n_1(E_{1i}) = |V(A_{1i})|$, $m_1(E_{1i}) = |E(A_{1i})|$, $n_2(E_{1i}) = |V(A_{2i})|$, $m_2(E_{1i}) = |E(A_{2i})|$, and $w^{\#}(E_{1i}) = \sum_{e \in E_{1i}} w^{\#}(e)$, where $\# \in \{+, \times\}$. Then

$$\begin{aligned} SZ_v(\Phi_1) &= \sum_{i=1}^{k} |E_{1i}|\ n_1(E_{1i})n_2(E_{1i}), \\ SZ_e(\Phi_1) &= \sum_{i=1}^{k} |E_{1i}|\ m_1(E_{1i})m_2(E_{1i}), \\ SZ_{ve}(\Phi_1) &= \frac{1}{2}\sum_{i=1}^{k} |E_{1i}|\ \big(n_1(E_{1i})m_2(E_{1i}) + n_2(E_{1i})m_1(E_{1i})\big), \\ PI_v(\Phi_1) &= \sum_{i=1}^{k} |E_{1i}|\ \big(n_1(E_{1i}) + n_2(E_{1i})\big), \\ PI_e(\Phi_1) &= \sum_{i=1}^{k} |E_{1i}|\ \big(m_1(E_{1i}) + m_2(E_{1i})\big), \\ w^{\#}SZ_v(\Phi_1) &= \sum_{i=1}^{k} w^{\#}(E_{1i})\ n_1(E_{1i})n_2(E_{1i}), \\ w^{\#}SZ_e(\Phi_1) &= \sum_{i=1}^{k} w^{\#}(E_{1i})\ m_1(E_{1i})m_2(E_{1i}), \end{aligned}$$

$$w^{\#}PI_v(\Phi_1) = \sum_{i=1}^{k} w^{\#}(E_{1i}) \ \big(n_1(E_{1i}) + n_2(E_{1i})\big),$$

$$w^{\#}PI_e(\Phi_1) = \sum_{i=1}^{k} w^{\#}(E_{1i}) \ \big(m_1(E_{1i}) + m_2(E_{1i})\big).$$

Computing $X(\Phi_2)$ from Equation (2) via the cut method is a tedious process. Therefore, in the forthcoming section, we utilize an algorithmic approach determine the Szeged-type indices of zeolite BCT network.

3 Szeged-type indices of zeolite BCT

The zeolite BCT's crystalline framework is built by setting up its unit cell in a $\alpha \times \beta$ mesh. The primitive unit cell of BCT consists of 12 vertices and 16 edges, with 2 squares and 4 hexagons linked by common edges. The schematic growth of unit cell into 2D BCT framework with α rows and β columns is illustrated in Figure 1.

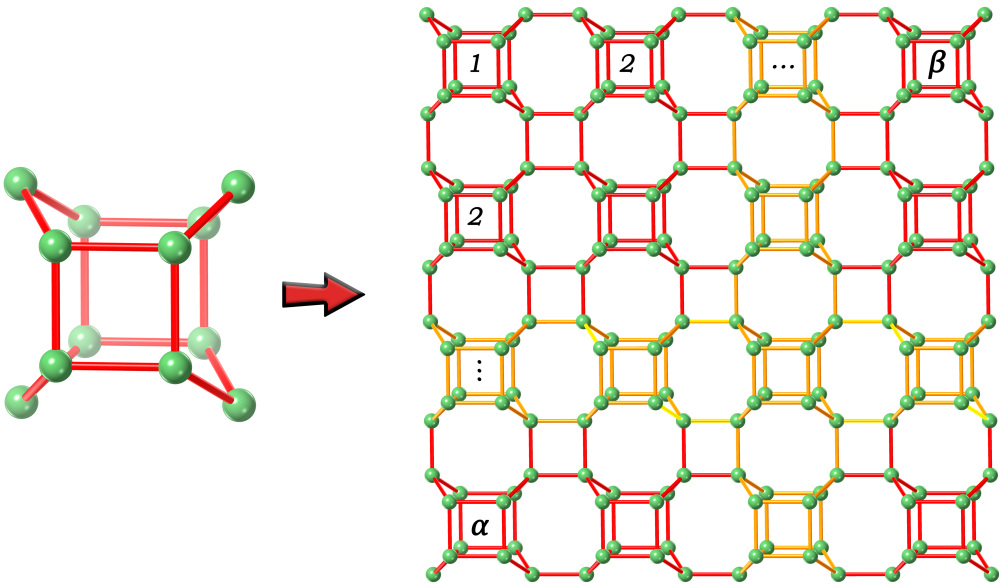


Figure 1: Construction of BCT framework from an unit cell

We denote the molecular graph of BCT as BCT(α, β), where α and β are isomorphic to cyclic permutation i.e. BCT$(\alpha, \beta) \cong$ BCT(β, α). The cardinality of vertex and edge set is given by $|V(\text{BCT}(\alpha, \beta))| = 12\alpha\beta$ and $|E(\text{BCT}(\alpha, \beta))| = 2(10\alpha\beta - \alpha - \beta)$ respectively.

While exploring the molecular graph of BCT with the aid of the Djoković-Winkler relation and its properties, BCT turned out to be a non-partial cube. To see it, consider the Θ^*-classes of the unit cell of the zeolite BCT, see Figure 2. Among the four Θ^*-classes, in three of them we find a situation

where certain pairs of edges are not in relation Θ. This property is then transferred to an arbitrary molecular graph of BCT, that is, BCT(α, β).

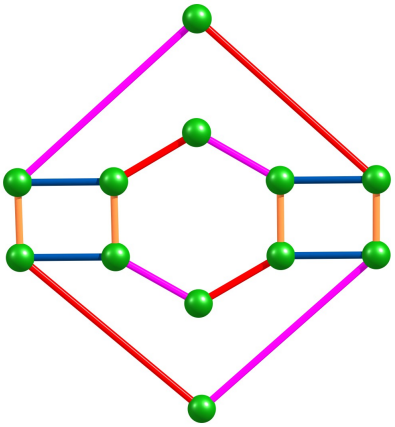


Figure 2: The unit cell of the zeolite BCT and its Θ^*-classes

Therefore, we split the edge set into Θ^*-classes E_{1i} and E_{2j}, where the topological function $\phi(e)$ for all $e \in \cup_i E_{1i}$ can be calculated using the standard cut method, while E_{2j} are all the remaining Θ^*-classes. In order to generalize the cuts in E_{1i} for $1 \leq i \leq 2(\alpha + \beta - 1)$, we classify the sets into four classes, where H_{1i} and H_{2i} represent horizontal cuts, similarly V_{1i} and V_{2i} represent vertical cuts. These classes of cuts are illustrated in Figure 3.

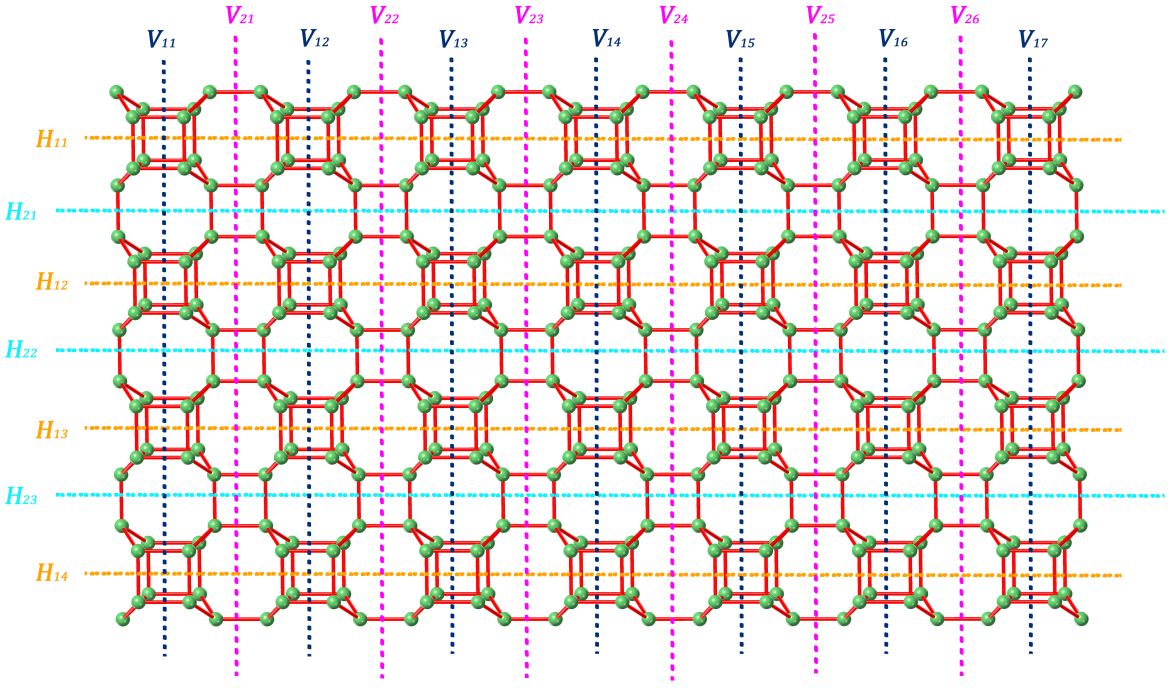


Figure 3: H_{1i}, H_{2i}, V_{1i} and V_{2i} cuts of BCT$(4, 7)$

The quotient graph for this class $E_{1i} \in \{H_{1i}, H_{2i}, V_{1i}, V_{2i}\}$ turns out to be the P_2, that is, the

removal of these edges disconnects the graph into exactly two components. We assign the parameters $[n_1(E_{1i}), m_1(E_{1i})]$ and $[n_2(E_{1i}), m_2(E_{1i})]$ to the vertices of the quotient graph along with the edge cardinality parameter $|E_{1i}|$. For each of the classes, the parameters of the quotient graph are presented Table 1.

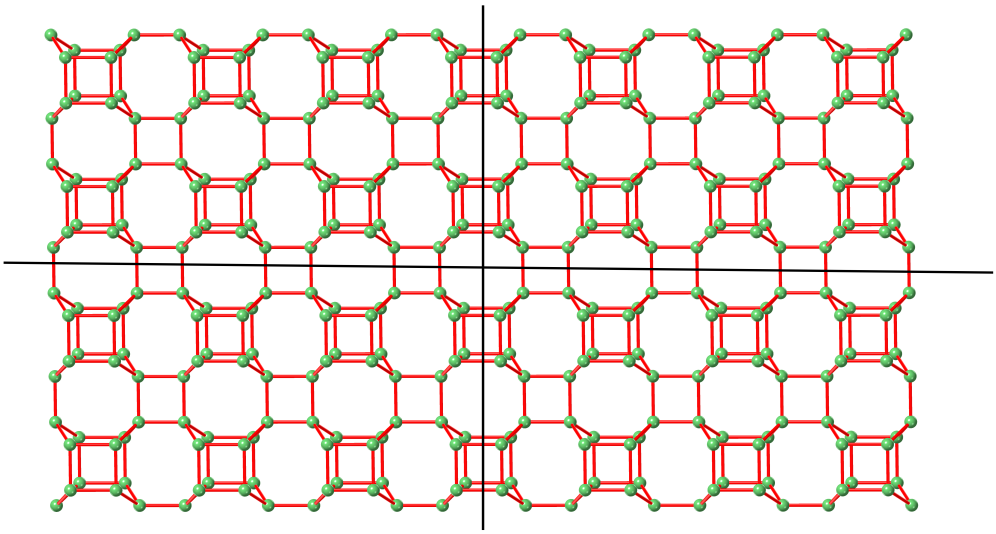
Table 1: Parameters associated with quotient graphs of each E_{1i} classes

$\boldsymbol{E_{1i}}$	**Range**	$\boldsymbol{n_1(E_{1i})}$	$\boldsymbol{m_1(E_{1i})}$	$\boldsymbol{\lvert E_{1i}\rvert}$	$\boldsymbol{w^+}$	$\boldsymbol{w^\times}$
V_{1i}	$1 \leq i \leq \beta$	$6\alpha(2i-1)$	$20\alpha i - 2i - 13\alpha + 1$	4α	24α	36α
V_{2i}	$1 \leq i \leq \beta - 1$	$12\alpha i$	$2(10\alpha i - i - \alpha)$	2α	$16\alpha - 4$	$32\alpha - 14$
H_{1i}	$1 \leq i \leq \alpha$	$6\beta(2i-1)$	$20\beta i - 2i - 13\beta + 1$	4β	24β	36β
H_{2i}	$1 \leq i \leq \alpha - 1$	$12\beta i$	$2(10\beta i - i - \beta)$	2β	$16\beta - 4$	$32\beta - 14$

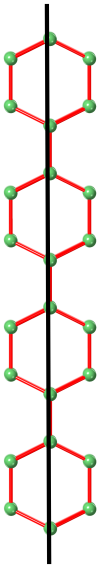
The remaining vertex parameters are given by the formula $n_2(E_{1i}) = |V(\mathrm{BCT})| - n_1(E_{1i})$ and $m_2(E_{1i}) = |E(\mathrm{BCT})| - m_1(E_{1i}) - |E_{1i}|$. The generalized expression to evaluate Szeged-type indices for E_{1i} edge classes of zeolite BCT is given as:

$$X(\Phi_1) = \sum_{i=1}^{\beta} X(V_{1i}) + \sum_{i=1}^{\beta-1} X(V_{2i}) + \sum_{i=1}^{\alpha} X(H_{1i}) + \sum_{i=1}^{\alpha-1} X(H_{2i}). \tag{3}$$

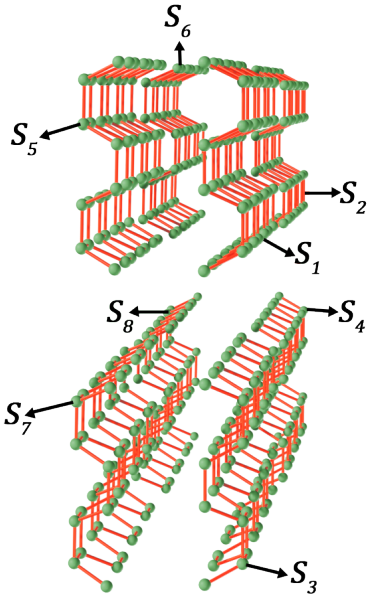
We employ the divide and conquer strategy for calculating $X(\Phi_2)$ of zeolite BCT(α, β) when $\alpha \leq \beta$. Initially, the molecular graph of the zeolite BCT framework is partitioned symmetrically into eight segments $S_1, \ldots, S_8$, let S denote the set of these segments. These eight segments are mutually isomorphic, which is achieved through horizontal and vertical front partitions, which divide the framework into four segments by removing the central connecting edges. Specifically, if α is even, the horizontal partition is introduced between the two central unit cell rows, whereas if α is odd, it passes through the middle of the central unit cell row. Similarly, if β is even, the vertical partition is introduced between the two central unit cell columns, whereas if β is odd, it passes through the middle of the central unit cell column. Subsequently, a vertical side partition is applied along the central plane of the framework, further dividing the framework into eight segments by duplicating the connecting vertices, as illustrated in Figure 4. The validity of this partitioning is independent of the parity of the framework dimensions. In particular, for all combinations of α and β (both even, both odd, or one even and the other odd), the partitioning procedure preserves the structural symmetry of the BCT framework and yields eight mutually isomorphic segments.



(a) Front view: Horizontal and vertical partitions



(b) Side view: Vertical partition



(c) Side view of all the eight segments

Figure 4: Partitioning of BCT$(4, 7)$ framework into 8 segments

Since each component is isomorphic to each other it is enough to compute the Szeged-type indices of E_{2j} class edges in any one of the segment and multiply it by 8 to obtain $X(\Phi_2)$. The single segment of zeolite BCT$(8, 14)$ is illustrated in Figure 5.

The cardinality of edges in each segment of S is given as $\alpha\beta$. We classify edges in S into 7 classes, say $C = \{C_{1r}, C_{2r}, C_{3r}, C_{4r}, C_{5r}, C_{6r}, C_{7r}\}$ to generalize the parameters required to compute Szeged-type indices. This classification is graphically presented in Figure 5. Manually determining the parameters such as $N_x(e|G)$, $N_y(e|G)$, $M_x(e|G)$, and $M_y(e|G)$ for each edge of the class C is a

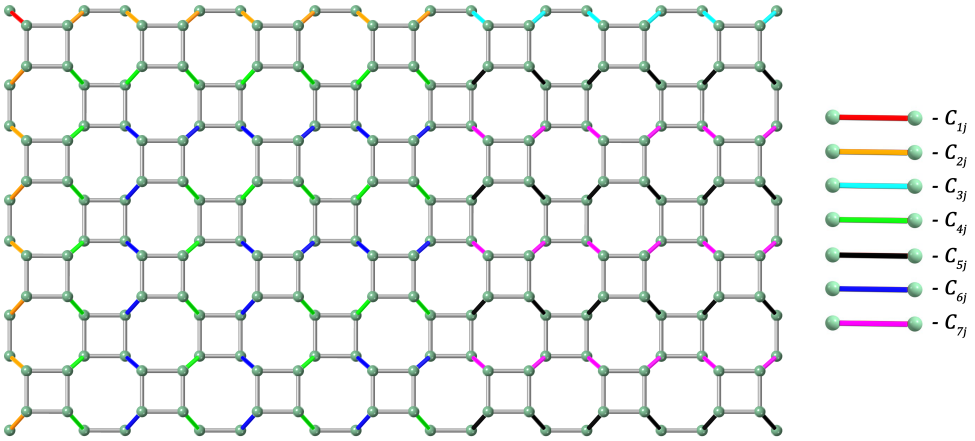


Figure 5: Single segment S_j of BCT$(8, 14)$ and its classifications

time-consuming and error-prone task, as these measures rely on computing the shortest paths between all pairs of vertices. To address this challenge, we employ Algorithm 1, which systematically computes the $N_x(e|G)$ and $N_y(e|G)$ values, the resulting patterns are identified and effectively generalized in Table 2.

Algorithm 1 Computing $N_x(e|G)$ and $N_y(e|G)$ for all edges in a graph

Input: Graph $G = (V, E)$
for each edge $e = (x, y) \in E$ **do**
  $N_x(e|G) \leftarrow 0, ; N_y(e|G) \leftarrow 0$
  for each vertex $w \in V$ **do**
    if $d_G(w, x) < d_G(w, y)$ **then**
      $N_x(e|G) \leftarrow N_x(e|G) + 1$
    else if $d_G(w, y) < d_G(w, x)$ **then**
      $N_y(e|G) \leftarrow N_y(e|G) + 1$
    end if
  end for
  Record $N_x(e|G)$ and $N_y(e|G)$
end for

Table 2: Parameters associated with an edge for each classes of C

C	$N_x(e\|G)$	$M_x(e\|G)$	$M_y(e\|G)$	w^+	$w^\times$
C_{1r}	5	5	$\|E(\text{BCT})\| - M_x(e\|G) - 4$	5	6
C_{2r}	$6r(r-1)+5$	$10r^2 - 14r + 9$	$\|E(\text{BCT})\| - M_x(e\|G) - 4r$	6	9
C_{3r}	$6\alpha(\alpha+1) + 12\alpha(r-1) + 4$	$20\alpha r - 2r - 14\alpha + 10\alpha^2 + 6$	$\|E(\text{BCT})\| - M_x(e\|G) - 4\alpha + 2$	6	9
C_{4r}	$6r(r-1) - 3$	$10r^2 - 14r - 3$	$\|E(\text{BCT})\| - M_x(e\|G) - 4r$	7	12
C_{5r}	$6\alpha(\alpha+1) + 12\alpha(r-1) - 4$	$6\alpha + (20\alpha - 2)(r-1) + 10\alpha^2 - 8$	$\|E(\text{BCT})\| - M_x(e\|G) - 4\alpha + 2$	7	12
C_{6r}	$6r(r-1)+5$	$10r^2 - 14r + 9$	$\|E(\text{BCT})\| - M_x(e\|G) - 4r$	7	12
C_{7r}	$6\alpha(\alpha+1) + 12\alpha(r-1) + 4$	$20\alpha r - 2r - 14\alpha + 10\alpha^2 + 6$	$\|E(\text{BCT})\| - M_x(e\|G) - 4\alpha + 2$	7	12

Similarly, Algorithm 2 is used in generalizing the patterns in $M_x(e|G)$ and $M_y(e|G)$ measures.

Algorithm 2 Computing $M_x(e|G)$ and $M_y(e|G)$ for all edges in a graph

Input: Graph $G = (V, E)$
for each edge $e = (x, y) \in E$ **do**
    $M_x(e|G) \leftarrow 0, ; M_y(e|G) \leftarrow 0$
    for each edge $s \in E$ **do**
        if $d_G(s, x) < d_G(s, y)$ **then**
            $M_x(e|G) \leftarrow M_x(e|G) + 1$
        else if $d_G(s, y) < d_G(s, x)$ **then**
            $M_y(e|G) \leftarrow M_y(e|G) + 1$
        end if
    end for
    Record $M_x(e|G)$ and $M_y(e|G)$
end for

The remaining parameter is $N_y(e|G) = |V(\mathrm{BCT})| - N_x(e|G)$. By substituting the parameters in the following equation, we can obtain the expression for computing Szeged-type indices for the edges in a E_{2j} class:

$$X(\Phi_2) = 8\Big[X(C_{1r}) + 2\sum_{r=2}^{\alpha} X(C_{2r}) + \sum_{r=1}^{\beta-\alpha} X(C_{3r}) + \sum_{t=2}^{\alpha}\sum_{r=t}^{\alpha} X(C_{4r}) + \frac{1}{4}(2\alpha + (-1)^{\alpha} - 1)\sum_{r=1}^{\beta-\alpha} X(C_{5r}) + \sum_{t=3}^{\alpha}\sum_{r=t}^{\alpha} X(C_{6r}) + \frac{1}{4}(2\alpha - (-1)^{\alpha} - 3)\sum_{r=1}^{\beta-\alpha} X(C_{7r})\Big]. \quad (4)$$

Adding Equations (3) and (4), and substituting the quantities from Tables 1 and 2, we obtain the following result that computes the various Szeged-type indices of zeolite $\mathrm{BCT}(\alpha, \beta)$.

Theorem 3.1. *If $G = \mathrm{BCT}(\alpha, \beta)$, $\alpha \leq \beta$, then the following hold.*

1. $SZ_v(G) = 8\alpha(60\alpha^2\beta^3 + 6\alpha^3 - 12\alpha^2\beta - 16\alpha^2 + 48\alpha\beta - 7\alpha - 16\beta + 8)$.
2. $SZ_e(G) = \frac{8}{3}(-2\alpha^5 + (50\beta + 30)\alpha^4 + (500\beta^3 - 330\beta^2 - 10\beta - 133)\alpha^3 + (-190\beta^3 - 18\beta^2 + 413\beta - 57)\alpha^2 + (50\beta^3 + 3\beta^2 - 144\beta + 54)\alpha - 3\beta^3)$.
3. $SZ_{ve}(G) = \frac{8}{5}\alpha(-\alpha^4 + (25\beta + 45)\alpha^3 + (500\beta^3 - 165\beta^2 - 75\beta - 130)\alpha^2 + (-95\beta^3 - 30\beta^2 + 400\beta - 55)\alpha + 15\beta^3 - 140\beta + 61)$.
4. $PI_v(G) = 24\alpha\beta(10\alpha\beta - \beta - \alpha)$.
5. $PI_e(G) = \frac{4}{3}(8\alpha^3 + (300\beta^2 - 99\beta + 6)\alpha^2 + (-75\beta^2 - 6\beta + 4)\alpha + 6\beta^2)$.
6. $w^+SZ_v(G) = \frac{8}{5}(12\alpha^5 + (-60\beta + 210)\alpha^4 + (2040\beta^3 - 60\beta^2 - 480\beta - 420)\alpha^3 + (-180\beta^3 + 1320\beta - 245)\alpha^2 + (-60\beta^3 + 60\beta^2 - 560\beta + 298)\alpha + 80\beta)$.

7. $w^{\times}SZ_v(G) = \frac{48}{5}(6\alpha^5+(-30\beta+60)\alpha^4+(580\beta^3-35\beta^2-155\beta-90)\alpha^3+(-95\beta^3+305\beta-70)\alpha^2+(-35\beta^3+35\beta^2-160\beta+89)\alpha+40\beta)$.

8. $w^{+}SZ_e(G) = \frac{8}{3}(6\alpha^5+(250\beta+210)\alpha^4+(3400\beta^3-2340\beta^2-91\beta-713)\alpha^3+(-1560\beta^3+162\beta^2+2306\beta-399)\alpha^2+(329\beta^3+108\beta^2-986\beta+413)\alpha-27\beta^3+105\beta)$.

9. $w^{\times}SZ_e(G) = \frac{4}{3}(72\alpha^5+(600\beta+720)\alpha^4+(11600\beta^3-8280\beta^2-379\beta-1891)\alpha^3+(-6120\beta^3+1428\beta^2+6444\beta-1362)\alpha^2+(1061\beta^3+636\beta^2-3354\beta+1507)\alpha-115\beta^3+6\beta^2+631\beta)$.

10. $w^{+}PI_v(G) = 48\alpha\beta(34\alpha\beta-7\beta-7\alpha+2)$.

11. $w^{\times}PI_v(G) = 24\alpha\beta(116\alpha\beta-35\beta-35\alpha+14)$.

12. $w^{+}PI_e(G) = \frac{8}{3}(28\alpha^3+(1020\beta^2-444\beta+33)\alpha^2+(-360\beta^2+78\beta+11)\alpha+33\beta^2-3\beta)$.

13. $w^{\times}PI_e(G) = 4(32\alpha^3+(1160\beta^2-614\beta+51)\alpha^2+(-518\beta^2+200\beta+7)\alpha+51\beta^2-9\beta)$.

In Theorem 3.1 we have assumed that $\alpha \leq \beta$. Note that this no no restriction, because if $\alpha > \beta$, then it is enough to interchange the parameters α and β. Further, the proposed algorithmic technique is applicable for indices that are formulated based on edge contribution therefore Wiener-type index are not focused as a part of the theorem. Apart from the zeolite BCT framework, this method can also be applied to other graphs that are non-partial cube and where the strength weighted cut method fails to compute the Szeged-type indices.

In order to graphically represent the derived expressions, we consider square dimension of the framework, which implies BCT(α, β) such that $\alpha = \beta$. For $2 \leq \alpha \leq 100$, the numerical values of vertex, edge and weighted versions of Szeged and PI indices of zeolite BCT framework is illustrated in Figures 6 and 7.

It is observed that PI_v index attains the least value, while the $w^{\times}SZ_e$ index attains the peak value. Further, the values of $w^{+}PI_e$ and $w^{\times}PI_v$ lie close to each other as shown in Figure 7. All the symbolic derivations presented in this section are performed using MATLAB software and the results are validated using ChemGraphX web tool [20].

4 Concluding remarks

In this article, we have presented a novel technique which is efficient in computing Szeged-type indices of certain molecular graphs that are more general than partial cubes. By implementing this technique, we have derived generalized analytical expressions that compute Szeged-type indices of zeolite BCT-type framework. The indices developed in this work are expected to have high correlation with physico-chemical properties of the framework. Further, the proposed method can be utilized for overcoming

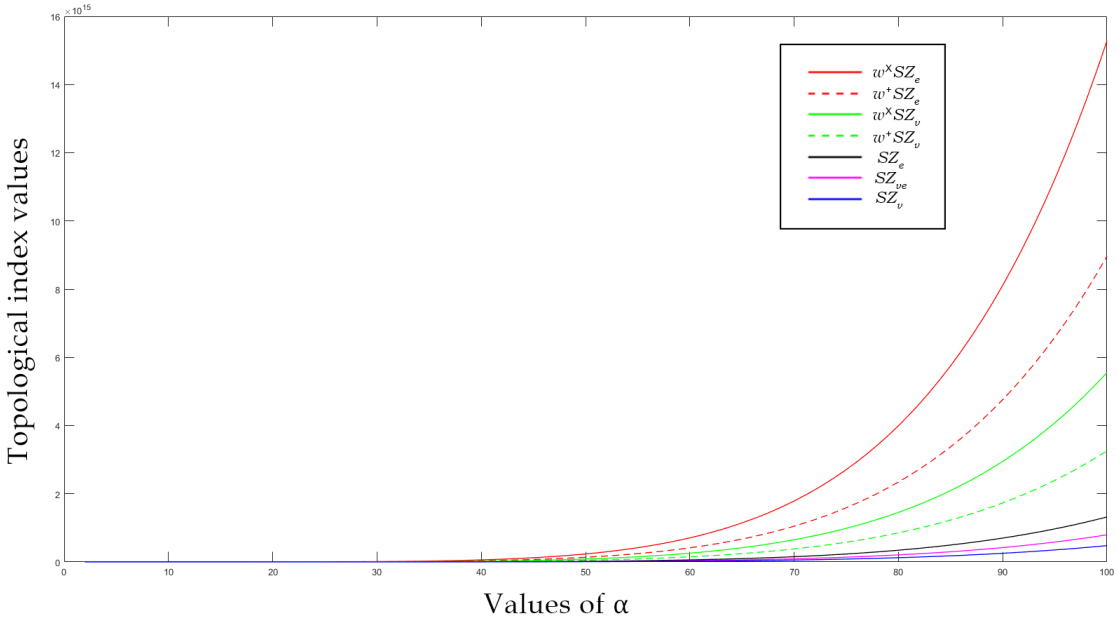


Figure 6: SZ_v, SZ_{ve}, SZ_e, $w^{+}SZ_v$, $w^{\times}SZ_v$, $w^{+}SZ_e$ and $w^{\times}SZ_e$ indices of BCT(α, β), when $\alpha = \beta$

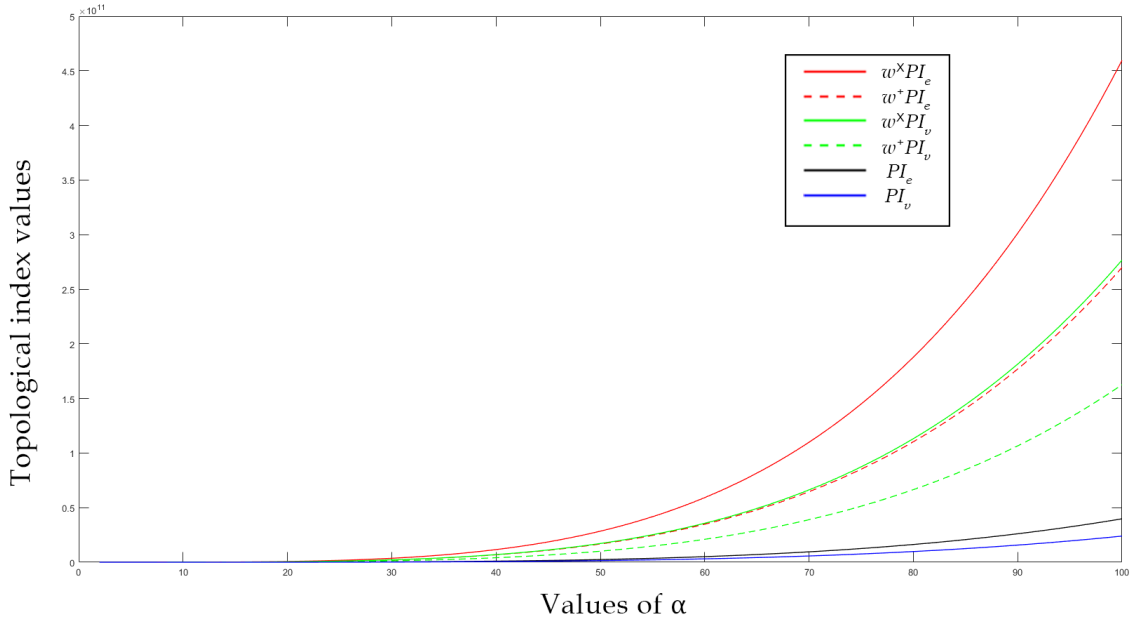


Figure 7: PI_v, PI_e, $w^{+}PI_v$, $w^{\times}PI_v$, $w^{+}PI_e$ and $w^{\times}PI_e$ indices of BCT(α, β), when $\alpha = \beta$

the challenges in computing the distance based topological indices of complex molecular graphs such as zeolites and other chemical frameworks that have similar attributes. In the future, this method can be enhanced to determine Szeged-type entropy measures of chemical graphs to understand the complexity of its framework.

Conflict of interest

The authors declare no conflicts of interest.

Data Availability statement

No data associated in the manuscript.

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