Relativistic Distance Based and Bond Additive Topological Descriptors of Zeolite RHO Materials

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Abstract

Topological indices are graph invariants which provide quantitative information on molecular structures and thus they yield quantitative structure activity relationships (QSAR) and quantitative structure property relationships (QSPR) for the prediction of physico chemical properties of compounds. The zeolite RHO frameworks have received considerable attention as they are extremely useful in trapping heavy metal ions and thus in environmental remediation. These frameworks contain optimal cavities to trap toxic medial ions and recently for heavier halogen substitution. We have applied an efficient technique to obtain exact analytical expressions for the various relativistic topological descriptors of the zeolite RHO structures by graph-theoretical cut methods that reduce the complex structures with tunnels and cages into simpler graphs. Our incorporation of relativistic parameters would be especially useful for the characterization of properties when heavier atoms are incorporated.

Keywords: Graph metrics; topological indices; cut method; zeolites; relativistic QSAR of materials.

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1 Introduction

Zeolites are crystalline microporous aluminosilicates with uniform cavities that can trap multiple toxic metal ions and environmental pollutant gases. Zeolite RHO is a material with considerable potential as it offers smaller pore sizes of $3.6 \, \text{Å} \times 3.6 \, \text{Å}$ with a relatively low Si/Al ratio of $2.5 - 3.0$. The zeolite offers significant flexibility during sorptions and thus these materials offer considerable promise to trap multiple metal ions of varying sizes such as Na$^+$, Cd$^{2+}$, Sr$^{2+}$, Rb$^+$, Ba$^{2+}$ etc. Moreover they have also been considered as potential candidates for the environmental remediation of high level nuclear wastes. The structure of zeolite RHO consists of a body centered cubic arrangement of $\alpha$-cages linked via double 8-rings [1] as shown in Figure 1. This framework displays a considerable flexibility during the sorption-desorption process with metal ions and molecules, and thus it is able to adapt to various cation sizes and shaped adsorbent molecules [2,3]. Johnson et al. [4] have reported the synthesis of a microporous aluminogerminate with a zeolite RHO topology of composition Na$_{16}$Cs$_8$Al$_{24}$Ge$_{24}$O$_{96}$. In this framework cation (sodium and cesium) sites can be substituted by a number of cations such as NH$_4^+$, Ba$^{2+}$, Sr$^{2+}$ and Cd$^{2+}$ etc. [4], thus acting as sorption sites for such metal ions. More recently Sun et al. [5] have reported a novel high-silica zeolite RHO that included a self-assembled Cs$^+$-18-crown -6 sandwich complex. The crown complex containing Cs$^+$ exhibits a greater catalytic activity for ethanol dehydration than other materials with a considerably enhanced selectivity toward ethylene. Zeolite RHO exhibits a high selectivity in catalyzing the production of dimethylamine from ammonia and methanol [6–11]. In addition, it can also serve as a hydrogen storage material with tailor-made pore sizes and cations that are suitable for hydrogen absorption [12–14] or as a CO$_2$ selective adsorbent [15]. The aluminosilicate framework of zeolite RHO undergoes a significant distortion and loss of symmetry upon dehydration. Ng et al. [16] have used an ultraviolet irradiation method for faster and efficient synthesis of zeolite RHO; the technique has yielded high crystallinity with a truncated octahedral morphology. Hence molecular sieves and zeolites are becoming important materials for gas sorptions catalysis and environmental remediation through sorption of toxic heavy metal ions including high level radioactive wastes [17,18] as they offer flexible pore size to accommodate multiple ions. Furthermore, heavier halogen substitution such as Br in scapolite-group minerals and sodalite has received experimental and mineralogical interest [19]. Typically the solid samples of these materials are characterized with X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA) and nitrogen adsorption-desorption analysis in order to establish their structures and pore sizes.

The design of new materials as well as proposed materials with novel architecture require theoretical insights and knowledge concerning feasible structures, their topologies, as well as short and long-
range orders. The topology of the zeolite RHO material is directly connected to tiling and sphere packings. The nomenclature of each material is based on its zeolite framework type and it is assigned a three letter code usually derived from the name of the source material; the code is used in describing the network of corner sharing tetrahedral of the atoms irrespective of its composition.

Chemical graph theory is a branch of discrete mathematics which facilitates the computation of topological descriptors of molecular structures which can then be used to predict the physico chemical properties of complex systems such as zeolite RHO materials. Molecular graphs are structural representations, where the vertices represent the atoms in the molecular structure and the edges represent the chemical bonds. As properties of molecules are functions of their structures, real numbers derived from the associated molecular graphs are called the graph invariants or more frequently structural descriptors (topological indices). In the study of QSAR and QSPR these parameters are utilized to compute the physico chemical and biological activities of chemical compounds from their molecular structures. In this regard, a topological index can be regarded as a score function which maps each molecular structure to a real number and then used as a descriptor of the molecule under consideration.

In the present study we consider the computation of relativistic topological indices for zeolite RHO materials that can incorporate heavy ions such as Cs$^+$, Ba$^{2+}$, Sr$^{2+}$, Cd$^{2+}$, Hg$^{2+}$, Br$^-$ as well as heavy metal oxide ions like UO$_2^{2+}$ that are present in high level nuclear wastes. For such systems containing very heavy atoms, relativistic effects including spin-orbit coupling alter the geometries, energetics, topological and reactivity properties of these compounds are extremely important. Thus any realistic development of topological indices must include the relativistic parameters into both vertices and edges of the molecular structures. Consequently, the present study considers such a development of topological indices that incorporate relativistic effects. Furthermore we have validated the derived
analytical results for the topological indices of zeolite RHO networks by computing several of the topological indices by the software Topochemie-2020 [67].

2 Computational Techniques

We start with some basic definitions and notations that will be used in the paper. Let \( G \) be a finite simple connected graph with vertex set and edge set respectively as \( V(G) \) and \( E(G) \). We define \( d_G(u,v) \) to be the usual shortest-path distance between vertices \( u,v \in V(G) \) and the distance between a vertex \( u \in V(G) \) and an edge \( f = xy \in E(G) \) is defined as \( d_G(u,f) = \min\{d_G(u,x),d_G(u,y)\} \). Moreover, the shortest-path distance between edges \( g = ab \) and \( f = xy \) is defined as \( D_G(g,f) = \min\{d_G(a,f),d_G(b,f)\} \). For an edge \( e = uv \in E(G) \), we propose the values \( n_u(e|G) \) and \( m_u(e|G) \) are defined as the number of vertices and edges of \( G \) respectively whose distance to the vertex \( u \) is smaller than the distance to the vertex \( v \). Similarly, \( n_v(e|G) \) and \( m_v(e|G) \) are defined as the number of vertices and edges of \( G \) respectively whose distance to the vertex \( v \) is smaller than the distance to the vertex \( u \).

Let \( \deg_G(u) \) be the number of edges that incident to \( u \) and the degree of an edge \( e = uv \in E(G) \) is defined as the number of edges adjacent to \( e \) and denoted by \( \deg_G(e) \). i.e., \( \deg_G(e) = \deg_G(u) + \deg_G(v) - 2 \). In addition to the degree measure of the edge, there are two types of measures defined based on the degrees of end vertices and given below:

- \( w^+(e) = \deg_G(u) + \deg_G(v) \).
- \( w^*(e) = \deg_G(u) \deg_G(v) \).

We now present the definitions of Wiener-type, Szeged-type, Mostar-type and degree-based topological indices for a simple graph \( G \) [28] [50].

(1) Wiener-type indices:

\[
\begin{align*}
\text{Wiener} & \quad W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) \\
\text{Edge Wiener} & \quad W_e(G) = \sum_{\{f,g\} \subseteq E(G)} D_G(f,g) \\
\text{Vertex-edge Wiener} & \quad W_{ev}(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{f \in E(G)} d_G(u,f) \\
\text{Schultz} & \quad S(G) = \sum_{\{u,v\} \subseteq V(G)} (\deg_G(u) + \deg_G(v))d_G(u,v)
\end{align*}
\]
\[ \text{Gutman}\hspace{1cm} \text{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} \text{deg}_G(u) \text{deg}_G(v) d_G(u,v) \]

(2) Szeged-type indices:

Vertex Szeged \[ S_{zv}(G) = \sum_{e=uv \in E(G)} n_u(e|G)n_v(e|G) \]

Edge Szeged \[ S_{ze}(G) = \sum_{e=uv \in E(G)} m_u(e|G)m_v(e|G) \]

Edge-vertex Szeged \[ S_{zev}(G) = \frac{1}{2} \sum_{e=uv \in E(G)} (n_u(e|G)m_v(e|G) + n_v(e|G)m_u(e|G)) \]

Padmakar-Ivan \[ PI(G) = \sum_{e=uv \in E(G)} (m_u(e|G) + m_v(e|G)) \]

\( w^+ \)-vertex Szeged \[ w^+S_{zv}(G) = \sum_{e=uv \in E(G)} w^+(e) n_u(e|G)n_v(e|G) \]

\( w^+ \)-edge Szeged \[ w^+S_{ze}(G) = \sum_{e=uv \in E(G)} w^+(e) m_u(e|G)m_v(e|G) \]

\( w^+ \)-PDMakar-Ivan \[ w^+PI(G) = \sum_{e=uv \in E(G)} w^+(e) (m_u(e|G) + m_v(e|G)) \]

\( w^* \)-vertex Szeged \[ w^*S_{zv}(G) = \sum_{e=uv \in E(G)} w^*(e) n_u(e|G)n_v(e|G) \]

\( w^* \)-edge Szeged \[ w^*S_{ze}(G) = \sum_{e=uv \in E(G)} w^*(e) m_u(e|G)m_v(e|G) \]

\( w^* \)-PDMakar-Ivan \[ w^*PI(G) = \sum_{e=uv \in E(G)} w^*(e) (m_u(e|G) + m_v(e|G)) \]

(3) Mostar-type indices:

Mostar \[ Mo(G) = \sum_{e=uv \in E(G)} |n_u(e|G) - n_v(e|G)| \]

Edge Mostar \[ Mo_e(G) = \sum_{e=uv \in E(G)} |m_u(e|G) - m_v(e|G)| \]

\( w^+ \)-Mostar \[ w^+Mo(G) = \sum_{e=uv \in E(G)} w^+(e) |n_u(e|G) - n_v(e|G)| \]

\( w^+ \)-edge Mostar \[ w^+Mo_e(G) = \sum_{e=uv \in E(G)} w^+(e) |m_u(e|G) - m_v(e|G)| \]

\( w^* \)-Mostar \[ w^*Mo(G) = \sum_{e=uv \in E(G)} w^*(e) |n_u(e|G) - n_v(e|G)| \]
\[ w^* - \text{edge Mostar} \quad w^*M_{\alpha}(G) = \sum_{e=uv \in E(G)} w^*(e) \left| m_u(e|G) - m_v(e|G) \right| \]

(4) Degree-based indices:

First Zagreb
\[ M_1(G) = \sum_{e=uv \in E(G)} w^+(e) \]

Second Zagreb
\[ M_2(G) = \sum_{e=uv \in E(G)} w^*(e) \]

Randić
\[ R(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{w^*(e)}} \]

Atom Bond Connectivity
\[ ABC(G) = \sum_{e=uv \in E(G)} \sqrt{w^+(e) - 2} \]

Harmonic
\[ H(G) = \sum_{e=uv \in E(G)} \frac{2}{w^+(e)} \]

Sum Connectivity
\[ SC(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{w^+(e)}} \]

Hyper Zagreb
\[ HM(G) = \sum_{uv \in E(G)} (w^+(e))^2 \]

Geometric Arithmetic
\[ GA(G) = \sum_{e=uv \in E(G)} 2^{\frac{w^*(e)}{w^+(e)}} \]

Irregularity Measure
\[ irr(G) = \sum_{e=uv \in E(G)} \left| \deg_G(u) - \deg_G(v) \right| \]

Sigma
\[ \sigma(G) = \sum_{e=uv \in E(G)} \left( \deg_G(u) - \deg_G(v) \right)^2 \]

Forgotten
\[ F(G) = \sum_{e=uv \in E(G)} \left( \deg_G(u)^2 + \deg_G(v)^2 \right) \]

Symmetric Division Degree
\[ SDD(G) = \sum_{e=uv \in E(G)} \left( \frac{\deg_G(u)}{\deg_G(v)} + \frac{\deg_G(v)}{\deg_G(u)} \right) \]

We expand this preliminary section by defining a few concepts related to the cut method \[52,53\], which has been used in the computation of relativistic topological descriptors of certain types of zeolite structures \[23,51\]. A subgraph \( H \) of a graph \( G \) is said to be isometric if \( d_H(u,v) = d_G(u,v) \) holds for all pairs of vertices \( u \) and \( v \) of \( H \). The family of graphs that comprises of all isometric subgraphs of hypercubes are known as partial cubes. The Djoković-Winkler relation \( \Theta \) \[54,55\], which acts a decisive part in our computations, is defined as follows: if \( e = ab \in E(G) \) and \( f = cd \in E(G) \), then \( e \Theta f \) if \( d_G(a,c) + d_G(b,d) \neq d_G(a,d) + d_G(b,c) \). The relation \( \Theta \) is reflexive and symmetric, but not
transitive in general. If $G$ is a partial cube, then $\Theta$ is also transitive and hence $G$ is an equivalence relation. Moreover, in that case for any $\Theta$-class $F_i$, the graph $G - F_i$ consists of exactly two connected components $52$. We now define the measures of $F_i$ based on $w^+$ and $w^*$ as $w^+(F_i) = \sum_{s \in F_i} w^+(s)$, and $w^*(F_i) = \sum_{s \in F_i} w^*(s)$. The standard cut method for the computation of topological indices $48,50,55–64$ can be now expressed as follows.

**Theorem 2.1.** Let $G$ be a partial cube with its $\Theta$-partition $\mathcal{F} = \{F_1, \ldots, F_k\}$. For each $1 \leq i \leq k$, let $XF_i$ and $YF_i$ be the connected components of $G$. Let $n_1(F_i) = |V(XF_i)|$, $n_2(F_i) = |V(YF_i)|$, $m_1(F_i) = |E(XF_i)|$ and $m_2(F_i) = |E(YF_i)|$. Then

1. $W(G) = \sum_{i=1}^{k} n_1(F_i) n_2(F_i)$,
2. $W_e(G) = \sum_{i=1}^{k} m_1(F_i) m_2(F_i)$,
3. $W_{ev}(G) = \sum_{i=1}^{k} \frac{1}{2} [n_1(F_i) m_2(F_i) + n_2(F_i) m_1(F_i)]$,
4. $Sz_v(G) = \sum_{i=1}^{k} |F_i| n_1(F_i) n_2(F_i)$,
5. $Sz_e(G) = \sum_{i=1}^{k} |F_i| m_1(F_i) m_2(F_i)$,
6. $Sz_{ev}(G) = \sum_{i=1}^{k} \frac{1}{2} |F_i| \{n_1(F_i) m_2(F_i) + n_2(F_i) m_1(F_i)\}$,
7. $PI(G) = |E(G)|^2 - \sum_{i=1}^{k} |F_i|^2$,
8. $S(G) = |E(G)||V(G)| + \sum_{i=1}^{k} 2[n_1(F_i) m_2(F_i) + n_2(F_i) m_1(F_i)]$,
9. $Gut(G) = 2|E(G)|^2 + \sum_{i=1}^{k} [4m_1(F_i) m_2(F_i) - |F_i|^2]$,
10. $Mo(G) = \sum_{i=1}^{k} |F_i| |n_1(F_i) - n_2(F_i)|$,
11. $Mo_e(G) = \sum_{i=1}^{k} |F_i| |m_1(F_i) - m_2(F_i)|$,

When $\# \in \{+,\ast\}$,
12. $w^\# Mo(G) = \sum_{i=1}^{k} w^\#(F_i) \ |n_1(F_i) - n_2(F_i)|$,
13. $w^\# Mo_e(G) = \sum_{i=1}^{k} w^\#(F_i) \ |m_1(F_i) - m_2(F_i)|$,
14. \( w^\#Sz_v(G) = \sum_{i=1}^{k} w^\#(F_i) \cdot n_1(F_i) \cdot n_2(F_i) \),

15. \( w^\#Sz_e(G) = \sum_{i=1}^{k} w^\#(F_i) \cdot m_1(F_i) \cdot m_2(F_i) \),

16. \( w^\#PI(G) = \sum_{i=1}^{k} w^\#(F_i) \cdot (m_1(F_i) + m_2(F_i)) \).

### 3 A Construction of Partial Cubes

In order to apply Theorem 2.1, we need to deal with partial cubes. To establish this fact for the key players of this paper, zeolite RHO materials, the theorem proved in this section is essential. To prove it, we recall the following two result, see [65, Lemma 11.2] and [65, Lemma 11.3], respectively.

**Lemma 3.1.** Let \( G \) be a bipartite graph and \( e = uv, f = xy \) be two edges of \( G \) with \( e \Theta f \). Then the notation can be chosen such that 
\[ d_G(u,x) = d_G(v,y) = d_G(u,y) - 1 = d_G(v,x) - 1 \]

**Lemma 3.2.** Suppose that a walk \( P \) connects the endpoints of an edge \( e \) but does not contain it. Then \( P \) contains an edge \( f \) with \( e \Theta f \). If it is the only edge of \( P \) with this property, then it cannot be incident with \( e \).

To state the key result recall that a subgraph \( H \) of a graph \( G \) is convex if for each pair of vertices \( x \) and \( y \) of \( G \), each shortest path between \( x \) and \( y \) in \( G \) lies completely in \( H \), and that a set of edges of \( G \) is called a perfect matching if it an independent edge set that covers every vertex of \( G \).

**Theorem 3.1.** Let \( G \) and \( H \) be partial cubes, and let \( C_G \) and \( C_H \) be convex cycles in \( G \) and \( H \), respectively, where \( |C_G| = |C_H| \). Let \( X \) be the graph obtained from the disjoint union of \( G \) and \( H \) by adding a perfect matching between \( C_G \) and \( C_H \) which induces an isomorphism between \( C_G \) and \( C_H \). Then \( X \) is a partial cube.

**Proof.** To prove the result we will use Winkler’s characterization that a connected graph \( G \) is a partial cube if and only if \( G \) is bipartite and \( \Theta \) is transitive on \( E(G) \) [55]. First, since \( G \) and \( H \) are partial cubes, they are bipartite graphs. It is then straightforward to see that \( X \) is bipartite as well. It remains to show that \( \Theta \) is transitive in \( X \).

Let \( e_1 = x_1y_1, e_2 = x_2y_2, \) and \( e_3 = x_3y_3 \) be arbitrary edged of \( X \) such that \( e_1 \Theta e_2 \) and \( e_2 \Theta e_3 \) hold.

We need to prove that \( e_1 \Theta e_3 \) holds as well. If \( e_1, e_2, e_3 \in E(G) \), then since \( G \) is convex in \( X \) and \( G \) is a partial cube, \( e_1 \Theta e_3 \) holds by Wikler’s theorem applied to \( G \) (as a subgraph of \( X \)). Similarly, if \( e_1, e_2, e_3 \in E(H) \), we have the same conclusion.

Consider next the case that \( e_1 \) is one of the matching edges between \( G \) and \( H \). Assume without loss of generality that \( x_1 \in V(G) \) and \( y_1 \in V(H) \). Then \( d_X(y_1,u) = d_X(x_1,u) + 1 \) holds for each
vertex \( u \in V(G) \). Using Lemma \([3.1]\) it follows that \( e_1 \) is not in relation \( \Theta \) with any of the edges from \( E(G) \). So \( e_1 \) can be only in relation \( \Theta \) with matching edges. It is straightforward to see that \( e_1 \) is in relation \( \Theta \) with all the matching edges. In particular, \( e_2 \) and \( e_3 \) are also matching edges and \( e_1 \Theta e_3 \) holds.

It remains to consider the case in which two of the edges \( e_1, e_2, e_3 \) lie in \( E(G) \) and one in \( E(H) \) or the other way around. Without loss of generality, there are two cases to be considered: (i) \( e_1, e_2 \in E(G) \) and \( e_3 \in E(H) \), and (ii) \( e_1, e_3 \in E(G) \) and \( e_2 \in E(H) \).

Suppose first that \( e_1, e_2 \in E(G) \) and \( e_3 \in E(H) \). Recall that \( e_1 \Theta e_2 \) and \( e_2 \Theta e_3 \). By Lemma \([3.1]\) we may assume that \( d_X(x_2, x_3) = d_X(y_2, y_3) = d_X(x_2, y_3) - 1 = d_X(y_2, x_3) - 1 \). Let \( P \) be an arbitrary shortest \( x_2, x_3 \)-path and let \( u \) be the first vertex on \( P \) which lies in \( C_G \). Denoting the neighbor of \( u \) in \( H \) by \( u' \) we may assume that \( u' \) also lies on \( P \). Since \( d_X(y_2, x_3) = d_X(x_2, x_3) + 1 \), we infer that \( d_X(y_2, u) = d_X(x_2, u) + 1 \). Consider next a shortest \( y_2, y_3 \)-path \( Q \), and let \( w \) be the first vertex of \( Q \) that lies on \( C_G \). Then \( w \neq u \), for otherwise we would have \( d_X(y_3, u') < d_X(x_3, u') \) which is not possible because it would imply that \( d_X(y_3, x_2) < d_X(x_3, x_2) \). Consider now the walk \( W \) which connects \( x_2 \) with \( y_2 \) and is composed of the subpath of \( P \) between \( x_2 \) and \( u \), a shortest path between \( u \) and \( w \) on \( C_G \), and the subpath of \( Q \) between \( w \) and \( y_2 \). By Lemma \([3.2]\) \( W \) contains an edge \( f \) such that \( e_2 \Theta f \).

Since no two edges of a shortest path are in relation \( \Theta \), we infer that \( f \) must be an edge of the cycle \( C_G \). Because \( e_1 \Theta e_2, e_2 \Theta f \), and \( e_1, e_2, f \in E(G) \), we get that \( e_1 \Theta f \). Denoting by \( f' \) the isomorphic copy of \( f \) in \( C_H \) we also get that \( e_1 \Theta f' \). But then, since the distance function between the end vertices of \( e_1 \) and \( f' \), and between \( f' \) and \( e_3 \) is additive, we conclude that \( e_1 \Theta e_3 \).

Suppose second that \( e_1, e_3 \in E(G) \) and \( e_2 \in E(H) \), where again \( e_1 \Theta e_2 \) and \( e_2 \Theta e_3 \). Considering the edges \( e_1 \) and \( e_2 \) and using an argument parallel to the above reasoning, we find that there exists an edge \( f \in C_G \) such that \( e_1 \Theta f \). Let \( f' \) be the isomorphic copy of \( f \) in \( C_H \). Similarly, considering the edges \( e_3 \) and \( e_2 \) we find that there exists an edge \( g \in C_G \) such that \( e_3 \Theta g \). Let \( g' \) be the isomorphic copy of \( g \) in \( C_H \). Since \( f' \Theta e_2 \) and \( e_2 \Theta g' \), and \( H \) is a partial cube, we see that \( f' \Theta g' \). Consequently, \( f \Theta g \). But now we have \( e_1 \Theta f \Theta g \Theta e_3 \), and as these are all edges of \( G \) (which is a partial cube and a convex subgraph of \( X \)), transitivity implies that \( e_1 \Theta e_3 \).

## 4 Results and Discussion

The primitive unit cell of zeolite RHO materials is a truncated cuboctahedron, called the \( \alpha \)-cage. It is an Archimedean solid consisting of 48 vertices and 72 edges with 26 faces made of 12 squares, 8 hexagons and 6 octagons that preserve the point group symmetry on each its face as depicted in Figure 2(a). That this \( \alpha \)-cage, that is, the truncated cuboctahedron, belongs to the class of partial cubes has
Figure 2: Primitive unit cell of zeolite RHO and its single layer

been shown in [66] where an extensive search for cubic partial cubes has been performed.

The zeolite RHO materials are designed by arranging the α-cages in a 3D mesh $a \times b \times c$ such that two α-cages are connected by two eight-membered rings (octagonal prism) in order that all cation sites are equally accessible for adsorbate molecules as shown in Figure 2(b). This 3D materials is denoted by $RHO(a, b, c)$ and by symmetrical arrangement of α-cages, $RHO(a, b, c) \cong RHO(b, c, a) \cong RHO(c, a, b)$. Inductively applying Theorem 3.1 we infer that the 3D material $RHO(a, b, c)$ is a partial cube.

From the octagonal-prism arrangement of α-cages, we can find the number of vertices and edges as $|V(RHO(a, b, c))| = 48abc$ and $|E(RHO(a, b, c))| = 96abc - 8(ab + bc + ca)$, respectively. It is clear that $RHO(a, b, c)$ contains $abc$ number of α-cages and we denote the α-cage in the $(x, y, z)$ position of $a \times b \times c$ mesh as $\alpha_{x,y,z}$.

The relativistic parameters for the various heavy atoms impregnated into zeolites can be derived by convenient localization of molecular orbitals as described in [51]. Hence, the topological indices in terms of relativistic quantum parameters can be computed by weighted graphs with weights $\gamma_x$ and $\rho_{xy}$ for each vertex $x$ and edge $xy$, respectively. Thus, the molecular graphs of doped or impregnated zeolite RHOS with heavy elements can be represented as a structural graphs with vertex-weights $\{\gamma_x, \gamma_y\}$ and edge-weights $\rho_{xy}$ such that $\gamma_x$ and $\gamma_y$ with equal ratio. Let $V_\gamma(RHO(a, b, c))$ and $E_\rho(RHO(a, b, c))$ be the structural vertex set and edge set of $RHO(a, b, c)$ respectively. Therefore, it can be seen that $|V_\gamma(RHO(a, b, c))| = \frac{1}{2}(\gamma_x + \gamma_y)|V(RHO(a, b, c))|$ and $|E_\rho(RHO(a, b, c))| = \rho_{xy}|E(RHO(a, b, c))|$. 
We now present the technique to compute the relativistic topological indices for single layered zeolite RHO materials, i.e. $RHO(a, b, 1)$ and then readily generalize the technique to multi-layered layers zeolite $RHO(a, b, c)$. For convenience, we use the notation $RHO(a, b)$ instead of $RHO(a, b, 1)$ and in the same way $\alpha_{x,y,1}$ by $\alpha_{x,y}$ as given in Figure 2(b). To proceed further, we first compute the $\Theta$-classes of single $\alpha$-cage and then identify the $\Theta$-classes of $RHO(a, b)$.

![Various $\Theta$-classes of $\alpha$-cage based on the front-, side- and top-view](image)

Figure 3: Various $\Theta$-classes of $\alpha$-cage based on the front-, side- and top-view

As a consequence of point group symmetry on each face of $\alpha$-cage, we could find nine types of $\Theta$-classes as shown in Figure 3. These types are denoted by front-view forward-slash $F/$, front-view
Theorem 4.1. Let $G$ be a zeolite RHO materials $RHO(a,b)$ where $1 \leq a \leq b$. Then,

1. $W(G) = \frac{48}{5}a(\gamma_{x} + \gamma_{y})^2(60ab^3 + (40a^2 + 15a + 5)b^2 + (10a^3 + 5a)b - 2a^4 + 2)$.

2. $W_{c}(G) = \frac{16}{15}\rho_{xy}^2((7260a^2 - 1320a + 60)b^3 + (4840a^3 - 5100a^2 + 1565a - 45)b^2 + (1210a^4 - 1320a^3 + 1595a^2 - 90a - 15)b - 242a^5 + 50a^3 - 45a^2 + 237a)$.

3. $W_{ce}(G) = \frac{32}{5}a\rho_{xy}(\gamma_{x} + \gamma_{y})((330a - 30)b^3 + (220a^2 - 75a + 35)b^2 + (55a^3 - 30a^2 + 35a)b - 11a^4 + 11)$.

4. $S_{x}(G) = 384a\rho_{xy}(\gamma_{x} + \gamma_{y})((23a^2 + 1)b^3 + 3a^2b - a^3 + a)$.

5. $S_{xy}(G) = \frac{256}{15}\rho_{xy}^3((6800a^3 - 2130a^2 + 790a - 30)b^3 + (-2570a^3 + 315a^2 - 85a)b^2 + (165a^4 + 1430a^3 - 360a^2 + 25a)b - 11a^5 - 320a^4 + 25a^3 + 320a^2 - 44a)$.

6. $S_{xy}(G) = \frac{128}{3}a\rho_{xy}(\gamma_{x} + \gamma_{y})((1250a^2 - 195a + 85)b^3 + (-235a^2 - 5)b^2 + (15a^3 + 195a^2 - 30a)b - a^4 - 55a^3 + 5a^2 + 55a - 4)$.

7. $PI(G) = \frac{128}{3}\rho_{xy}^2((180a^2 - 39a + 3)b^2 + (-42a^2 + 3a)b + a^3 + 3a^2 - a)$.

8. $S(G) = \frac{64}{5}a\rho_{xy}(\gamma_{x} + \gamma_{y})((660a - 60)b^3 + (440a^2 + 15a + 55)b^2 + (110a^3 - 60a^2 + 55a)b - 22a^4 + 22)$.

9. $Gut(G) = \frac{64}{15}\rho_{xy}^2((7260a^2 - 1320a + 60)b^3 + (4840a^3 - 1485a^2 + 845a)b^2 + (1210a^4 - 1320a^3 + 845a^2 - 30a - 15)b - 242a^5 + 60a^3 + 227a)$.

10. $Mo(G) = 96\rho_{xy}(\gamma_{x} + \gamma_{y})((10a^2 - 2a + (-1)a - 1)b^2 - 2b^2 - ((-1)a + b - 2)a^2)$.

11. $Mo_{s}(G) = \frac{32}{3}\rho_{xy}((330a^2 - 84a + 33(-1)a - 33)b^2 + (-78a^2 + 12a - 3(-1)a + 3)b - 2a^2 - (33(-1)a + b - 33(-1)b - 66)a^2 + 3(-1)a + b - 3(-1)b + 8)a)$.

12. $w^{+}Mo(G) = 16\rho_{xy}(\gamma_{x} + \gamma_{y})((456a^2 - 144a + 45(-1)a - 21)b^2 + (-150a^2 - 9(-1)a + 9)b + 2a^3 - (42(-1)a + b - 51)a^2 + 3(-1)a + b - 9(-1)a + 10)$.

13. $w^{+}Mo_{e}(G) = 16\rho_{xy}((1672a^2 - 618a + 165(-1)a - 69)b^2 + (-612a^2 + 84a - 48(-1)a + 40)b - 2a^2 + (-154(-1)a + 165(-1)b - 179)a^2 + (25(-1)a + b - 48(-1)b + 59)a + 2(-1)a + b - 5)$.

14. $w^{*}Mo(G) = 8\rho_{xy}(\gamma_{x} + \gamma_{y})((1752a^2 - 750a + 171(-1)a + 21)b^2 + (-798a^2 + 24a - 63(-1)a + 63)b + 16a^3 + (-150(-1)a + b + 171(-1)b - 57)a^2 + 2(-1)a + b - 63(-1)b + 71)$.
(15) \( w^* \Omega_e(G) = \frac{8}{3} \rho_{xy} (19272a^2 - 9276a + 1881(-1)a + 405)b^2 + (-9504a^2 + 1512a - 864(-1)a + 648)b + 76a^3 + (-1650(-1)a + b + 1881(-1)b - 453)a^2 + (414(-1)a + b - 864(-1)b + 842)a + 39(-1)a + b - 102). \)

(16) \( w^* \Sigma v(G) = \frac{384}{5} \rho_{xy} (\gamma_x + \gamma_y)^2 ((880a^3 - 55a^2 - 25a + 30)b^3 + (-45a^3 - 15a)b^2 + (-5a^4 + 45a^3 - 15a^2)b + a^5 - 35a^4 + 30a^3 + 35a^2 - a). \)

(17) \( w^* \Sigma e(G) = \frac{128}{75} \rho_{xy} ((103960a^3 - 39100a^2 + 7185a + 2975)b^3 + (-4050a^3 + 10020a^2 - 2330a - 660)b^2 + (1705a^3 + 16145a^3 - 6195a^2 + 780a + 25)b - 33a^5 - 4480a^4 + 3750a^3 + 3820a^2 - 717a). \)

(18) \( w^* P I(G) = \frac{64}{7} \rho_{xy}^2 (2748a^2 - 837a + 71)b^2 + (-879a^2 + 144a - 3)b + 14a^3 + 75a^2 - 17a). \)

(19) \( w^* \Sigma v(G) = \frac{192}{5} \rho_{xy}^3 (\gamma_x + \gamma_y)^2 ((3400a^3 - 395a^2 - 355a + 240)b^3 + (-315a^3 - 105a)b^2 + (-40a^4 - 105a^3 - 105a^2)b + 8a^5 - 125a^4 + 240a^3 + 125a^2 - 8a). \)

(20) \( w^* \Sigma e(G) = \frac{64}{15} \rho_{xy}^4 ((401320a^3 - 17260a^2 + 6655a + 25765)b^3 + (-184990a^3 + 55680a^2 - 11090a - 5280)b^2 + (3410a^4 + 38655a^3 - 24960a^2 + 4030a + 215)b + 418a^5 - 16000a^4 + 28555a^3 + 10720a^2 - 2993a). \)

(21) \( w^* P I(G) = \frac{64}{3} \rho_{xy}^3 (5298a^2 - 2043a + 198)b^2 + (-2118a^2 + 459a - 12)b + 25a^3 + 198a^2 - 37a). \)

**Proof.** We begin the proof by identifying the \( \Theta \)-classes of \( RHO(a, b) \) based on the \( \Theta \)-classes of \( \alpha \)-cage as shown in Figure 4. For \( 1 \leq i \leq a + b - 1 \), let \( F/_{i} = \{ e \in \alpha_{x,y} : e \in F/ \text{ such that } x + y - 1 = i \} \), \( F\backslash_{i} = \{ e \in \alpha_{x,y} : e \in F \backslash \text{ such that } y - x + a = i \} \) and \( F|_{i} = \{ e \in \alpha_{x,y} : e \in F\} \) be \( \text{the} \text{front-view type of} \Theta\text{-classes.} \) For \( 1 \leq i \leq a \), let \( S/_{i} = \{ e \in \alpha_{x,y} : e \in S/ \text{ such that } x = i \} \), \( S\backslash_{i} = \{ e \in \alpha_{x,y} : e \in S \backslash \text{ such that } x = i \} \) and \( S|_{i} = \{ e \in \alpha_{x,y} : e \in S \} \text{ such that } y = i \} \) be \( \text{the side-view type of} \Theta\text{-classes.} \) For \( 1 \leq i \leq b \), let \( T/_{i} = \{ e \in \alpha_{x,y} : e \in T/ \text{ such that } y = i \} \), \( T\backslash_{i} = \{ e \in \alpha_{x,y} : e \in T \backslash \text{ such that } y = i \} \) and \( T|_{i} = \{ e \in \alpha_{x,y} : e \in T \} \text{ such that } x = i \} \) be \( \text{the top-view type of} \Theta\text{-classes.} \)

For \( 1 \leq i \leq b - 1 \), let \( S\backslash_{i} \) be a set of edges connecting \( \alpha_{x,i} \) and \( \alpha_{x,i+1} \), called \( \text{side-view horizontal-slash type} \Theta\text{-classes.} \) Similarly, for \( 1 \leq i \leq a - 1 \), let \( T\backslash_{i} \) be a set of edges connecting \( \alpha_{i,y} \) and \( \alpha_{i+1,y} \), called \( \text{top-view horizontal-slash type} \Theta\text{-classes.} \) Since \( |V(RHO(a, b))| = 48ab \) and \( |E(RHO(a, b))| = 8[11ab - (a + b)] \), we have \( |V\gamma(RHO(a, b))| = \frac{1}{2} (\gamma_x + \gamma_y) |V(RHO(a, b))| \) and \( |E\rho(RHO(a, b))| = \rho_{xy} |E(RHO(a, b))| \). The graph theoretical parameters of Front-view \( \Theta \)-classes are given below:

\[
|F/_{i}| = \begin{cases} 
8i\rho_{xy} & \text{if } 1 \leq i \leq a - 1 \\
8a\rho_{xy} & \text{if } a \leq i \leq b \\
|F/_{a+b-i}| & \text{if } b + 1 \leq i \leq a + b - 1 
\end{cases}
\]
Figure 4: Various Θ-classes of $RHO(2,2)$ based on the front-, side-, top-, horizontal- and vertical-view
\[ n_1(F_i) = \begin{cases} 
12i^2 \{\gamma_x + \gamma_y\} & \text{if } 1 \leq i \leq a - 1 \\
12a(2i - a) \{\gamma_x + \gamma_y\} & \text{if } a \leq i \leq b \\
n_1(F_{a+b-i}) & \text{if } b + 1 \leq i \leq a + b - 1 
\end{cases} \]

\[ n_2(F_i) = |V_\gamma(RHO(a,b))| - n_1(F_i), \]

\[ m_1(F_i) = \begin{cases} 
4i(11i - 3)\rho_{xy} & \text{if } 1 \leq i \leq a - 1 \\
8(11a - 1)i - 4a(11a + 1)\rho_{xy} & \text{if } a \leq i \leq b \\
m_1(F_{a+b-i}) & \text{if } b + 1 \leq i \leq a + b - 1 
\end{cases} \]

\[ m_2(F_i) = |E_\rho(RHO(a,b))| - m_1(F_i) - |F_i|. \]

\[ w^+(F_i) = \begin{cases} 
4(14i - 1)\rho_{xy} & \text{if } 1 \leq i \leq a - 1 \\
8(7a - 1)\rho_{xy} & \text{if } i = a, \ a = b \\
2(28a - 3)\rho_{xy} & \text{if } i = a, \ a < b \\
4(14a - 1)\rho_{xy} & \text{if } a < i < b \\
w^+(F_{a+b-i}) & \text{if } b \leq i \leq a + b - 1 
\end{cases} \]

\[ w^+(F_i) = \begin{cases} 
4(25i - 4)\rho_{xy}^2 & \text{if } 1 \leq i \leq a - 1 \\
4(25a - 7)\rho_{xy}^2 & \text{if } i = a, \ a = b \\
2(50a - 11)\rho_{xy}^2 & \text{if } i = a, \ a < b \\
4(25a - 4)\rho_{xy}^2 & \text{if } a < i < b \\
w^+(F_{a+b-i}) & \text{if } b \leq i \leq a + b - 1 
\end{cases} \]

\[ |F_1| = 8ab\rho_{xy}, \]

\[ n_1(F_1) = n_2(F_1) = 12ab\{\gamma_x + \gamma_y\}, \]

\[ m_1(F_1) = m_2(F_1) = (40ab - 4(a + b))\rho_{xy}, \]

\[ w^+(F_1) = 8(8ab - (a + b))\rho_{xy}, \]

\[ w^+(F_1) = 4(32ab - 7(a + b))\rho_{xy}^2. \]

The graph theoretical parameters of \( S/ \) and \( S\) as well as \( T/ \) and \( T\) are the same. In addition, the parameters of \( S/ \) and \( T/ \) are symmetrical with respect to \( a \) and \( b \) whereas \( S\) and \( T\) as well as
If we denote $TI$ then the proof is complete by the following equation.

$S$- and $T$- are symmetrical with respect to $b$ and $a$. Hence, we have the following measures for only $S$-type classes.

$$|S/| = 8b \rho_{xy}, \ 1 \leq i \leq a$$

$$n_1 (S/|i) = 12b(2i - 1){\gamma}_x + {\gamma}_y, \ 1 \leq i \leq a$$

$$n_2 (S/|i) = |V_\gamma (RHO(a, b))| - n_1 (S/|i), \ 1 \leq i \leq a$$

$$m_1 (S/|i) = 8(11b - 1)i - 4(13b - 1) \rho_{xy}, \ 1 \leq i \leq a$$

$$m_2 (S/|i) = |E_\rho (RHO(a, b))| - m_1 (S/|i) - |S/|i, \ 1 \leq i \leq a$$

$$w^+ (S/|i) = \begin{cases} 4(15b - 2) \rho_{xy} & \text{if } i = 1, a \\ 8(8b - 1) \rho_{xy} & \text{if } 1 < i < a \end{cases}$$

$$w^* (S/|i) = \begin{cases} 28(4b - 1) \rho_{xy}^2 & \text{if } i = 1, a \\ 4(32b - 7) \rho_{xy}^2 & \text{if } 1 < i < a \end{cases}$$

$$|S|i = 8a \rho_{xy}, \ 1 \leq i \leq b$$

$$n_1 (S|i) = 12a(2i - 1){\gamma}_x + {\gamma}_y, \ 1 \leq i \leq b$$

$$n_2 (S|i) = |V_\gamma (RHO(a, b))| - n_1 (S|i), \ 1 \leq i \leq b$$

$$m_1 (S|i) = 8(11a - 1)i - 4(13a - 1) \rho_{xy}, \ 1 \leq i \leq b$$

$$m_2 (S|i) = |E_\rho (RHO(a, b))(\rho_{xy})| - m_1 (S|i) - |S|i, \ 1 \leq i \leq b$$

$$w^+ (S|i) = 8(7a - 1) \rho_{xy}, \ 1 \leq i \leq b$$

$$w^* (S|i) = 4(25a - 7) \rho_{xy}^2, \ 1 \leq i \leq b$$

$$|S−i| = 8a \rho_{xy}, \ 1 \leq i \leq b - 1$$

$$n_1 (S−i) = 24ai{\gamma}_x + {\gamma}_y, \ 1 \leq i \leq b - 1$$

$$n_2 (S−i) = |V_\gamma (RHO(a, b))| - n_1 (S−i), \ 1 \leq i \leq b - 1$$

$$m_1 (S−i) = 8(11a - 1)i - 8a \rho_{xy}, \ 1 \leq i \leq b - 1$$

$$m_2 (S−i) = |E_\rho (RHO(a, b))| - m_1 (S−i) - |S−i|, \ 1 \leq i \leq b - 1$$

$$w^+ (S−i) = 64a \rho_{xy}, \ 1 \leq i \leq b - 1$$

$$w^* (S−i) = 128a \rho_{xy}^2, \ 1 \leq i \leq b - 1$$

If we denote $TI(X)$ to represent the numerical number induced by the class $X$ with respect to $TI$, then the proof is complete by the following equation.
\[ TI(G) = 4 \sum_{i=1}^{a-1} TI(F/i) + 2 \sum_{i=a}^{b} TI(F/i) + TI(F/i) \]
\[ + 2 \sum_{i=1}^{a} TI(S\backslash i) + \sum_{i=1}^{b} TI(S\backslash i) \sum_{i=1}^{b} TI(S-i) \]
\[ + 2 \sum_{i=1}^{a} TI(T\backslash i) + \sum_{i=1}^{a} TI(T\backslash i) + \sum_{i=1}^{a-1} TI(T-i). \]

\[ \square \]

**Theorem 4.2.** Let \( TI \in \{W, W_e, W_{ew}, S_{zv}, S_{ze}, S_{zy}, PI, S, Gut, Mo, Mo_e, w^+Mo, w^+Mo_e, w^+S_{ze}, w^+Mo_e, w^+S_{ze}, w^+PI, \} \). For \( a \leq b \leq c \),

\[ TI(RHO(a, b, c)) = TI(a, b, c) + TI(a, c, b) + TI(b, c, a), \]

where we use \( TI(a, b, c) \) from the following expressions, \( TI(a, c, b) \) and \( TI(b, c, a) \) are obtained from \( TI(a, b, c) \) by replacing suitable values.

1. \( W(a, b, c) = \frac{48}{5} ac(\gamma_x + \gamma_y)^2((20ab^2)c^2 + (-2a^4 + 10a^3b + 20ab^3 + 2)c - 5ab^2). \)
2. \( W_e(a, b, c) = \frac{16}{15} \rho_{xy}^2(2880a^2b^2 - 480a^2b - 20a^2 - 480ab^2 + 40ab + 20b^2)c^3 + (288a^5 + 1440a^4b - 480a^3b + 10a^3 + 2880a^2b^2 - 2880a^2b^2 + 270a^2b - 480ab^3 + 240ab^2 + 240ab + 278a + 20b^3 - 20b)c^2 + (48a^5 - 40a^4b + 40a^3b - 480a^2b^3 + 240a^2b^2 + 60a^2b - 5a^2 + 40ab^3 + 60ab^2 - 30ab - 48a - 5b^2)c - 2a^5 + 10a^4b + 20a^2b^3 - 60a^2b^2 + 2a). \)
3. \( W_{ew}(a, b, c) = \frac{16}{5} ac\rho_{xy}(\gamma_x + \gamma_y)((20ab - 240ab^2 + 20b^2)c^2 + (24a^4 - 120a^3b + 20a^2b - 240ab^3 + 120ab^2 + 20b^3 - 10b - 24)c - 2a^4 + 10a^3b + 20ab^3 + 30ab^2 - 5ab - 5b^2 + 2). \)
4. \( S_{zv}(a, b, c) = 384a^2c\rho_{xy}(\gamma_x + \gamma_y)^2((-a^2 + 8a^3 + 2ab + 1)c^2 - ab^3). \)
5. \( S_{ze}(a, b, c) = \frac{128}{5} \rho_{xy}^2((-24a^4 + 360a^3b - 755a^3 + 5760a^2b^3 - 1920a^2b^2 + 1550a^2b + 120a^2 - 960ab^3 + 160a^2b - 600ab + 755a + 40b^3 + 40b - 96)c^3 + (2a^3 - 30a^3b + 120a^3 - 1920a^2b^3 + 240a^2b^2 - 240a^2b - 10a^2 + 160ab^3 + 50ab - 120a + 8)c^2 + (-5a^3 + 140a^2b^3 + 60a^2b^2 + 5a^2b + 60ab^3 - 10ab^2 + 5a - 5b^3)c - 60a^2b^3). \)
6. \( S_{zy}(a, b, c) = \frac{128}{5} ac\rho_{xy}^2(\gamma_x + \gamma_y)((-a^4 + 15a^3b - 60a^3 + 480a^2b^3 - 80a^2b^2 + 120a^2b + 5a^2 - 40ab^3 - 25ab + 60a - 4)c^2 + (5a^3 - 80a^2b^3 - 10a^2b - 5a)c - 30a^2b^3 + 5a^2b^2 + 5ab^3). \)
7. \( PI(a, b, c) = \frac{64}{3} \rho_{xy}^2((2a^3 + 144a^2b^2 - 30a^2b + a^2 - 24ab^2 + 2ab - 2a + b^2)c^2 + (-30a^2b^2 + 2a^2b + 2ab^2)c + 4a^2b^2). \)
(8) \( S(a, b, c) = \frac{64}{3} a c \rho_{xy}(\gamma_x + \gamma_y)((240a^2b - 20ab - 20b^2)c^2 + (-24a^4 + 120a^3b - 20a^2b + 240ab^3 - 60ab^2 - 5ab - 20b^3 - 5b^2 + 10b + 24)c + 2a^4 - 10a^3b - 20ab^3 - 35ab^2 + 5ab + 5b^2 - 2). \)

(9) \( \text{Gut}(a, b, c) = \frac{64}{3} a^2 \rho_{xy}^2 ((2880a^2b^2 - 480a^2b + 20a^2 - 480ab^2 + 40ab + 20b^2)c^3 + (-288a^4 + 1440a^3b - 480a^3b + 20a^3 + 2880a^2b^2 - 1440a^2b^2 + 10a^2 - 480ab^2 + 260ab + 268a + 20b^3 + 10b^2 - 20b)c^2 + (48a^5 - 240a^4b + 40a^3b - 480a^2b^2 - 30a^2b^2 + 80a^2b - 5a^2 + 40ab^3 + 80ab^2 - 30ab - 48a - 5b^2)c - 2a^5 + 10a^4b + 20a^2b^3 - 35a^2b^2 + 2a). \)

(10) \( M_o(a, b, c) = 96a^2 c \rho_{xy}(\gamma_x + \gamma_y)((2b^2 - 1(c^{(a+b)} - 1)c - 2b^2). \)

(11) \( M_o(a, b, c) = \frac{32}{3} a^2 \rho_{xy}^2 (144ab^2 - 6ab - 36(-1)^{(a+b)}a - 36a + 3(-1)^{(a+b)} - 2a^2 - 12b^2 + 5)c + 3a + 6ab + 3(-1)^{(a+b)}a - 78ab^2 + 6b^2). \)

(12) \( w^+ M_o(a, b, c) = 16a \rho_{xy}(\gamma_x + \gamma_y)(192ab^2 - 18ab - 48(-1)^{(a+b)}a - 36a + 3(-1)^{(a+b)} + 2a^2 - 12b^2 + 1)c^2 + (6a + 6(-1)^{(a+b)}a - 108ab^2)c + 3a + 3b^2 - 3(-1)^{c}b^2 - 3(-1)^{c}ab. \)

(13) \( w^+ M_o(a, b, c) = \frac{16}{3} a^2 \rho_{xy}^2 (68a + 24ab - 336ab^2 - 312a^2b - 420a^2 - 8a^3 + 12b^2 - 3(-1)^{a}(-1)^{b} + 2304a^2b^2 + 84(-1)^{a}(-1)^{b}a - 576(-1)^{(a)b}a + 3)(c^2 + (114ab^2 - 11a + 108ab^2 + 108a^2^2 + 2a^3 - 1392a^2b^2 - 9(-1)^{(a)}(-1)^{b}a + 120(-1)^{(a)}(-1)^{c}b^2c + 36ab^2 - 6a + 36ab^2 + 9a^2 - 3b^2 + 12a^2b^2 + 3(-1)^{a}a^2 + 3(-1)^{c}b^2 - 36(-1)^{(a)}ab^2 - 36(-1)^{(c)}a^2b - 6(-1)^{a}(-1)^{b}a^2 + 6(-1)^{c}ab). \)

(14) \( w^+ M_o(a, b, c) = 8a \rho_{xy}(\gamma_x + \gamma_y)(24b - 120a - 138ab - 192(-1)^{(a+b)}a + 768ab^2 + 24(-1)^{(a+b)} + 16a^2 - 90b^2 + 8)c^2 + (42a + 42(-1)^{(a+b)}a - 468ab^2)c + 21ab + 21b^2 - 21(-1)^{c}b^2 - 21(-1)^{c}b. \)

(15) \( w^+ M_o(a, b, c) = \frac{8}{3} a^2 \rho_{xy}^2 (248a - 24b + 468ab - 184ab^2 - 2040a^2b - 1350a^2 + 64a^3 + 90b^2 - 24(-1)^{(a+b) + 9216a^2b^2 + 480(-1)^{(a+b)}a - 2304(-1)^{(a+b)}a^2 + 24)c^2 + (516ab^2 - 24ab - 78a + 480a^2b + 624a^2 + 12a^3 - 600a^2b^2 - 66(-1)^{(a+b)}a + 696(-1)^{(a+b)}a^2)c + 252ab^2 - 42ab + 52a^2b - 63a^2 - 21b^2 + 84a^2b^2 + 21(-1)^{c}a^2 + 21(-1)^{c}b^2 - 252(-1)^{c}ab^2 - 252(-1)^{c}a^2b + 24(-1)^{(a+b)}a^2 + 42(-1)^{c}a. \)

(16) \( w^+ S_z(a, b, c) = \frac{32}{3} a c \rho_{xy}(\gamma_x + \gamma_y)((a^4 - 5a^3b - 25a^2b + 320a^2b^2 - 10a^2b^2 + 50a^2b + 20ab^3 + 40a - 1)c^2 + (5a^3 - 20a^2b^2 - 10a^2b - 5a)c - 40a^2b^2 - 5a^2b^2 - 5a^2b^3). \)

(17) \( w^+ S_z(a, b, c) = \frac{128}{15} \rho_{xy}^2 ((48a^5 + 216a^4b - 3880a^4 + 46080a^3b^3 - 16800a^3b^2 + 8560a^3b + 585a^3 - 10560a^2b^3 + 2480a^2b^2 - 3465a^2b + 995a^2 + 800a^3b - 90ab^2 + 110ab - 907a - 20b^3 + 10b)c^3 + (16a^5 - 480a^4b + 1355a^4 - 18240a^3b^3 + 4080a^3b^2 - 2810a^3b - 170a^3 + 2720a^2b^3 - 300a^2b^2 + 850a^2b - 1715a^2 - 100ab^3 - 30ab + 184ac)^2 + (-a^5 + 25a^4b - 145a^4 + 1600a^3b^3 - 420a^2b + 370a^3b + 5a^3 - 350a^2b^3 + 160a^2b^2 - 65a^2b + 160a^2 + 80ab^3 - 15ab^2 - 9a - 5b^3)c + 5a^4 + 500a^3b^3 - 10a^3b - 5a^2). \)

(18) \( w^+ P(a, b, c) = \frac{64}{3} \rho_{xy}^2 ((16a^3 + 1152a^2b^2 - 216a^2b + 6a^2 - 168ab^2 + 15ab - 13a + 6b^2)c^2 + (-2a^3 - 504a^2b^2 + 45a^2b^2 + 39ab^2 + 2a)c + 54a^2b^2). \)
(19) \( w^* \text{Sz}_v(a, b, c) = \frac{192}{5} acp_{xy}^2 (\gamma_x + \gamma_y)^2 ((8a^4 - 40a^3b - 70a^3 - 1280a^2b^3 - 70a^2b^2 + 140a^2b - 150ab^3 + 160a - 8)b)^2 + (35a^3 - 140a^2b^3 - 70a^2b - 35ac - 160a^2b^3 - 35a^2b^2 - 35ab^3). \)

(20) \( w^* \text{Sz}_e(a, b, c) = \frac{64}{15} p_{xy}^2 ((384a^3 + 5760a^2b - 11200a^2 + 184320a^3b^3 + 27280b^3 + 1570a^3 - 52320a^2b^3 + 14240a^2b^2 - 11370a^2b + 23890a^2 + 4880a^3b^3 - 690ab^2 - 220ab - 4184a - 150b^3 + 80b)c^3 + (40a^5 - 2520a^4b + 6965a^4 - 81600a^2b^2 + 22800a^2b^2 - 14650a^3b - 980a^3 + 15440a^2b^3 - 2160a^2b^2 + 5080a^2b - 9125a^2 - 720ab^3 - 200ab + 1120a)c^2 + (6a^5 - 170a^4b - 910a^4 + 7840a^3b^3 - 4380a^3b^2 + 2500a^3b + 70a^3 - 3900a^2b^2 + 1360a^2b^2 - 455a^2b + 1000a^2 + 680ab^3 - 105ab^2 - 64a - 35b^3)c + 35a^4 - 260a^3b^3 - 70a^2b - 35a^2). \)

(21) \( w^* \text{PI}(a, b, c) = \frac{32}{3} p_{xy}^3 ((64a^3 + 4608a^2b^2 - 11160a^2b + 45a^2 - 924ab^2 + 186ab - 52a + 45b^2 - 6b)c^2 + (14a^3 - 2232a^2b^2 + 246a^2b + 204ab - 6ab + 14a)c + 234a^2b^2). \)

**Proof.** We complete the proof by enumerating the \( \Theta \)-classes of zeolite RHO structures and then applying Theorem \[2.1\] The \( \Theta \)-classes of zeolite RHO structures are classified into three types as follows:

1. Front-view: \( \{ F/_{i}^{ab}, F\setminus_{i}^{ab} : \leq i \leq a + b - 1 \} \), \( \{ F|_{i}^{ab} : \leq i \leq c \} \) and \( \{ F-^{ab}_i : \leq i \leq c - 1 \} \).
2. Side-view: \( \{ S/_{i}^{ac}, S\setminus_{i}^{ac} : \leq i \leq a + c - 1 \} \), \( \{ S|_{i}^{ac} : \leq i \leq b \} \) and \( \{ S-^{ac}_i : \leq i \leq b - 1 \} \).
3. Top-view: \( \{ T/_{i}^{bc}, T\setminus_{i}^{bc} : \leq i \leq b + c - 1 \} \), \( \{ T|_{i}^{bc} : \leq i \leq a \} \) and \( \{ T-^{bc}_i : \leq i \leq a - 1 \} \).

From the construction of forward-slash and backward-slash of \( \Theta \)-classes, it is easily seen that the graph theoretical parameters of \( F/_{i}^{ab} \) and \( F\setminus_{i}^{ab} \) are same and similarly true for \( S/_{i}^{ac} \), \( S\setminus_{i}^{ac} \), \( T/_{i}^{ab} \) and \( T\setminus_{i}^{ab} \) of \( \Theta \)-classes. In addition, the graph theoretical parameters of \( S\setminus_{i}^{ac} \) and \( T\setminus_{i}^{bc} \) are similar to \( F\setminus_{i}^{ab} \) with respect to superfix variables. Also, the graph theoretical parameters of \( F|_{i}^{ab} \), \( S|_{i}^{ac} \) and \( T|_{i}^{bc} \) as well as \( F-^{ab}_i \), \( S-^{ac}_i \) and \( T-^{bc}_i \) are similar with respect to superfix variables respectively. Bearing the above relations in our mind, it is enough to perform the computation for front-view related \( \Theta \)-classes and the other classes can be easily manipulated from the following equations.

If we denote \( TI(a, b, c) = \sum_{i=1}^{a+b-1} TI(F/_{i}^{ab}) + TI(F\setminus_{i}^{ab}) + \sum_{i=1}^{c} TI(F|_{i}^{ab}) + \sum_{i=1}^{c-1} TI(F-^{ab}_i) \),

then \( TI(a, c, b) = \sum_{i=1}^{a+c-1} TI(S/_{i}^{ac}) + TI(S\setminus_{i}^{ac}) + \sum_{i=1}^{b} TI(S|_{i}^{ac}) + \sum_{i=1}^{b-1} TI(S-^{ac}_i) \),

and \( TI(b, c, a) = \sum_{i=1}^{b+c-1} TI(T/_{i}^{bc}) + TI(T\setminus_{i}^{bc}) + \sum_{i=1}^{a} TI(T|_{i}^{bc}) + \sum_{i=1}^{a-1} TI(T-^{bc}_i) \).

Combining the above three equations, we have

\[ TI(Z(a, b, c)) = TI(a, b, c) + TI(a, c, b) + TI(b, c, a). \]
We now present the graph theoretical parameters related to $F_{i}^{ab}$, $F_{i}^{\backslash ab}$, $F_{i}^{ab}$ and $F_{i}^{-ab}$ inorder to compute the expressions of $TI(a,b,c)$. As we mentioned earlier, the expressions of $TI(a,c,b)$ and $TI(b,c,a)$ are easily derived by replacing the values of $a, b$ and $c$ in $TI(a,b,c)$.

The number of elements and weighted bond measures in the $\Theta$-classes of $F_{i}^{ab}$, $F_{i}^{\backslash ab}$, $F_{i}^{ab}$ and $F_{i}^{-ab}$ are given below:

\[
\begin{align*}
|F_{i}^{ab}| &= |F_{i}^{\backslash ab}| = \begin{cases} 
8ci\rho_{xy} & \text{if } 1 \leq i \leq a-1 \\
8ac\rho_{xy} & \text{if } a \leq i \leq b \\
F_{a+b-i}^{\backslash ab} & \text{if } b+1 \leq i \leq a+b-1 
\end{cases} \\
|F_{i}| &= 8a\rho_{xy}, \quad 1 \leq i \leq c \\
|F_{i}^{-}| &= 8a\rho_{xy}, \quad 1 \leq i \leq c-1 
\end{align*}
\]

\[
\begin{align*}
w^{+}(F_{i}^{ab}) &= w^{+}(F_{i}^{\backslash ab}) = \begin{cases} 
(8i(8c-1) - 4c)\rho_{xy} & \text{if } 1 \leq i \leq a-1 \\
(8a(8c-1) - 8c)\rho_{xy} & \text{if } i = a, \ a = b \\
(8a(8c-1) - 6c)\rho_{xy} & \text{if } i = a, \ a < b \\
(8a(8c-1) - 4c)\rho_{xy} & \text{if } a < i < b \\
w^{+}(F_{a+b-i}^{\backslash ab}) & \text{if } b \leq i \leq a+b-1 
\end{cases} \\
w^{*}(F_{i}^{ab}) &= w^{*}(F_{i}^{\backslash ab}) = \begin{cases} 
(4i(32c - 7) - 16c)\rho_{xy}^{2} & \text{if } 1 \leq i \leq a-1 \\
(4a(32c - 7) - 28c)\rho_{xy}^{2} & \text{if } i = a, \ a = b \\
(4a(32c - 7) - 22c)\rho_{xy}^{2} & \text{if } i = a, \ a < b \\
(4a(32c - 7) - 16c)\rho_{xy}^{2} & \text{if } a < i < b \\
w^{*}(F_{a+b-i}^{\backslash ab}) & \text{if } b \leq i \leq a+b-1 
\end{cases} \\
w^{+}(F_{i}) &= 8(8ab - (a+b))\rho_{xy}, \quad 1 \leq i \leq c \\
w^{*}(F_{i}) &= 4(32ab - 7(a+b))\rho_{xy}^{2}, \quad 1 \leq i \leq c \\
w^{+}(F_{i}^{-}) &= 64a\rho_{xy}, \quad 1 \leq i \leq c-1 \\
w^{*}(F_{i}^{-}) &= 128a\rho_{xy}^{2}, \quad 1 \leq i \leq c-1 
\end{align*}
\]

Finally, we present the number of vertices and edges in the components which are obtained by removal of $\Theta$-classes from zeolites.
For $1 \leq TI \leq 4$, we use the edge partition technique based on the degrees of terminal vertices of each edge to find the expressions of degree-based topological indices of the zeolite RHO materials. Since zeolite RHO contains only $\rho_{xy}$ bond type, it is sufficient to consider the computation of degree-based topological indices.

\[ n_1 \left( F/_{i}^{ab} \right) = n_1 \left( F\backslash_{i}^{ab} \right) = \begin{cases} 12ci^2(\gamma_x + \gamma_y) & \text{if } 1 \leq i \leq a - 1 \\ 12ac(2i - a)(\gamma_x + \gamma_y) & \text{if } a \leq i \leq b \\ n_1 \left( F\backslash_{a+b-i}^{ab} \right) & \text{if } b + 1 \leq i \leq a + b - 1 \end{cases} \]

\[ n_2 \left( F/_{i}^{ab} \right) = n_2 \left( F\backslash_{i}^{ab} \right) = |V_\gamma(RHO(a,b,c))| - n_1 \left( F\backslash_{i}^{ab} \right) \]

\[ m_1 \left( F/_{i}^{ab} \right) = m_1 \left( F\backslash_{i}^{ab} \right) = \begin{cases} 4((12c - 1)i^2 - 3ci)\rho_{xy} & \text{if } 1 \leq i \leq a - 1 \\ 4(2(12ac - a - c)i - ac(12a + 1) + a^2)\rho_{xy} & \text{if } a \leq i \leq b \\ m_1 \left( F\backslash_{a+b-i}^{ab} \right) & \text{if } b + 1 \leq i \leq a + b - 1 \end{cases} \]

\[ m_2 \left( F/_{i}^{ab} \right) = m_2 \left( F\backslash_{i}^{ab} \right) = |E_\rho(RHO(a,b,c))| - m_1 \left( F\backslash_{i}^{ab} \right) - |F\backslash_{i}^{ab}| \]

For $1 \leq i \leq c$,

\[ n_1 \left( F/_{i} \right) = 12ab(2i - 1)(\gamma_x + \gamma_y), \]

\[ n_2 \left( F/_{i} \right) = |V_\gamma(RHO(a,b,c))| - n_1 \left( F/_{i} \right), \]

\[ m_1 \left( F/_{i} \right) = 4(2(12ab - a - b)i - (14ab - a - b))\rho_{xy}, \]

\[ m_2 \left( F/_{i} \right) = |E_\rho(RHO(a,b,c))| - m_1 \left( F/_{i} \right) - |F/_{i}|. \]

For $1 \leq i \leq c - 1$,

\[ n_1 \left( F-_{i} \right) = 24abi(\gamma_x + \gamma_y), \]

\[ n_2 \left( F-_{i} \right) = |V_\gamma(RHO(a,b,c))| - n_1 \left( F-_{i} \right), \]

\[ m_1 \left( F-_{i} \right) = 8((12ab - (a + b)i - ab)\rho_{xy}, \]

\[ m_2 \left( F-_{i} \right) = |E_\rho(RHO(a,b,c))| - m_1 \left( F-_{i} \right) - |F-_{i}|. \]

Then, $TI(a,b,c) = 4 \sum_{i=1}^{a-1} TI(F/_{i}^{ab}) + 2 \sum_{i=a}^{b} TI(F\backslash_{i}^{ab}) + \sum_{i=a}^{c} TI(FB/_{i}^{ab}) + \sum_{i=1}^{c-1} TI(F-_{i}^{ab})$, which completes the proof. \(\square\)

### 4.1 Degree-based Topological Indices

In this section, we use the edge partition technique based on the degrees of terminal vertices of each edge to find the expressions of degree-based topological indices of the zeolite RHO materials. Since zeolite RHO contains only $\rho_{xy}$ bond type, it is sufficient to consider the computation of degree-based
indices without weights. We now partition the edge set of zeolite \( \text{RHO}(a, b, c) \) as follows:

Let \( E_1 = \{ uv \in E(\text{RHO}(a, b, c)) : (\deg_G(u), \deg_G(v)) = (3, 3) \} \),

\[ E_2 = \{ uv \in E(\text{RHO}(a, b, c)) : (\deg_G(u), \deg_G(v)) = (3, 4) \} \],

\[ E_3 = \{ uv \in E(\text{RHO}(a, b, c)) : (\deg_G(u), \deg_G(v)) = (4, 4) \} \].

Then \( E(\text{RHO}(a, b, c)) = E_1 \cup E_2 \cup E_3 \) and

\[ |E_1| = 8(2(ab + bc + ac) + (a + b + c)), \]

\[ |E_2| = 16((ab + bc + ac) - (a + b + c)), \]

\[ |E_3| = 8(12abc - 5(ab + bc + ac) + (a + b + c)). \]

In addition, there are 16\((ab + ac + bc)\) vertices of degree 3 and 48\(abc - 16(ab + ac + bc)\) vertices are of degree 4. We now present the degree-based topological measures of zeolite RHO materials in view of the above edge partition by simple mathematical calculations.

**Theorem 4.3.** Let \( G \) be a Zeolite RHO materials \( \text{RHO}(a, b, c) \) where \( a, b, c \geq 1 \). Then,

1. \( M_1(G) = 16(48abc - 7(ab + bc + ca)) \).
2. \( M_2(G) = 8(192abc - 38(ab + bc + ca) + (a + b + c)) \).
3. \( R(G) = \frac{2}{3}(36abc + (4\sqrt{3} - 7)(ab + bc + ca) - (4\sqrt{3} - 7)(a + b + c)) \).
4. \( ABC(G) = \frac{2}{3}(36\sqrt{6}abc + (4\sqrt{15} - 15\sqrt{6} + 16)(ab + bc + ca) + (3\sqrt{6} - 4\sqrt{15} + 8)(a + b + c)) \).
5. \( H(G) = \frac{2}{21}(252abc - (ab + bc + ca) + (a + b + c)) \).
6. \( HM(G) = \frac{2}{21}(252\sqrt{2}abc + (28\sqrt{6} - 105\sqrt{2} + 24\sqrt{7})(ab+bc+ca) + (21\sqrt{2}+14\sqrt{6}-24\sqrt{7})(a+b+c)) \).
7. \( SC(G) = 16(384abc - 75(ab + bc + ca) + (a + b + c)) \).
8. \( GA(G) = \frac{8}{7}(84abc + (8\sqrt{3} - 21)(ab + bc + ca) - (8\sqrt{3} - 14)(a + b + c)) \).
9. \( \text{irr}(G) = 16((ab + bc + ca) - (a + b + c)) \).
10. \( \sigma(G) = 16((ab + bc + ca) - (a + b + c)) \).
11. \( F(G) = 16(192abc - 37(ab + bc + ca)) \).
12. \( SDD(G) = \frac{4}{3}(144abc - 11(ab + bc + ca) - (a + b + c)) \).
4.2 Numerical Values

By considering the relativistic parameters as $\gamma_x = \gamma_y = \rho_{xy} = 1$, the numerical topological descriptor values are presented in Tables 2 and 3 and the comparative study between the descriptors are displayed in Figures 5 and 6. The numerical results for the topological indices derived from the expressions were also validated against the results computed from the TopoChemie-2020 software [67].

Table 2: TI values of $RHO(a,b)$

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<th>a = 3</th>
</tr>
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<td>b = 2</td>
<td>b = 3</td>
<td>b = 3</td>
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<td></td>
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<tr>
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Figure 5: Comparison of $TI$ values for $RHO(a,b)$
Table 3: \(TI\) values of \(RHO(a,b,c)\) when \(a = b = c\)

<table>
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<tr>
<th>(TI)</th>
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<th>(a = 3)</th>
<th>(a = 4)</th>
<th>(a = 5)</th>
<th>(a = 6)</th>
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<tr>
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<td>647.14</td>
<td>1534.28</td>
<td>2997.13</td>
<td>5179.69</td>
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<tr>
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<td>1491.90</td>
<td>3593.26</td>
<td>7084.51</td>
<td>12318.40</td>
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Figure 6: Comparison of $TI$ values for $RHO(a, b, c)$
One can visualize from the above numerical values and 3D-bar graphs that the degree-based TIs have the smaller quantity values compared to distance-based indices. Among all the distance-based TIs, Mostar type indices acquire the least values while Szeged type indices expose the largest values implying the peripheral perfection of the materials. On the other hand, the correlation between the pairs of TIs such as \((M_1, M_2)\), \((R, ABC)\), \((W, W_e)\), \((S, Gut)\), \((M, Mo_e)\) and etc., was found to be greater than 0.99. Hence, all the acquired topological descriptors are highly significant for the characterization of the QSAR properties of zeolite frameworks. Relativistic effects in both scalar form and vector form (spin-orbit coupling) are extremely important for molecules and materials that contain very heavy atoms \([24, 25]\). Both computational and experimental studies have been carried out on such molecules with heavy atoms \([17, 18, 24, 27, 67, 70]\), and all of these studies have demonstrated the importance of relativistic effects including spin-orbit coupling. Consequently, the techniques developed in the current study can provide rapid quantitative measures of phase transformations and other structural and topological modifications that occur in materials through the incorporation of such heavy atoms through sorption, environmental pollutants and so forth. Such relativistic computations of the topological indices of these materials would involve two-component Wannier function spinors obtained from localization of Bloch spinors by localization techniques such as the Pipek-Mezey localization technique \([71]\). The technique would yield a number of localized properties including localized charges, populations and bond parameters which can then be used in the relativistic topological indices formulated in this study.

5 Conclusion

In this study we have computed relativistic structural descriptors for 3D zeolite RHO frameworks by employing cut methods for vertex and edge weighted molecular graphs. These materials exhibit extremely complex framework of topologies in multiple layers, cages and pores. Such relativistic topological descriptors of zeolite RHOs can provide for QSAR correlations for rapid computations of their physico chemical properties and thus enhance future applications of these materials for catalysis and sorptions. These techniques can also pave the way for future synthesis of novel and complex 2D and 3D structures comprising of tunnels and cages. An important feature of the developments considered here is that relativistic effects are included in here. Thus applications to a number of structural and reactivity problems pertaining to very heavy elements are feasible. For example, environmental remediation of mercury ions and actinyl ions found in environmental and high-level nuclear wastes requires such developments and consequently, the developed techniques are of paramount importance to the environmental management of pollutants, green-house gases and mitigation of heavy metal.
toxins including the ones in high level nuclear wastes. Moreover the developed topological indices that have the capability to include relativistic effects would be especially useful in the characterization of morphological changes to the materials that occur by the incorporation of heavier elements into the zeolite. The topological techniques can also provide quantitative measures for phase transitions and other modifications to the materials through interaction with chemicals, pollutants, and heavy metal ions.

References


