Quantitative structural descriptors of sodalite materials

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ABSTRACT
Topological characterization of 3D molecular structures is an emerging research area in the fields of theoretical and computational chemistry. Such a characterization of the underlying connectivity and molecular structure yields quantitative structural descriptors, also called topological indices (TIs) that aim to predict chemical properties and biological activities. Sodalite is a complex three dimensional crystalline structure consisting of a network of interconnected tunnels and cages. Due to the shape selective properties, sodalite structures are grasped in molecular sieving applications for sequestering molecules on the basis of size, shape and polarity. We have derived the exact analytical expressions of various topological descriptors for the sodalite structures by employing graph-theoretical cut method techniques that reduce the complex structures with tunnels and cages into simpler graphs.

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1. Introduction
Zeolites and macromolecular sieves have received considerable attention over the years [1–4] because of their importance in tailor-made molecular captures. Hence they are widely utilized catalysts, ion exchange and environmental remediation through selective sorptions. Currently there are around 248 types of zeolites and they can be identified by their Silicon–Aluminium (Si/Al) ratio present the atomic structure of the zeolites which comprises of building blocks of various complexity exhibiting tunnels and cages [5]. The current nomenclature and classification of zeolite materials has been provided by the Structure Commission of the International Zeolite Association (IZA) that identifies each material based on their zeolite framework type with a three letter code usually derived from the name of the source material which are used in describing the network of corner sharing tetrahedral of the atoms irrespective of its composition [6,7]. Furthermore, natural zeolites are utilized in bulk mineral applications because of their lower cost [4]. Zeolites of varying sizes and complexity have been synthesized over the years due to their structural relationships with other members of the group and also based on their fractal dimensions. Some of these molecular sieves have found commercial applications, for example: Linde Type A (LTA), Sodalite (SOD), Faujasite (FAU), ZSM-5, Chabazite, Mordenite, Stilbite and Tschemnichtite [8]. The crystal structures of minerals and synthetic compounds with a sodalite type frameworks are the most frequently studied structures among all zeolite-types [9,10], and some of the topological indices have been analyzed for the zeolite group of minerals [11–13]. The structures of sodalites are intriguing not only from crystallographic and materials science standpoints, but these materials have exhibit one of the highest thermodynamic stability among all zeolites [14–16]. The sodalite mineral exhibits a cubic structure with an ideal formula Na8(Al6Si6O24) and it is typically assigned to feldspathoids in the mineralogical classification [17]. The sodalite unit cell is comprised of two cages each one composed of four and six membered rings that are shared by two cages. The six membered rings form a set of channels parallel to the body diagonals of the cube, and intersect at the corners and centers of the unit cells to form large cavities. The cavities in the sodalites can be tailor-made to trap molecules such as water and CO2, and they have the capability of adsorbing and desorbing molecules without damage to the crystal structure. Consequently, zeolites can be used in selective removal of water and greenhouse gases.
Quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) models provide for powerful tools to predict the properties and activities of materials by harnessing the underlying topological features of the molecular structure. Such functional representations of the structural information have applications in coding, database search, retrieval, physicochemical property predictions and biological activity prediction of materials and molecules [18]. One of the most significant features of the QSPR/QSAR modelling is to provide structural descriptors, called the topological indices which have the power to predict the properties. In the field of computational and theoretical chemistry, TIs have emerged to be important descriptors because the activity of molecules depends on their 3D structures and the relative ease with which these indices can be employed in computing the molecular properties compared to numerically intensive quantum chemical computations [19–21]. A variety of TIs are available, among which the most commonly utilized in QSPR/QSAR study for grasping the relationships between the molecular structure and the potential physicochemical characteristics are vertex-distance based [22–30] and vertex degree-based topological indices [31–45]. Some progress has been made in quantitative characterization of complex 3D structures through quantitative shape and hypercube formulations [46–48]. The topological structures of such hollow materials are observed to be governed by rules for example, Loewenstein’s rule, which stipulates avoidance of unstable Al—O—Al bridges in these structures as O prefers Si over Al in bridges. This has been justified by both electronic and structural results based on quantum chemical methods as shown by Mezey and co-workers [49,50].

In this present article, we explore a collection of relativistically weighted-topological indices for molecules from which the correlation in QSPR and QSAR models can be improved by assigning optimized weights for the vertices and edges of the structure so that one may obtain realistic topological models that include such characteristics as structural instabilities and other quantum chemically derived features that govern the overall structural stability of hollow materials.

2. Graph theoretical terminologies

Throughout the paper, we write $G$ to denote a finite simple connected graph with vertex set and edge set respectively as $V(G)$ and $E(G)$. The distance $d_{G}(u,v)$ between vertices $u, v \in V(G)$ is the length of a shortest path between $u$ and $v$. If $x \in V(G)$ and $e = uw \in E(G)$, then the distance $d_{G}(x,e)$ between them is defined as $\min\{d_{G}(x,u), d_{G}(x,v)\}$. In Ref. [51] several possible definitions for the distance between two edges of a graph were considered and it was concluded that the distance between edges $f = ab$ and $g = cd$ should be the distance between the corresponding vertices in the line graph of $G$. In this paper, we consider that the distance $d_{G}(f, g)$ between edges $f$ and $g$ as the minimum number of edges along a shortest (f, c)-path or a shortest (f, d)-path. The degree of a vertex $v \in V(G)$ is the number of edges incident to $v$ and denoted by $\deg_{G}(v)$. In the same way, 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 degrees of end vertices and given below:

\[ \psi^{+}(e) = \deg_{G}(u) + \deg_{G}(v). \]

\[ \psi^{-}(e) = \deg_{G}(u)\deg_{G}(v). \]

For an edge $e = uv \in E(G)$, we now recall the following four quantities based on vertex-vertex and vertex-edge distance functions which will give the number of vertices and edges closer to the end vertices of $e$.

\[ n_{u}(e) = |\{x \in V(G) : d_{G}(u,x) < d_{G}(v,x)\}|. \]

\[ n_{v}(e) = |\{x \in V(G) : d_{G}(v,x) < d_{G}(u,x)\}|. \]

\[ m_{u}(e) = |\{f \in E(G) : d_{G}(u,f) < d_{G}(v,f)\}|. \]

\[ m_{v}(e) = |\{f \in E(G) : d_{G}(v,f) < d_{G}(u,f)\}|. \]

In addition, we denote $t_{u}(e) = n_{u}(e) + m_{u}(e)$ and $t_{v}(e) = n_{v}(e) + m_{v}(e)$. From the above quantitative measures based on vertices and edges, we are ready to present the definitions of distance-based and/or degree-based, and bond additive topological indices in the Table 1. It is to be noted that the vertex-edge Wiener index was defined in Ref. [52] without the additional factor (1/2) in order to count the vertex-edge pair exactly once. However, we use the original definition [27] of vertex-edge Wiener index by considering the additional factor (1/2).

It is essential to recall the prominent preliminaries with respect to the cut method, which are beneficial for our computations. A subgraph $H$ of a graph $G$ is said to be convex if for any two vertices $u, v \in H$, any shortest path between them in $G$ lies completely in $H$. But, the subgraph $H$ is said to be isometric if $d_{H}(u,v) = d_{G}(u,v)$. Any isometric subgraph of a hypercube is called a partial cube. The Djoković-Winkler relation $\Theta$[54,55] on the edge set of a graph $G$ is defined as follows: For two edges $f = ab$ and $g = cd$ in $E(G)$, $f$ is said to be adjacent to $g$ if $d_{G}(a,c) + d_{G}(b,d) = d_{G}(a,d) + d_{G}(b,c)$. If $G$ is a partial cube, then $\Theta$ is always an equivalence relation. Clearly, $G$ is a partial cube if and only if each $\Theta$-class of $G$ leaves exactly two convex components [55,56].

Let $S \subseteq E(G)$, the quotient graph $G/S$ is the graph whose vertices are the connected components of the graph $G - S$ and two components $X$ and $Y$ are adjacent in $G/S$ if some vertex of $X$ is adjacent to a vertex of $Y$ in $G$. In addition, we define the measures of $S$ based on $w$ and $w^*$ as $w(S) = \sum_{x \in S} w^*(x)$, and $w^*(S) = \sum_{x \in S} w^*(x)$.

Let $G$ be a partial cube with its $\Theta$-partition $\mathcal{F} = \{F_{1}, F_{2}, \ldots, F_{k}\}$. For each $F_{i}$, the quotient graph $G/F_{i}$ has exactly two components [55,56] of $G$ as vertices, say $GF_{i}^{1}$ and $GF_{i}^{2}$, $1 \leq i \leq k$, as shown in Fig. 1 and they are adjacent in $G/F_{i}$. For $j = 1, 2$, we write $n_{j}(F_{i}) = |V(GF_{i}^{j})|$, $m_{j}(F_{i}) = |E(GF_{i}^{j})|$ and $t_{j}(F_{i}) = n_{j}(F_{i}) + m_{j}(F_{i})$.

Now, we denote
## Summary of topological indices

<table>
<thead>
<tr>
<th>Classification</th>
<th>Mathematical expressions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>(1) Wiener type indices:</strong></td>
<td></td>
</tr>
<tr>
<td>Topological indices</td>
<td>Mathematical expressions</td>
</tr>
<tr>
<td>Wiener [30]</td>
<td>$W(G) = \sum_{[u,v] \in V(G)} d_{2}(u,v)$</td>
</tr>
<tr>
<td>Edge-Wiener [27]</td>
<td>$W_{e}(G) = \sum_{(f,g) \in E(G)} D_{2}(f,g)$</td>
</tr>
<tr>
<td>Vertex-edge-Wiener [27]</td>
<td>$W_{ve}(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{[u,f] \in E(G)} d_{2}(u,f)$</td>
</tr>
<tr>
<td>Hyper-Wiener index [28]</td>
<td>$W_{H}(G) = \frac{1}{2} \sum_{[u,v] \in V(G)} d_{2}(u,v) + \frac{1}{2} \sum_{[u,v] \in E(G)} d_{2}^{2}(u,v)$</td>
</tr>
<tr>
<td><strong>(2) Szeged type indices:</strong></td>
<td></td>
</tr>
<tr>
<td>Vertex-Szeged [22]</td>
<td>$Sz_{v}(G) = \sum_{e \in E(G)} n_{u}(e) n_{v}(e)$</td>
</tr>
<tr>
<td>Edge-Szeged [24]</td>
<td>$Sz_{e}(G) = \sum_{e \in E(G)} m_{u}(e) m_{v}(e)$</td>
</tr>
<tr>
<td>Edge-vertex-Szeged [26]</td>
<td>$Sz_{ev}(G) = \frac{1}{2} \sum_{e \in E(G)}</td>
</tr>
<tr>
<td>Padmakar-Ivan [25]</td>
<td>$PI(G) = \sum_{e \in E(G)}</td>
</tr>
<tr>
<td><strong>(3) Degree and distance-based indices:</strong></td>
<td></td>
</tr>
<tr>
<td>Schultz [29]</td>
<td>$S(G) = \sum_{(u,v) \in V(G)} (\deg_{G}(u) + \deg_{G}(v))d_{2}(u,v)$</td>
</tr>
<tr>
<td>Gutman [22]</td>
<td>$Gut(G) = \sum_{[u,v] \in V(G)} \deg_{G}(u)\deg_{G}(v)d_{2}(u,v)$</td>
</tr>
<tr>
<td><strong>(4) Mostar type indices:</strong></td>
<td></td>
</tr>
<tr>
<td>Mostar [53]</td>
<td>$Mo(G) = \sum_{e \in E(G)}</td>
</tr>
<tr>
<td>Edge-Mostar [59]</td>
<td>$Mo_{e}(G) = \sum_{e \in E(G)}</td>
</tr>
<tr>
<td>Total-Mostar [60]</td>
<td>$Mo_{t}(G) = \sum_{e \in E(G)}</td>
</tr>
<tr>
<td><strong>(5) Weighted plus Mostar type indices:</strong></td>
<td></td>
</tr>
<tr>
<td>$w^{+}$-Mostar [19]</td>
<td>$w^{+}Mo(G) = \sum_{e \in E(G)} w^{+}(e)</td>
</tr>
<tr>
<td>$w^{+}$-edge-Mostar [19]</td>
<td>$w^{+}Mo_{e}(G) = \sum_{e \in E(G)} w^{+}(e)</td>
</tr>
<tr>
<td>$w^{+}$-total-Mostar [19]</td>
<td>$w^{+}Mo_{t}(G) = \sum_{e \in E(G)} w^{+}(e) l_{u}(e) - l_{v}(e)$</td>
</tr>
<tr>
<td><strong>(6) Weighted product Mostar type indices:</strong></td>
<td></td>
</tr>
<tr>
<td>$w^{*}$-Mostar [19]</td>
<td>$w^{<em>}Mo(G) = \sum_{e \in E(G)} w^{</em>}(e)</td>
</tr>
<tr>
<td>$w^{*}$-edge-Mostar [19]</td>
<td>$w^{<em>}Mo_{e}(G) = \sum_{e \in E(G)} w^{</em>}(e)</td>
</tr>
<tr>
<td>$w^{*}$-total-Mostar [19]</td>
<td>$w^{<em>}Mo_{t}(G) = \sum_{e \in E(G)} w^{</em>}(e) l_{u}(e) - l_{v}(e)$</td>
</tr>
<tr>
<td><strong>(7) Degree-based bond additive indices:</strong></td>
<td></td>
</tr>
<tr>
<td>First Zagreb [32]</td>
<td>$M_{1}(G) = \sum_{e \in E(G)} (\deg_{G}(u) + \deg_{G}(v))$</td>
</tr>
<tr>
<td>Second Zagreb [32]</td>
<td>$M_{2}(G) = \sum_{e \in E(G)} \deg_{G}(u)\deg_{G}(v)$</td>
</tr>
<tr>
<td>Randić [34]</td>
<td>$R(G) = \sum_{e \in E(G)} \frac{1}{\sqrt{\deg_{G}(u)\deg_{G}(v)}}$</td>
</tr>
<tr>
<td>Atom Bond Connectivity [33]</td>
<td>$ABC(G) = \sum_{e \in E(G)} \frac{\deg_{G}(u) + \deg_{G}(v) - 2}{\deg_{G}(u)\deg_{G}(v)}$</td>
</tr>
<tr>
<td>Harmonic [35]</td>
<td>$H(G) = \sum_{e \in E(G)} \frac{1}{\deg_{G}(u) + \deg_{G}(v)}$</td>
</tr>
<tr>
<td>Sum Connectivity [36]</td>
<td>$SC(G) = \sum_{e \in E(G)} \frac{1}{\sqrt{\deg_{G}(u)\deg_{G}(v)}}$</td>
</tr>
<tr>
<td>Hyper Zagreb [45]</td>
<td>$HM(G) = \sum_{e \in E(G)} (\deg_{G}(u) + \deg_{G}(v))^{2}$</td>
</tr>
<tr>
<td>Geometric Arithmetic [37]</td>
<td>$GA(G) = \sum_{e \in E(G)} \frac{\deg_{G}(u)\deg_{G}(v)}{\deg_{G}(u) + \deg_{G}(v)}$</td>
</tr>
<tr>
<td>Irregularity Measure [38]</td>
<td>$irr(G) = \sum_{e \in E(G)}</td>
</tr>
<tr>
<td>Sigma [39]</td>
<td>$\sigma(G) = \sum_{e \in E(G)} (\deg_{G}(u) - \deg_{G}(v))^{2}$</td>
</tr>
<tr>
<td>Forgotten [40]</td>
<td>$F(G) = \sum_{e \in E(G)} (\deg_{G}(u)^{2} + \deg_{G}(v)^{2})$</td>
</tr>
<tr>
<td>Symmetric Division Degree [41]</td>
<td>$SDD(G) = \sum_{e \in E(G)} \frac{\deg_{G}(u) + \deg_{G}(v)}{\deg_{G}(u)\deg_{G}(v)}$</td>
</tr>
</tbody>
</table>
Theorem 2.1. Let $G$ be a partial cube with its $\Theta$-classes $\mathcal{F} = \{F_1, F_2, \ldots, F_k\}$. Let $T_l \in \{W, W_{c}, W_{e}, S_{Z}, S_{Z_{c}}, S_{Z_{e}}, S_{Z_{m}}, P, S, \Gamma, Mo, Mo_{e}, Mo_{m}, w^+ Mo, w^+ Mo_{e}, w^+ Mo_{m}, w^+ Mo_{e}, w^+ Mo_{m}\}$. Then,

$$T_l(G) = \sum_{l=1}^{k} T_l(G / F_i).$$

Even though the cut method is applicable for hyper-Wiener index [57], but the computation process is a bit tedious because of considering all the possible pairs of $\Theta$-classes. Thus, we do not wish to obtain here.

3. Results and discussion

Natural minerals are known to act as potential iodine disposal forms because of successful incorporation of iodine and/or iodide species. Iodosodalite is one such mineral that can accommodate iodine in its atomic structure and it is readily synthesized at low temperatures. Yet, the natural sodalite contains only trace quantities of iodine and synthetic versions have been produced with iodine or iodide species in the unit cell of sodalite structures, see the review paper for details [67]. The building block (unit cell) of the sodalite structures is usually called a $\beta$-cage which is a truncated octahedron containing 24 vertices and 36 edges among which 6 squares and 8 hexagons are connected by sharing a common edge as shown in Fig. 2(a).

The structurally interconnected arrangement of $\beta$-cages in the $n \times m \times l$ mesh results a single layer of sodalite materials, see Fig. 2(b) and this layer can be easily extended to many layers by arranging in $n \times m \times l$ mesh, denoted by $SOD(n, m, l)$. This 3D structure is isomorphic to a cyclic permutation of its coordinates, i.e., $SOD(n, m, l) \equiv SOD(l, n, m) \equiv SOD(m, l, n)$. It is easily seen from the arrangements of $\beta$-cages that $|V(SOD(n, m, l))| = 12nm + 4(nm + nl + ml)$ and $|E(SOD(n, m, l))| = 24nm + 4(nm + nl + ml)$.

The main objectives of this section are twofold. One is to derive the analytic expressions of the distance-based and bond additive topological indices such as variants of Wiener, Szeged and Mostar indices of sodalite structures. Second is to compute several significant degree-based indices of the same structures.

3.1. Distance-based and bond additive topological indices

In this section, we use the cut method to find the quantitative expressions of topological indices of the sodalite materials based on the distance and edge measures.

We first classify the $\Theta$-classes of the $\beta$-cage which can be readily generalized to sodalite structures. There are three types of $\Theta$-classes on $\beta$-cage as defined below:

- Front-to-Back $\Theta$-classes: $FB_L$ and $FB_R$
- Side-to-Side $\Theta$-classes: $SS_L$ and $SS_R$
- Top-to-Bottom $\Theta$-classes: $TB_L$ and $TB_R$

Here the suffixes $L$ and $R$ stand for $\Theta$-classes covering the squares of two parallel sides, respectively as displayed in Fig. 3. Moreover, it is interesting to see that by rotation of $\beta$-cage horizontally and vertically $90^\circ$ respectively the Side-to-Side $\Theta$-classes and Top-to-Bottom $\Theta$-classes are symmetrical to Front-to-Back $\Theta$-classes. Hence, the removal of any $\Theta$-class from $\beta$-cage results the same convex components as shown in the Fig. 4 and proving that $\beta$-cage belongs to the family of partial cubes. Now, the $\Theta$-classes of the $\beta$-cage can be extended to the entire sodalite structures because two $\beta$-cages are shared by common 4-cycle and in no other way as displayed in the Figs. 5 and 6. Therefore, the sodalite materials also belong to the family of partial cubes.

Theorem 3.1. Let $T_l \in \{W, W_{c}, W_{e}, S_{Z}, S_{Z_{c}}, S_{Z_{e}}, S_{Z_{m}}, P, S, \Gamma, Mo, Mo_{e}, Mo_{m}, w^+ Mo, w^+ Mo_{e}, w^+ Mo_{m}, w^+ Mo_{e}, w^+ Mo_{m}\}$. For $2 \leq n \leq m \leq l$, $T_l(SOD(n, m, l)) = T_l(n, m, l) + T_l(n, l, m) + T_l(m, l, n)$.

where we use

Fig. 1. Cut $F_i$ on $G$. 

$W(G / F_i) = n_1(F_i)n_2(F_i)$,

$W_o(G / F_i) = m_1(F_i)m_2(F_i)$,

$W_{o_v}(G / F_i) = \frac{1}{2}[n_1(F_i)m_2(F_i) + n_2(F_i)m_1(F_i)]$,

$Sz(G / F_i) = |F_1|n_1(F_i)n_2(F_i)$,

$Sz_o(G / F_i) = |F_1|m_1(F_i)m_2(F_i)$,

$Sz_{o_v}(G / F_i) = \frac{1}{2}|F_1|[n_1(F_i)m_2(F_i) + n_2(F_i)m_1(F_i)]$,

$Pl(G / F_i) = \frac{1}{k}E(G)^2 - |F_i|^2$,

$S(G / F_i) = \frac{1}{k}E(G)|V(G)| + 2[n_1(F_i)m_2(F_i) + n_2(F_i)m_1(F_i)]$.

$Gut(G / F_i) = \frac{2}{k}E(G)^2 + \left[4m_1(F_i)m_2(F_i) - |F_i|^2\right]$.

$Mo(G / F_i) = |F_1||n_1(F_i) - n_2(F_i)|$,

$Mo_o(G / F_i) = |F_1|m_1(F_i) - m_2(F_i)|$,

$Mo_{o_v}(G / F_i) = |F_1||t_1(F_i) - t_2(F_i)|$

When $\# \in \{+, *, \}$.

$w^\# Mo(G / F_i) = w^\# |n_1(F_i) - n_2(F_i)|$,

$w^\# Mo_o(G / F_i) = w^\# |m_1(F_i) - m_2(F_i)|$,

$w^\# Mo_{o_v}(G / F_i) = w^\# |t_1(F_i) - t_2(F_i)|$.
$W(x, y, z) = \frac{8}{15} \left[ \left( -9z^2 - 6z - 1 \right)x^3 + \left( 45yz^2 + 30yz + 5y \right)x^4 + \left( 20yz + 60yz^2 + 10z^2 \right)x^3 + \left( 90y^3z^2 + 60y^3z + 10y^2z + 30yz^2 \right)x^2 + \left( 60y^3z^2 + 20y^3z + 30y^2z^2 - 30yz^2 - 10yz - z^2 + 6z + 1 \right)x + 10y^3z^2 - 10yz \right]$

$W_e(x, y, z) = \frac{2}{15} \left[ \left( -144z^2 - 48z - 2 \right)x^3 + \left( 720yz^2 + 240yz + 20y \right)x^4 + \left( 80yz - 20z + 480yz^2 + 20z^2 - 5 \right)x^3 + \left( 1440y^3z^2 + 480y^3z + 40y^3 - 360y^2z - 60y^2 + 60yz^2 + 15y \right)x^2 + \left( 480y^3z^2 + 80y^3z - 60y^2z - 240yz^2 - 40yz + 124z^2 + 68z + 9 \right)x + 40y^3z^2 - 40yz \right]$

$W_{en}(x, y, z) = \frac{4}{15} \left[ \left( -36z^2 - 18z - 2 \right)x^3 + \left( 180yz^2 + 90yz + 10y \right)x^4 + \left( 40yz + 180yz^2 + 20z^2 \right)x^3 + \left( 360y^3z^2 + 180y^3z + 20y^3 + 180y^2z^2 - 15y^2z - 15y^2 + 30yz^2 - 15yz \right)x^2 + \left( 180y^3z^2 + 40y^3z + 30y^2z^2 - 15y^2z - 90yz^2 - 20yz + 16z^2 + 18z + 2 \right)x + 20y^3z^2 - 20yz \right]$

$S_z(x, y, z) = \frac{8}{15} \chi(2z + 1) \left[ \left( 6z^2 + 2z \right)x^4 + \left( -30z - 10yz - 30y^2z - 45z^2 - 5 \right)x^3 + \left( 180y^3z^2 + 120y^3z + 20y^3 + 180y^2z^2 + 60yz^2 + 60yz + 10y - 30z^2 - 10z \right)x^2 + \left( 120y^3z^2 + 40y^3z + 60y^2z^2 + 90yz^2 + 30yz + 45z^2 + 30z + 5 \right)x + 20y^3z^2 + 20yz^2 + 24z^2 + 8z \right]$

Fig. 2. Sodalite 3D structures.
Fig. 3. Three types of Θ-classes on the β-cage.

\[
S_{\beta}(x, y, z) = \frac{2}{15}(2z + 1) \left[ (48z^2 + 8z)x^4 + (40y - 260z + 280yz + 240y^2z^2 - 700z^2 - 35)x^3 + (2880y^2z^2 + 960y^3 + 32y^3z - 720y^2z - 120y^2 + 1480y^2z^2 + 520yz + 70y - 240z^2 - 40z)x^2 + (960y^3z^2 + 160y^3z - 120y^2z + 240yz^2 - 200yz - 40y + 700z^2 + 260z + 35)x + 80y^3z^2 - 40yz + 192z^2 + 32z \right]
\]
Fig. 4. $\Theta$-class of $\beta$-cage and its convex components.

Fig. 5. Front-to-Back $\Theta$-classes of SOD(2, 3, 2) and similar to Top-to-Bottom $\Theta$-classes by rotation of 90° vertically.

$$S_{eo}(x, y, z) = \frac{8}{15} x(2z + 1) \left[ (9z^2 + 2z) x^4 + \left( 5y - 40z + 15yz - 15yz^2 - 80z^2 - 5 \right) x^3 + \left( 360y^3 z^2 + 180y^2 z^2 - 15y^2 z - 15y^2 + 180yz^2 + 80yz + 10y - 45z^2 - 10z \right) x^2 + \left( 180y^3 z^2 + 40y^2 z^2 - 15y^2 z + 105yz^2 + 5yz - 5y + 80z^2 + 40z + 5 \right) x + 20y^3 z^2 + 10yz^2 - 5yz + 36z^2 + 8z \right]$$

$$P_{l}(x, y, z) = \frac{8}{3(2x + 2y + 2z - 3)} \left[ (8z^2 + 8z + 2) x^4 + \left( 216y^2 z^2 + 72y^2 z + 6y^2 + 56yz^2 - 4yz - 4y + 8z^3 + 2z^2 - 10z - 3 \right) x^3 + \left( 216y^3 z^2 + 72y^3 z + 6y^3 - 96y^2 z^2 - 72y^3 z - 12y^2 - 24yz^3 - 42yz^2 + 18yz + 9y - 14z^2 - 8z - 2 \right) x^2 + \left( 72y^3 z^2 + 12y^3 z - 54y^2 z^2 - 12y^2 z - 20yz^2 - 8yz - 2y - 8z^3 + 4z^2 + 10z + 3 \right) x + 6y^3 z^2 - 6y^2 z^2 \right]$$
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\[ S(x,y,z) = \frac{16}{15(2x + 2y + z - 3)} \left[ \left( -72z^2 - 36x - 4 \right)x^6 + \left( 16y + 50z + 144yz + 288yz^2 + 72z^2 - 72z^3 + 6 \right) \right] \]
\[ + \left( 360y^2z^2 + 180y^2z + 20y^2 + 360yz^3 - 170yz - 30y + 40z^3 \right) \]
\[ + \left( 720y^3z^2 + 360yz^3 + 40y^3 + 990y^2z^2 + 185yz^2 - 15y^2 + 360yz^3 - 225yz^2 - 120yz + 40z^3 - 45z^2 \right) \]
\[ + \left( 720y^4z^3 + 360y^3z^3 + 270y^2z^3 - 315y^3z - 75y^3 + 360y^2z^3 - 450y^2z^2 - 120y^2z + 30y^2 + 60yz^3 \right. \]
\[ \left. - 390yz^2 - 25yz + 17z^2 + 36z + 4 \right) \]
\[ + \left( 360y^4z^2 + 80y^4z + 360y^3z^2 - 225y^3z^2 - 120y^3z + 60y^2z^3 - 390y^2z^2 - 25yz^2 - 180yz^3 + 192yz^2 + 96yz + 4y + 32z^3 \right. \]
\[ \left. - 12z^2 - 50z - 6 \right) \times 40y^4z^2 + 40y^3z^2 - 45y^2z^2 - 55y^2z^2 - 40yz^2 + 60yz^2 \]
\[ \frac{Gut(x,y,z) = \frac{32}{15(2x + 2y + z - 3)} \left[ \left( -72z^2 - 24x - 2 \right)x^6 + \left( 8y + 34z + 96yz + 288yz^2 + 84z^2 - 72z^3 + 3 \right) \right] \]
\[ + \left( 360y^2z^2 + 120yz^2 + 10y^2 + 360yz^3 - 180yz^2 - 130yz - 15y + 20z^2 \right) \]
\[ + \left( 720y^3z^2 + 240yz^2 + 20y^3 + 780y^2z^2 + 40y^2z + 15y^2 + 24yz^3 - 120yz^2 - 60yz - 80z^3 - 15z^2 \right) \]
\[ + \left( 720y^4z^3 + 240yz^2 + 20y^4 + 720y^3z^3 - 60y^3z^2 - 300y^2z^3 - 45y^3 + 360y^2z^2 + 60y^2z + 30y^2 - 585yz^2 - 5yz + 37z^2 + 24z + 2 \right) \]
\[ + \left( 240y^4z^2 + 40y^4z + 240y^3z^2 - 120y^3z - 285yz^2 - 5yz^2 - 120yz^3 + 162yz^2 + 54yz + 2y + 52z^3 - 54z^2 - 34z - 3 \right) \]
\[ + \left( 20y^4z^2 + 20yz^3 - 15y^2z^2 - 35y^2z^2 - 20yz^3 + 30yz^2 \right) \]
\[ \frac{M_o(x,y,z) = \frac{2}{3} \left( 2x + 1 \right) \left[ -4x^3 + \left( 18z - 36yz^2 - 12y^2 + 6 \right) \times 10z - 12y^2z + (-1)^{(y-x)} (6z + 6x + 18y) \right] \]
\[ \frac{M_e(x,y,z) = \frac{2}{3} \left( 2x + 1 \right) \left[ 4x^2 + \left( 72y^2z - 36z + 12y^2 + 6 \right) \times 12y^2z - 10z - 6(-1)^{(y-x)} (6xz - 6x - z) \right] \]
\[ \frac{M_{ot}(x,y,z) = \frac{2}{3} \left( 2x + 1 \right) \left[ 8x^2 + \left( 108y^2z - 54z + 24y^2 - 12 \right) \times 24y^2z - 20z - 6(-1)^{(y-x)} (2z + 2x + 9xz) \right] \]
\[ \frac{w^+M_o(x,y,z) = \frac{8}{3} \left( 22z + 5 \right)x^3 + \left( 48x^2z^2 + 28y^2z^2 + 4y^2 - 6y^2z^2 - 2yz - 19z^2 - 12 - 2 \right)x^2 \]
\[ \frac{4}{3} \left( 78y^2z - 12yz - 53z + 18y^2 - 19 \right) \times 8y^2z^2 - 4z^2 - 4(-1)^{(y-x)} \left( 48x^2z^2 + 28x^2z + 4x^2 + 13xz^2 + 3xz - z^2 \right) \]
\[ \frac{w^+M_{ot}(x,y,z) = \frac{8}{3} \left( 41z + 10 \right)x^3 + \left( 16 \left( 72y^2z^2 + 34y^2z^2 + 4y^2 - 8y^2z - 12yz - 52z^2 - 15z - 2 \right) \right)x^2 \]
\[ \frac{4}{3} \left( 138y^2z - 24yz - 103z + 36y^2 - 38 \right) \times 16y^2z^2 - 8z^2 - 4(-1)^{(y-x)} \left( 144x^2z^2 + 68x^2z + 8x^2 + 23xz + 6xz - 2xz^2 \right) \]
\[ \frac{w^+M_{ot}(x,y,z) = \frac{16}{3} \left( 22z + 3 \right)x^3 + \left( 96y^2z^2 + 38y^2z^2 + 2y^2 - 24yz^2 - 8yz - 34z^2 - 13 \right)^2 \right)x^2 \]
\[ \frac{8}{3} \left( 6y - 32z - 6yz + 60y^2z - 6y^2 - 3 \right) \times 32y^2z^2 + 16yz^2 - 16z^2 - 8(-1)^{(y-x)} \left( 48x^2z^2 + 19x^2z + x^2 + 10xz - xz - 2z \right) \]
\[ w^* Mo_e(x, y, z) = \frac{16}{3} z(28z + 3)x^3 + 8\left(192y^2z^2 + 44y^2z + 2y^2 - 48yz^2 - 8yz - 64z^2 - 16z - 1\right)x^2 + \]
\[ \frac{8}{3} z^2\left(6y - 26z + 12yz + 24y^2z - 6y^2 - 3\right)x - 32y^2z^2 + 16yz^2 - 16z^2 - 8(-1)^{(y-x)}\left(96x^2z^2 + 22x^2z + x^2 + 4xz^2 - xz - 2z^2\right) \]
\[ w^* Mo_i(x, y, z) = \frac{32}{3} z(25z + 3)x^3 + 8\left(288y^2z^2 + 82y^2z + 4y^2 - 72yz^2 - 16yz - 98z^2 - 29z - 2\right)x^2 + \]
\[ \frac{16}{3} z\left(6y - 29z + 3yz + 42y^2z - 6y^2 - 3\right)x - 64y^2z^2 + 32yz^2 - 32z^2 - 8(-1)^{(y-x)}\left(144x^2z^2 + 41x^2z + 2x^2 + 14xz^2 - 2xz - 4z^2\right) \]

Proof. We first locate the \( \Theta \)-classes of \( SOD(n, m, l) \) on the basis of single \( \beta \)-cage to cover the edge set of sodalite structures, and then apply Theorem 2.1 to complete the proof as the sodalite structures belong to the family of partial cubes. The \( \Theta \)-classes of sodalite structures are Front-to-Back \( \{FB_{Li}^{mn} : 1 \leq i \leq n + m - 1\} \), Side-to-Side \( \{SS_{Li}^{nl} : 1 \leq i \leq n + l - 1\} \), and Top-to-Bottom \( \{TB_{Li}^{nl} : 1 \leq i \leq m + l - 1\} \) as displayed in the Figs. 5 and 6.

Then, we have the number of elements in the \( \Theta \)-classes as given below:

\[
|FB_{Li}^{mn}| = \begin{cases} 2i(2m + 1) & \text{if } 1 \leq i \leq n - 1 \\ 2n(2i + 1) & \text{if } n \leq i \leq m \\ |FB_{Li(n+m-i)}^{mn}| & \text{if } m + 1 \leq i \leq n + m - 1 \end{cases}
\]

\[
|SS_{Li}^{nl}| = \begin{cases} 2i(2m + 1) & \text{if } 1 \leq i \leq n - 1 \\ 2n(2i + 1) & \text{if } n \leq i \leq l \\ |SS_{Li(n+l-i)}^{nl}| & \text{if } l + 1 \leq i \leq n + l - 1 \end{cases}
\]

\[
|TB_{Li}^{nl}| = \begin{cases} 2i(2m + 1) & \text{if } 1 \leq i \leq m - 1 \\ 2m(2i + 1) & \text{if } m \leq i \leq l \\ |TB_{Li(m+l-i)}^{nl}| & \text{if } l + 1 \leq i \leq m + l - 1 \end{cases}
\]

We notice that \( |FB_{Li}^{mn}| = |FB_{Li}^{m}|, \quad |SS_{Li}^{nl}| = |SS_{Li}|, \quad \text{and } \quad |TB_{Li}^{nl}| = |TB_{Li}| \).

Following this, we now compute the edge measures based on \( w^* \) and \( w^* \) for \( \Theta \)-classes.

\[
w^* (FB_{Li}^{mn}) = \begin{cases} 8i(4l + 1) - 2l & \text{if } 1 \leq i \leq n - 1 \\ 8n(4l + 1) - 4l & \text{if } i = n, n = m \\ 8n(4l + 1) - 2l & \text{if } n < i < m \end{cases}
\]

\[
w^* (FB_{Li}^{mn}) = \begin{cases} 4i(16l + 1) - 8l & \text{if } 1 \leq i \leq n - 1 \\ 4n(16l + 1) - 14l & \text{if } i = n, n = m \\ 4n(16l + 1) - 11l & \text{if } n < i < m \end{cases}
\]

\[
w^* (FB_{Li}^{mn}) = \begin{cases} 8i(4m + 1) - 2m & \text{if } 1 \leq i \leq n - 1 \\ 8n(4m + 1) - 3m & \text{if } i = n, l \end{cases}
\]

\[
w^* (SS_{Li}^{nl}) = \begin{cases} 8i(2l + 1) & \text{if } 1 \leq i \leq n - 1 \\ 2n(2i + 1) & \text{if } n \leq i \leq l \\ |SS_{Li(n+l-i)}^{nl}| & \text{if } l + 1 \leq i \leq n + l - 1 \end{cases}
\]

\[
w^* (SS_{Li}^{nl}) = \begin{cases} 4i(16m + 1) - 8m & \text{if } 1 \leq i \leq n - 1 \\ 4n(16m + 1) - 11m & \text{if } i = n, l \end{cases}
\]

Fig. 6. Side-to-Side \( \Theta \)-classes of SOD(2, 3, 2), displayed by rotation of 90° horizontally.

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\[ w^+(TB_{Li}^{nm}) = \begin{cases} 
8i(4n+1) - 2n & \text{if } 1 \leq i \leq m - 1 \\
8m(4n+1) - 3n & \text{if } i = m,l \\
8m(4n+1) - 2n & \text{if } m < i < l \\
w^+(TB_{L(m+l-i)}^{nm}) & \text{if } l + 1 \leq i \leq m + l - 1 
\end{cases} \]

\[ m_1(FB_{Li}^{nm}) = \begin{cases} 
2(6l + 1)^2 + (2l - 1)i & \text{if } 1 \leq i \leq n - 1 \\
4(6nl + n + l)i - 2n^2(6l + 1) - n(2l + 1) & \text{if } n \leq i \leq m \\
m_1(FB_{L(n+m-l)}^{nm}) & \text{if } m + 1 \leq i \leq n + m - 1 
\end{cases} \]

\[ m_2(FB_{Li}^{nm}) = |E(SOD(n, m, l))| - m_1(FB_{Li}^{nm}) - |FB_{Li}^{nm}| \]

\[ w^+(TB_{Li}^{nm}) = \begin{cases} 
4i(16n + 1) - 8n & \text{if } 1 \leq i \leq m - 1 \\
4m(16n + 1) - 11n & \text{if } i = m,l \\
4m(16n + 1) - 8n & \text{if } m < i < l \\
w^+(TB_{L(m+l-i)}^{nm}) & \text{if } l + 1 \leq i \leq m + l - 1 
\end{cases} \]

\[ n_1(SS_{Li}^{nm}) = \begin{cases} 
2(3m + 1)^2 + 4mi & \text{if } 1 \leq i \leq n - 1 \\
4(3mn + n + m)i - 2n^2(3m + 1) & \text{if } n \leq i \leq l \\
n_1(SS_{L(n+m-l)}^{nm}) & \text{if } l + 1 \leq i \leq n + l - 1 
\end{cases} \]

\[ n_2(SS_{Li}^{nm}) = |V(SOD(n, m, l))| - n_1(SS_{Li}^{nm}) \]

\[ m_1(SS_{Li}^{nm}) = \begin{cases} 
2(6m + 1)^2 + (2m - 1)i & \text{if } 1 \leq i \leq n - 1 \\
4(6mn + n + m)i - 2n^2(6m + 1) - n(2m + 1) & \text{if } n \leq i \leq l \\
m_1(SS_{L(n+m-l)}^{nm}) & \text{if } l + 1 \leq i \leq n + l - 1 
\end{cases} \]

\[ m_2(SS_{Li}^{nm}) = |E(SOD(n, m, l))| - m_1(SS_{Li}^{nm}) - |SS_{Li}^{nm}| \]
It is crucial to note that the Θ-classes of the above theorem is not applicable in the cases of Side-to-Side and Top-to-Bottom when sodalite materials reduced to a single layer as shown in Fig. 7. We now derive the exact expressions of distance-based and bond additive topological indices of sodalite SOD(n, m, 1). For convenience, we write SOD(n, m) instead of SOD(n, m, 1).

**Theorem 3.2.** Let \( \mathcal{T}_I \in \{W, We, Sz, Sz_e, Pl, S, Gut, Mo, Mo_e, Mo_i, w^+Mo, w^+Mo_e, w^+Mo_i, w^+Mo_e, w^+Mo_i\} \). For \( 1 \leq n \leq m \)

\[
\mathcal{T}_I(SOD(n, m)) = \mathcal{T}_I(n, m) + \mathcal{T}_I(n, m) + \mathcal{T}_I(m, n),
\]

where we use \( \mathcal{T}_I(x, y, z) \) from Theorem 3.1 and

\[
W(x, y) = \frac{8}{3}x \left[ \left( 32y^2 + 16y + 2 \right)x^2 + \left( 24y^2 + 6y \right)x + 19y^2 + 8y + 1 \right]
\]

\[
W_e(x, y) = \frac{2}{3}x \left[ \left( 392y^2 + 112y + 8 \right)x^2 + \left( -84y - 12 \right)x + 196y^2 + 56y + 7 \right]
\]

\[
W_{ev}(x, y) = \frac{4}{5}x \left[ \left( 112y^2 + 44y + 4 \right)x^2 + \left( 42y^2 - 6y - 3 \right)x + 56y^2 + 19y + 2 \right]
\]

\[
S_{ze}(x, y) = \frac{16}{3}x(2y + 1) \left[ \left( 32y^2 + 16y + 2 \right)x^2 + \left( 24y^2 + 6y \right)x + 19y^2 + 8y + 1 \right]
\]

\[
S_{ze}(x, y) = \frac{4}{5}x(2y + 1) \left[ \left( 392y^2 + 112y + 8 \right)x^2 + \left( -84y - 12 \right)x + 196y^2 + 56y + 7 \right]
\]

\[
S_{ze}(x, y) = \frac{8}{5}x(2y + 1) \left[ \left( 112y^2 + 44y + 4 \right)x^2 + \left( 42y^2 - 6y - 3 \right)x + 56y^2 + 19y + 2 \right]
\]

\[
PL(x, y) = \frac{8}{(2x + 2y - 1)} \left[ \left( 98y^2 + 28y + 2 \right)x^2 + \left( 20y^2 - 4y + 2 \right)x - 8y^2 - 2y^2 + 2y + 1 \right]
\]

\[
S(x, y) = \frac{16x}{3(2x + 2y - 1)} \left[ \left( 224y^2 + 88y + 8 \right)x^3 + \left( 224y^3 + 144y^2 - 15y - 7 \right)x^2 + \left( 84y^3 + 91y^2 + 44y + 7 \right)x + 112y^2 - 15y - 2 \right]
\]

\[
Gut(x, y) = \frac{32x}{3(2x + 2y - 1)} \left[ \left( 196y^2 + 56y + 4 \right)x^3 + \left( 196y^3 + 105y^2 - 24y - 5 \right)x^2 + \left( 92y^2 + 43y + 5 \right)x + 92y^2 - 21y^2 - 9y - 1 \right]
\]

\[
Mo(x, y) = 2(2y + 1)(4y + 1) \left[ 4x^2 + 2(-1)^x - 2 \right]
\]

\[
Mo_e(x, y) = 2(2y + 1)(7y + 1) \left[ 4x^2 + 2(-1)^x - 2 \right]
\]

\[
Mo_i(x, y) = 2(2y + 1)(11y + 2) \left[ 4x^2 + 2(-1)^x - 2 \right]
\]
whereas the Side-to-Side and the Top-to-Bottom

\[ \text{SSI}_{(n,m)} = \left\{ (V(SOD(n,m))) \right\} = 16nm + 4(n + m), \quad \text{and} \quad E(SOD(n,m)) = 28nm + 4(n + m). \]

The Front-to-Back Θ-classes \{FB_{1,i}, FB_{2,i} : 1 \leq i \leq n + m - 1\} of SOD(n,m) are the same to \{FB_{1,i}, FB_{2,i} : 1 \leq i \leq n + m - 1\} as in Theorem 2.1 for SOD(n,m,l) whereas the Side-to-Side and the Top-to-Bottom Θ-classes are respectively \{SSI_{1,i}, SSI_{2,i} : 1 \leq i \leq n\} and \{TBI_{1,i}, TBI_{2,i} : 1 \leq i \leq m\} as depicted in Fig. 7. Since the graph theoretical parameters of SSI_{1,i} and SSI_{2,i} (respectively TBI_{1,i} and TBI_{2,i}) are the same, SSI_{1,i} and SSI_{2,i} are symmetrical with respect to \( n \) and \( m \). Hence, we focus our attention only to SSI_{1,i} in order to derive \( TII(n,m) \). The graph theoretical parameters of SSI_{1,i} are given below:

\[ |SSI_{1,i}| = 4m + 2, \quad 1 \leq i \leq n \]

\[ n_1(SSI_{1,i}) = 4(4m + 1)i - 2(3m + 1), \quad 1 \leq i \leq n \]

\[ n_2(SSI_{1,i}) = |V(SOD(n,m))| - n_1(SSI_{1,i}), \quad 1 \leq i \leq n \]

\[ m_1(SSI_{1,i}) = 4(7m + 1)i - (14m + 3), \quad 1 \leq i \leq n \]

\[ m_2(SSI_{1,i}) = |E(SOD(n,m))| - m_1(SSI_{1,i}) - |SSI_{1,i}|, \quad 1 \leq i \leq n \]

\[ w^{+}(SSI_{1,i}) = \begin{cases} 29m + 8 & \text{if } i = 1, n \\ 30m + 8 & \text{if } 1 < i < n \end{cases} \]

\[ w^{-}(SSI_{1,i}) = \begin{cases} 53m + 4 & \text{if } i = 1, n \\ 56m + 4 & \text{if } 1 < i < n \end{cases} \]

If we denote

\[ TII(n,m) = \sum_{i=1}^{n} |TII(SOD(n,m), SSI_{1,i})| + |TII(SOD(n,m), SSI_{2,i})|, \]

then

\[ \sum_{i=1}^{m} |TII(SOD(n,m), TBI_{1,i})| + |TII(SOD(n,m), TBI_{2,i})| = TII(n,m). \]

By Theorem 3.1, we have

\[ \sum_{i=1}^{m} |TII(SOD(n,m), TBI_{1,i})| + |TII(SOD(n,m), TBI_{2,i})| = TII(n,m). \]

and hence,

\[ TII(SOD(n,m)) = TII(n,m,1) + TII(n,m,2) + TII(n,m,3). \]

Based on the above measures, we now apply the following equation to obtain the explicit expressions of \( TII(n,m) \) and the other term \( TII(m,n) \) can be obtained similarly.

\[ TII(n,m) = 2 \sum_{i=1}^{n} |TII(SOD(n,m), SSI_{1,i})|, \]

Since we have computed Szeged-like topological indices and weighted (plus/product) Mostar indices for sodalite materials, it can be easily derived the weighted (plus/product) Szeged-like indices [68,69] from the cut method [69].

### 3.2. Degree-based topological indices

In this section, we use the edge partition technique based on the degrees of end vertices of each edge to find the quantitative expressions of degree-based topological indices of the sodalite materials. We now partition the edge set of sodalite SOD(n,m,1) as follows: Let \( E_1 = \{ uv \in E(SOD(n,m,1)) : (deg_{G_0}(u), deg_{G_0}(v)) = (3,3) \}, \)

\[ E_2 = \{ uv \in E(SOD(n,m,1)) : (deg_{G_0}(u), deg_{G_0}(v)) = (3,4) \}, \]

\[ E_3 = \{ uv \in E(SOD(n,m,1)) : (deg_{G_0}(u), deg_{G_0}(v)) = (4,4) \}. \]

Then, \( E(SOD(n,m,1)) = E_1 \cup E_2 \cup E_3 \). Then, \( |E_1| = 8(nm+nl+ml) + 4(n+m+l) \), \( |E_2| = 8(nm+nl+ml+nl+nl+nl) + (16 - 9\sqrt{6} + 12\sqrt{15})(nm+ml+ln) + 18\sqrt{6}nl \), \( |E_3| = 24nm - 12(nm+ml+nl) + 4(n+m+l) \).

In addition, there are \( 8(nm+ml+ln) \) vertices of degree 3 and \( 12nm-4(nm+ml+ln) \) vertices are of degree 4. We now present the degree-based topological measures of sodalite materials in view of the above edge partition by simple mathematical calculations.

**Theorem 3.3.** Let \( G \) be a sodalite materials \( SOD(n,m,1) \) where \( n, m, l \geq 1 \). Then,

\[ M_1(G) = 8(nm+ml+ln) + 192nmnl \]

\[ M_2(G) = 4(n+m+l) - 24(nm+ml+ln) + 384nmnl \]

\[ R(G) = \frac{1}{3}\left(7 - 4\sqrt{3}\right)(n+m+l) + \left(4\sqrt{3} - 1\right)(nm+ml+ln) + 18\sqrt{6}nm \]

\[ ABC(G) = \frac{1}{3}\left(8 + 3\sqrt{6} - 12\sqrt{15}\right)(n+m+l) + \left(16 - 9\sqrt{6} + 12\sqrt{15}\right)(nm+ml+ln) + 18\sqrt{6}nl \]

\[ H(G) = \frac{1}{2}(n+m+l) + 41(nm+ml+ln) + 126nmnl \]

\[ HM(G) = 196(n+m+l) - 1272(nm+ml+ln) + 6144nmnl \]
terization of minerals such as iodosodalites. Previous studies and/or iodide species. Relativistic effects [70]

\[ SC(G) = \frac{1}{\sqrt{42}} \left( [4\sqrt{7} - 8\sqrt{6} + 2\sqrt{21}] (n + m + l) \\
+ (8\sqrt{7} + 8\sqrt{6} - 6\sqrt{21}) (nm + ml + ln) + 12\sqrt{21}nmll \right) \]

\[ GA(G) = \frac{1}{7} \left( [56 - 32\sqrt{3}] (n + m + l) + [32\sqrt{3} - 28] \\
(nm + ml + ln) + 168nmll \right) \]

irr(G) = 8(nm + ml + ln − n − m − l)

\( \sigma(G) = 8(nm + ml + ln − n − m − l) \)

\[ F(G) = 768nmll - 40(nm + ml + ln) \]

\[ SDD(G) = \frac{1}{3} [26(nm + ml + ln) - 2(n + m + l) + 144nmll] \]

\[
\begin{align*}
\left(1/2\right)_{g}^{1/2} &= \left(\sigma_{g}\right)_{g} \left(\pi_{g}^{+}\right)_{g} ,
\left(1/2\right)_{g}^{-1/2} &= \left(\pi_{g}^{-}\right)_{g} ,
\left(1/2\right)_{u}^{1/2} &= \left(\sigma_{u}\right)_{u} \left(\pi_{u}^{+}\right)_{u} ,
\left(1/2\right)_{u}^{-1/2} &= \left(\pi_{u}^{-}\right)_{u} \\
\left(3/2\right)_{g}^{1/2} &= \left(-\sigma_{g}\right)_{g} \left(\pi_{g}^{+}\right)_{g} ,
\left(3/2\right)_{g}^{-1/2} &= \left(\pi_{g}^{-}\right)_{g} ,
\left(3/2\right)_{u}^{1/2} &= \left(-\sigma_{u}\right)_{u} \left(\pi_{u}^{+}\right)_{u} ,
\left(3/2\right)_{u}^{-1/2} &= \left(\pi_{u}^{-}\right)_{u} \\
\left(3/2\right)_{g}^{3/2} &= \left(\pi_{g}^{+}\right)_{g} ,
\left(3/2\right)_{g}^{-3/2} &= \left(\sigma_{g}\right)_{g} ,
\left(3/2\right)_{u}^{3/2} &= \left(\pi_{u}^{+}\right)_{u} ,
\left(3/2\right)_{u}^{-3/2} &= \left(\sigma_{u}\right)_{u} \\
\alpha &= \left(1\right) ,
\beta &= \left(0 \quad 1\right)
\end{align*}
\]

Thus the various molecular states of \( I_{2} \) can be expressed as product of these spinors, for example, the \( O_{g}^{1/2} \) ground state of \( I_{2} \) can be written as

\[
\begin{pmatrix}
\sigma_{g} \\
\pi_{g}^{+} \\
-\sigma_{g} \\
\pi_{g}^{-}
\end{pmatrix}
\begin{pmatrix}
\sigma_{u} \\
\pi_{u}^{+} \\
-\sigma_{u} \\
\pi_{u}^{-}
\end{pmatrix}
\begin{pmatrix}
-\sigma_{g} \\
\pi_{g}^{+} \\
\sigma_{g} \\
\pi_{g}^{-}
\end{pmatrix}
\begin{pmatrix}
-\sigma_{u} \\
\pi_{u}^{+} \\
\sigma_{u} \\
\pi_{u}^{-}
\end{pmatrix}
\begin{pmatrix}
\pi_{u}^{-} \\
\sigma_{u} \\
0 \\
\pi_{u}^{-}
\end{pmatrix}
\begin{pmatrix}
\pi_{u}^{+} \\
0 \\
\pi_{u}^{+} \\
0
\end{pmatrix}
\]

4. Relativistic formulations of topological indices

As noted earlier, iodosodalites are specific tailor-made molecular sieves that have the capability to selectively sequester iodine and/or iodide species. Relativistic effects [70–75] are known to be significant especially for atoms with \( Z > 50 \) and thus it would be important to incorporate relativistic effects in topological characterization of minerals such as iodosodalites. Previous studies [71–75] on clusters of atoms of tin and other heavier elements and their reactivities have demonstrated not only substantial scalar relativistic effects but also two-component spin-orbit effects. Moreover several quantum chemically based Le Chatelier principle such as the ones made by Mezey and co-workers [76–79] exemplify enhanced role of compensation effects as well as shape-complementarity, an enhanced role of the combination of both throug-space and through-bond interactions, as well as multicenter interactions. Likewise the intimate connection between the symmetry and periodicity of potential energy surfaces is reflected in the final equilibrium structures governed by such multiple forces arising from electronic factors, through bond and space interactions. Consequently, we develop here integrated relativistic quantum topological models that account for such different effects in these hollow structures. In the case of systems containing heavier atoms, the spin-orbit effects are best described by two-component molecular spinors. For example, the two component molecular spinors [70], for the molecular orbitals of diatomic iodine can be written in terms of the 5p orbitals of iodine as:

\[
\begin{pmatrix}
\pi_{g}^{+} \\
\pi_{g}^{-} \\
-\sigma_{g} \\
-\sigma_{u}
\end{pmatrix}
\begin{pmatrix}
\pi_{u}^{+} \\
\sigma_{u} \\
0 \\
\pi_{u}^{-}
\end{pmatrix}
\begin{pmatrix}
\pi_{g}^{+} \\
\pi_{g}^{-} \\
-\sigma_{g} \\
-\sigma_{u}
\end{pmatrix}
\begin{pmatrix}
\pi_{u}^{+} \\
\sigma_{u} \\
0 \\
\pi_{u}^{-}
\end{pmatrix}
\begin{pmatrix}
\pi_{u}^{-} \\
\sigma_{u} \\
0 \\
\pi_{u}^{-}
\end{pmatrix}
\begin{pmatrix}
\pi_{u}^{+} \\
0 \\
\pi_{u}^{+} \\
0
\end{pmatrix}
\]

There are other combinations which also give rise to the same \( O_{g}^{1/2} \) state, where \( \sigma_{g} \) and \( \sigma_{u} \) are the bonding and antibonding molecular orbitals along the molecular axis arising from the 5p orbitals of iodine, while \( \pi_{u} \) and \( \pi_{g} \) are the perpendicular bonding and antibonding orbitals arising from the 5p. The expansion of the above terms in terms of the spin orbitals reveals that two different electronic states such as \( 1S_{g}^{1/2} \) and \( 3P_{g} \) can mix for \( I_{2} \) which would...
normally not mix in non-relativistic theory. This is because the spin-orbit splitting of the $P_{3/2}$/$P_{1/2}$ states of iodine is 7603.2 cm$^{-1}$ or 0.94 eV [80], which is quite substantial. Thus the electronic states are not only split by spin-orbit coupling but there is also substantial mixing of different electronic states as a consequence of spin-orbit coupling.

Topological models considered here for sodalites can be extended for iodosodalites by incorporating spin-orbit and other relativistic effects through the use of relativistically weighted graphs. We can incorporate relativistic parameters for the edges between iodine and other atoms in the molecular sieve. In a recent study [81], it has been demonstrated how such relativistically weighted graphs can be handled, and how the various topological indices can be derived for such weighted graphs. As expressions get quite complex, we refer the readers to the previous work [81] for extensions that incorporate such relativistic effects into topological models considered here.

5. Conclusion

In this paper, by the use of powerful graph-theoretical tools, we have computed the exact analytical expressions of different versions of topological indices for 3D complex sodalite crystalline structures that contain tunnels and cages. The techniques that we have outlined do not require any intensive preprocessing steps such as 3D coordinate generation and conformational analysis, and yet have the predictive power for structure-property relations. These complex structures have been topologically characterized by the elegant use of powerful graph-theoretical cut methods that yield the topological indices of varied complexities. The mathematical techniques developed here should be extended to even more complex structures comprised of spinels, super lattices, complex weaving patterns, and other complex polyhedral metal organic frameworks which are becoming the novel materials of the future.

CRediT authorship contribution statement

Micheal Arockiaraj: Conceptualization, Supervision, Writing - review & editing. Joseph Clement: Investigation, Writing - original draft. Daniel Paul: Validation, Visualization. Krishnan Balasubramanian: Conceptualization, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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