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On certain distance and degree based topological indices of Zeolite LTA frameworks

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Abstract

Zeolites are aluminosilicates with extensive application both commercially and in materials science. Current applications include dehydrating natural gas and in humidity sensors. Synthesis of new frameworks is an important area of research in chemistry and materials science. The Zeolite LTA framework in particular is getting much attention in this area due to its potential for application. Topological indices are graph invariants which provide information on the structure of graphs and have proven very useful in quantitative structure activity relationships (QSAR) and quantitative structure property relationships (QSPR) at predicting important chemico-physical aspects of chemical compounds. In this paper we compute nine of the most significant distance based topological indices of the Zeolite LTA framework and thirteen valency based molecular descriptors.

1. Introduction

Zeolites are naturally occurring aluminosilicates commonly used as catalysts [1]. Due to their widespread application and diversity of possible frameworks, the synthesis of new zeolite frameworks is an important area of research in materials science. While computer simulations have shown there to be millions of possible zeolite frameworks, only just over forty have been found naturally [2]. In addition to these naturally occurring zeolite frameworks, approximately 250 more have been synthetically created [3]. Given the chemical and commercial importance of zeolites, further development of new zeolite frameworks is an important area of research in chemistry and materials science [4].

To aid in this developmental process, foreknowledge of the structure of possible candidate frameworks is critical. To aid in this endeavor, computation of the topological indices of the molecular graphs of candidate frameworks has proven to be a useful tool. In fact, topological indices of molecular graph families have a long history of contributing to the developmental process; for example, consider [5–10]. While other important computational studies have been carried out on various zeolite frameworks [2, 11], computation of the most important topological indices has not yet occurred. This is precisely the contribution of this paper. We compute nine of the most important topological indices specifically for the Zeolite LTA framework.

Topological indices are graph invariants in the form of real numbers which reflect the structure of the graph. In the case of molecular graphs, topological indices correlate to important structural characteristics and consequences such as the boiling point via quantitative structure activity relationships (QSAR) and quantitative structure property relationships (QSPR) [12]. These regression methods allow for researchers to estimate important properties of potential zeolite framework candidates for synthesis, including reactivity and solubility, in order to determine ideal candidate frameworks for a given purpose [13].

Zeolite LTA frameworks are experiencing widespread development and finding greater practical use. For example, they have proven extremely useful at dehydrating natural gas [14, 15]. Additionally, they have found...
use in humidity sensors due to their extremely hydrophilic nature \[16–18\]. With such commercial potential, furthering our knowledge of the underlying structure of the Zeolite LTA framework is economically imperative.

The molecular graph of the Zeolite LTA framework (see figure 1) has been previously studied \[19\]. Molecular graphs in general are graph theoretical representations of the structure of a chemical compound. Figures 2(a) and (b) explains about the unit cell of Zeolite LTA and \(Z(2 \times 2 \times 2)\). Thus we may define a molecular graph \(G = (V, E)\) where the vertex set \(V\) represent the atoms comprising the chemical compound and the edge set \(E\) represents the various bonds of the chemical compound \[20\]. In order to quantify the information encoded in the molecular graph, we compute topological indices which take the general form

\[
TI(G) = \sum_{\{u,v\} \subseteq V \times V} f(u, v)
\]

(1)

where \(TI(G)\) is the topological index in question and \(f(u, v)\) is particular to our choice of topological index.

Many standard graph theoretical properties allow for more efficient analyses of the structural characteristics of molecular graphs. For example, a vertex cut method for molecular graphs has been developed \[21\]. This approach relies on the existence of a vertex whose removal creates two disconnected subgraphs. Similarly, the notion of Hamilton-connectedness of molecular graphs and of subgraphs of molecular graphs has been studied \[12\]. In that approach the existence of certain Hamiltonian paths (paths that contain every vertex in the graph) was related to a topological index known as the Detour index. Other topics, such as dominating sets (sets of vertices which are collectively adjacent to every vertex in the graph), have also proven extremely useful in aiding in the computation of topological indices \[22, 23\]. For more references on dominating sets in particular, the reader is referred to several quality works \[24–26\].

**Figure 1.** Construction of Zeolite LTA Structures.
While important topological indices have been computed for a variety of important families of molecular graphs \[27, 28\], this problem remains open for Zeolite LTA frameworks. In particular, we compute the following topological indices: Wiener, Edge-Wiener, Vertex-edge Wiener, Vertex Szeged, Edge Szeged, Edge-vertex Szeged, Padmukar-Ivan, Schultz, and Gutman.

In order to compute these topological indices using the novel combination of methods in this paper, we used MATLAB\textsuperscript{®}. However, readers are interested in computing topological indices for any purpose are referred to the open source Python package MathChem \[29\].

For further information on Zeolites and their applications, the reader is referred to the following reference texts \[30–35\]. For general information on related chemistry and materials science matters, the reader is referred to the following texts \[36–38\]. For more on algebraic graph theory and the algebraic and graph theoretical tools used herein, the reader is referred to the standard text by Godsil \[39\].

2. Preliminaries

As all graphs referred to in this paper are molecular graphs, we simply use the term graph. For any vertex \( v \in V(G) \) we denote the degree of \( v \) by \( d_G(v) \) and the neighborhood of \( v \) by \( N_G(v) \). The degree of a vertex \( v \) is simply the cardinality of the neighborhood of that vertex, i.e., \( d_G(v) = |N_G(v)| \), and the neighborhood of a vertex \( v \) is the set of vertices connected to \( v \) by an edge. When the graph is known, we shorten these notations to \( d(v) \) for the degree of \( v \) and \( N(v) \) for the neighborhood of \( v \). The distance between two vertices \( u, v \in V(G) \), denoted \( d(u, v) \), is the length of a shortest path in \( G \) between \( u \) and \( v \). Since all graphs are undirected, the relation \( d(u, v) \) is symmetric, i.e., \( d(u, v) = d(v, u) \) for all pairs \( u, v \subseteq V \times V \).

We can define an analog for edges as follows. First we define the distance between a vertex \( w \) and an edge \( e = uv \) by \( d(w, e) = \min\{d(w, u), d(w, v)\} \). Extending this concept to edges \( e, f \in E(G) \) where \( e = uv \) and \( f = xy \), the distance between \( e \) and \( f \) is given by \( d(e, f) = \min\{d(u, f), d(v, f)\} = \min\{d(x, e), d(y, e)\} \).

As analogous concepts to \( N_G(v) \), we present four measures of partitioning the vertices and edges of \( G \) by relative proximity. Let \( e = uv \in E(G) \). These four measures tell us the relative size of the set of vertices (or edges) closer to either \( u \) or \( v \) than the other. They are defined as follows.

\[
\begin{align*}
    n_u(e) &= \{|x \in V(G) : d(u, x) < d(v, x)\} \\
    n_v(e) &= \{|x \in V(G) : d(v, x) < d(u, x)\} \\
    m_u(e) &= \{|f \in E(G) : d(u, f) < d(v, f)\} \\
    m_v(e) &= \{|f \in E(G) : d(v, f) < d(u, f)\}
\end{align*}
\]

(2)

Related to this concept is the notion of partitioning a graph into \( \Theta \)-classes, or subgraphs whose edges satisfy an asymmetric distance property. This property will be useful in several of the following preliminary results and is formally defined below.
Definition 1. [40] Two edges \( e = xy \) and \( f = uv \) in a graph belong to the same \( \Theta \)-class if they satisfy the relation \( e \Theta f \) where \( d(x, u) + d(y, v) = d(x, v) + d(y, u) \).

Theorem 1. [41] Let \( G \) be a partial cube and let \( F_1, F_2, \ldots, F_k \) be its \( \Theta \)-classes. Let \( n_1 \) and \( n_2 \) be the number of vertices in the two connected components of \( G - F_i \). Then \( W(G) = \sum_{i=1}^{k} n_1 n_2 \).

Lemma 1. A connected graph \( G \) admits a partition \( \{F_i\}_{i=1}^{k} \) of \( E(G) \) into convex cuts with components \( GF_1 \) and \( GF_2 \) for each \( i \). Let \( R \) be the set of all shortest paths with the property that for each pair of vertices of \( G \) there exists a unique path in \( R \) connecting them. For any \( P_i(e, f) \in R \) and each \( i \), the following statements hold:

1. If \( \{u, v\} \subseteq V(GF_1) \) or \( \{u, v\} \subseteq V(GF_2) \), then \( |E(P_i(u, v)) \cap F_i| = 0 \)
2. If \( u \in V(GF_1) \) and \( v \in V(GF_2) \), then \( |E(P_i(u, v)) \cap F_i| = 1 \)

Lemma 2. A connected graph \( G \) admits a partition \( \{F_i\}_{i=1}^{k} \) of \( E(G) \) into convex cuts with components \( GF_1 \) and \( GF_2 \) for each \( i \). Let \( S \) be a set of shortest paths with the property that for each pair of edges of \( G \) there exists a unique path in \( S \) connecting them. For any \( P_i(e, f) \in S \) and each \( i \), the following statements hold:

1. If \( \{e, f\} \subseteq E(GF_1) \) or \( \{e, f\} \subseteq E(GF_2) \), then \( |E(P_i(e, f)) \cap F_i| = 0 \)
2. If \( e \in F_i \) and \( f \in E(GF_1) \) or \( f \in E(GF_2) \), then \( |E(P_i(e, f)) \cap F_i| = 0 \)
3. If \( e \in E(GF_1) \) and \( f \in E(GF_2) \), then \( |E(P_i(e, f)) \cap F_i| = 1 \).

Theorem 2. Let \( H \) be a cube (partial) and let \( S_1, S_2, \ldots, S_k \) be its \( \Theta \)-classes with \( |S_i| = s_i \) such that \( H - S_i \) has exactly 2 convex components \( HS_i \) and \( HS_i^1 \) for \( 1 \leq i \leq k \) with \( |V(HS_i)| = n_i \), \( |V(HS_i^1)| = n - n_i \), \( |E(HS_i^1)| = m_i \) and \( |E(HS_i^1)| = m_i - n_i \). Then

1. [41] \( W(G) = \sum_{i=1}^{k} n_i (n - n_i) \)
2. [42] \( W_1(G) = \sum_{i=1}^{k} m_i (m - m_i) \)
3. [42] \( W_2(G) = \frac{1}{2} \sum_{i=1}^{k} [n_i (m - m_i - s_i) + (n - n_i) m_i] \)
4. [43] \( W_3(G) = \frac{1}{2} \sum_{i=1}^{k} [n_i (m - m_i - s_i) + (n - n_i) m_i] \)
5. [42] \( Sz_1(G) = \sum_{i=1}^{k} s_i n_i (n - n_i) \)
6. [44] \( Sz_2(G) = \sum_{i=1}^{k} s_i m_i (m - m_i - s_i) \)
7. [45] \( Sz_{ev} = \frac{1}{2} \sum_{i=1}^{k} [n_i (m - m_i - s_i) + (n - n_i) m_i] \)
8. [46] \( PI(G) = m^2 - \sum_{i=1}^{k} s_i^2 \)
9. [46] \( S(G) = mn + 2 \sum_{i=1}^{k} [n_i (m - m_i - s_i) + (n - n_i) m_i] \)
10. [47] \( Gut(G) = 2m^2 + \sum_{i=1}^{k} [4m_i (m - m_i - s_i) - s_i^2] \)

With these definitions in place, we are now ready to present the formulae for the nine topological indices to be computed in the following section. These formulae are presented in the following table 1.

3. Various distance based topological indices of Zeolite LTA

In this section we present exact expression of various distance based topological indices of Zeolite LTA using the well known cut method and theorem 2. These results were obtained using MATLAB® code which implements the methods discussed throughout this paper.

Theorem 3. For \( G = Z(p, q, r) \), \( p \leq q \leq r \) we have

1. \( W(G) = (-96p^3r + 480p^3q^2r + 1440pq^3r + 480pq^2r^2 - 480pq^2 - 480pqq - 480q^2r + r)/5 \).
2.
\[ W_1(G) = (-6912p^5q^2 + 1152p^5q - 2232p^5r - 56p^5 + 23040p^4q^r + 1200p^4q^2 + 9000p^4q^2 - 4800p^4q + 1000p^4q^2 + 7620p^4r^2 + 700p^4r - 10 080p^3q^r^2 - 11640p^3q^r - 14 820p^3r^2 - 16320p^3r^2 + 4680p^3q - 2040p^3q - 10 910p^3q + 840p^3r - 80^3 - 2232p^2q^2 + 9000p^2r^2 + 4500p^2q^2^2 - 5120p^2q^2^2 - 17400p^2q^r^2 - 4270p^2q^2 - 21 600p^2q^r^2 - 8010p^2q^r^2 + 23 010p^2q^r^2 + 4680p^2q^r^2 + 2760p^2q^r^2 + 4770p^2q^r^2 + 240p^2q^r^2 + 522p^2q^r^2 - 480p^2q^r^2 + 5100p^2q^r^2 - 380p^2q^r + 312pq^2 - 1320pq^2 + 308pq^4 - 2640pq^2^2 + 1440pq^4 + 360pq^4^2 + 14 040pq^4^2 + 5520pq^4^2 + 4470pq^4^2 - 1440pq^4^2 + 602pq^4 - 2160pq^4 + 1920pq^4^2 - 120pq^4^2 - 240pq^4 - 384pq^4 - 120pq^4 + 240pq^4 - 240pq^4^2 + 782pq^4 - 192pq + 16p - 8q^2 + 40pqr + 120pqr^2 - 4680pqr^2 - 2940pqr^2 - 7630pqr^2 + 1680pqr^2 - 120pqr + 840pqr + 280pqr^2 + 1680pqr - 280pqr^2 + 8q - 40pq - 80r^2 + 80r^2)/15.\]

3. \[ W_2(G) = (-840q^r^5 + 80q^r^5 + 2520pq^r^2^2 - 240pq^r^4 - 280q^r^4^2 + 3360p^2q^r^2 + 360p^2q^r^2 + 360p^2q^r^2 + 240p^2q^r^2 + 1680q^r^5 + 160q^r^5 - 312p^2q^r^2 + 4200q^4q^r^2 + 700p^4q^r^2 + 1440p^4q^r^2 + 640p^2q^r^2 + 840p^2q^r^2 + 2640p^2q^r^2 + 1440p^2q^r^2 + 480p^2q^r^2 + 260p^2q^r^2 - 240pq^r^2 + 720pq^r^2 - 80pq^2 + 192pqr + 160pqr^2 - 72p^3q^r^2 + 16p^r + 2880pq^r^2^2 - 180pq^r^2 - 1940pq^r^2 - 360pq^r^2 + 1320pq^r^2 + 1440pq^r^2 + 1980pq^r^2 + 300pq^r^2 - 80pq^r^2 - 80pq^r^2 - 16p - 86pq^r^2 + 132pq^2 + 715pq + 60pq - 20pq^r + 180pq^r - 312pq^2 + 380pq^4 + 360pq^4^2^2 + 255pq^2^2 + 192pq^2 + 16pq^4 + 144pq^4 - 28pq)./5.\]

4. \[ S_{ev}(G) = (-576p^4q^2 + 1728p^4q^2 - 1440p^4q^2 - 288pq^4^2 + 288pq^4^2 + 288pq^4^2 + 1728pq^4^2 + 768p^6q^3 - 576p^5q^6 - 1152q^r^6).\]

5. \[ S_{ev}(G) = (5760p^6q^3 - 34560p^6q^3 - 240p^6q - 60p^6q^r + 10368p^6q^r - 6912p^6q^r - 8640p^6q^r - 576p^5q^2 + 19440p^5q^3 - 8640p^5q^2 - 2220p^5q^r + 5867p^5q^r - 3696p^5q^r - 66240p^4q^r - 107 130p^4q^r + 19440p^4q^r + 15120p^4q^r - 720p^4q^r + 16 560pq^4^2 - 66240p^4q^r + 22560pq^4^2 - 1440pq^4q^r - 600pq^4q^r - 81 750pq^4q^r + 7920pq^4q^r - 120pq^4 + 6480p^3q^4 + 19 440p^3q^4^2 + 26712p^3q^4^2 - 19440p^3q^4^2 - 38340p^3q^4^2 + 100pq^4q^r - 49 100pq^4q^r + 144720pq^4q^r^3 - 82920pq^4q^r^3 + 188 540pq^4q^r^3 + 38120pq^4q^r^3 + 5160pq^4q^r^3 + 4160pq^4q^r^3 - 20160pq^4q^r^3 +64 16 230pq^4q^r^3 + 8102pq^4q^r^3 - 2160pq^4q^r^3 + 160pq^4q^r^3 - 4032pq^4q^r^3 + 39240pq^4q^r^3 + 2400pq^4q^r^3 + 720pq^4q^r^3 - 2160pq^4q^r^3 - 2256pq^4q^r^3 + 2160pq^4q^r^3 + 2640pq^4q^r^3 + 5040pq^4q^r^3 + 19440pq^4q^r^3 + 38280pq^4q^r^3 + 27 200pq^4q^r^3 + 45600pq^4q^r^3 + 16710pq^4 + 10 800pq^4q^r - 1792pq^4q^r^3 + 1840pq^4q^r - 5760pq^4q^r - 1440pq^4q^r - 2560pq^4q^r + 4240pq^4q^r^3 + 456pq^2 + 13 350pq^2 + 2880pq^2 + 120pq^2 - 120pq^2 + 8424pq^2q^r - 15120pq^2q^r + 26 660pq^2q^r - 5760pq^2q^r + 2800pq^2q^r - 4032pq^2q^r - 12960pq^2q^r^3 + 12 240pq^2q^r^4 - 7200pq^2q^r^3)\]
The graph $G_{12} = (\{p, q\} - \{p, q\} \cup \{p, q\} \cup \{p, q\})$.

6. $S_2(G) = \{4320p^4q^6 - 3569p^6q^3 - 648p^6q^4 - 720p^6q^7
\}
  + 12960p^3q^6 + 4392p^6q + 11520p^3q^6 + 9312p^6q^3 - 365p^3q^6 + 2160p^3q^6 - 720p^3q^6
+ 369p^3q^6 - 12480p^3q^6 - 14220p^3q^6 - 2160p^3q^6
+ 1623p^4q^7 - 504p^4q^7 - 1380p^4q^7 - 6240p^4q^7 + 1440p^4q^7 - 7920p^4q^7
+ 240p^4q^7 - 720p^4q^7 + 2160p^4q^7 - 2256p^4q^7 - 2160p^3q^7 - 2640p^3q^7 - 504p^3q^7
+ 23760p^3q^7 + 7360p^3q^7 + 21720p^3q^7 + 2040p^3q^7 - 160p^3q^7 - 2880p^3q^7 - 1120p^3q^7
+ 2880p^3q^7 + 7440p^3q^7 - 880p^3q^7 - 336p^3q^7 + 2400p^3q^7 + 242p^3q^7 + 2160p^3q^7 - 3520p^3q^7
+ 1920p^3q^7 - 2440p^3q^7 + 2160p^4q^7 + 1440p^4q^7 - 1920p^4q^7 - 480p^4q^7
+ 576p^4q^7 - 468p^4q^7 - 1840p^4q^7 + 2880p^4q^7 - 240p^4q^7 - 15120p^4q^7 - 720p^4q^7
+ 5760p^4q^7 - 640pq^7 - 252pq^7 - 1440pq^7
+ 1440pq^7 - 48pq^7 - 336p^3q^7 - 5040p^3q^7 - 1680p^3q^7 - 1008p^3q^7
+ 960p^3q^7 + 480pq^7 - 960pq^7)/5.

7. $P(I(G)) = -48p^2q^2 + 24pq^2 + 24pq^2
\}
  + 2304p^2q^2 - 856p^2q^2 + 80pq^2 - 88pq^2 + 24pq^2
+ 16pq^2 - 328pq^2 - 64pq^2 - 24pq^2 - 24pq^2 - 72pq^2 + 32pq^2
+ 108pq^2

8. $S(G) = (-3360p^7 + 320p^7 + 1008pq^7 - 960pq^7 - 1120p^7
+ 13440p^7 - 1440p^7 - 1440p^7 - 960p^7 - 6720pq^7 + 640pq^7 + 768pq^7 + 320pq^7
+ 2880pq^7 - 1920pq^7 - 960pq^7 + 2560pq^7 + 1680pq^7 + 1040pq^7 - 3360pq^7
+ 2800pq^7 - 1248pq^7 + 640pq^7 + 5760pq^7
+ 10560pq^7 - 5760pq^7 - 480pq^7 + 5760pq^7
+ 2880pq^7 + 64pq^7 + 11520pq^7 - 7480pq^7 - 7760pq^7 - 1440pq^7
+ 5380pq^7 - 5760pq^7 + 6960pq^7
+ 1200pq^7 - 320pq^7 + 320pq^7 - 645pq^7 + 456pq^7 + 352pq^7 + 288pq^7 + 240pq^7 - 804pq^7
+ 720pq^7 - 128pq^7 + 1520pq^7 + 1440pq^7
+ 1020pq^7 + 768pq^7 + 64pq^7 + 576pq^7 - 112pq^7)/5.

9. $Gat(G) = (-2764pq^5 - 4605pq^5 - 8928pq^5 - 1248pq^5 - 224pq^5 + 92160pq^5 + 480pq^5
+ 36000pq^5 - 1920pq^5 + 400pq^6
+ 30480pq^6 + 2800pq^6 - 40 320pq^6 - 46560pq^6 + 6000pq^6 + 65280pq^6
+ 18720pq^6 + 8160pq^6 + 4320pq^6 + 3360pq^6 + 320pq^6 = 8928pq^6 + 18000pq^6
+ 60480pq^6 - 6960pq^6 - 16 720pq^6
+ 86400pq^6 + 5042pq^6 + 67 680pq^6 + 20 880pq^6
+ 11040pq^6 + 17 760pq^6 + 960pq^6 + 1728pq^6 - 1920pq^6
+ 20640pq^6 + 1520pq^6 + 1248pq^6 - 5280pq^6 + 1520pq^6 + 10560pq^6
+ 5760pq^6 + 1440pq^6 + 56 160pq^6 + 2208pq^6
+ 7200pq^6 + 3840pq^6 + 2048pq^6 + 8640pq^4
+ 7680pq^4 - 480pq^4 - 960pq^4 - 1536pq^4 + 480pq^4 - 960pq^4
+ 2768pq^4 - 768pq^4 + 64pq^4 - 32pq^4 + 160pq^4 + 480pq^4 - 18720pq^4 - 11760pq^4 - 3160pq^4
+ 7440pq^4 - 480pq^4 + 3360pq^4 + 1120pq^4 + 6720pq^4 - 1120pq^4 + 32q - 160q - 320q)/15.

Proof. The graph $Z(p, q, r)$, $p \leq q \leq r$ has $n = 24pq^r$ number of vertices and $m = 48pqr - 4(pq + qr + pr)$ number of edges. The sets $\{S_j : 1 \leq j \leq 6\}$ divides graph $Z(p, q, r)$ into two convex components. We have

$s_1 = 4pr : 1 \leq i \leq q - 1$

$n_1 = 24pr : 1 \leq i \leq q - 1$

$m_1 = \{36p + 4r(p - 1) + 4(p - 1)i + 4pr(i - 1) : 1 \leq i \leq q - 1\}

$s_2 = 4pq : 1 \leq i \leq r - 1$

$n_2 = 24pq : 1 \leq i \leq r - 1$

$m_2 = \{36pq + 4(p - 1) + 4q(p - 1)i + 4pq(i - 1) : 1 \leq i \leq r - 1\}

$s_3 = 4qr : 1 \leq i \leq p - 1$

$n_3 = 24qri : 1 \leq i \leq p - 1$

$m_3 = \{36qr + 4(q - 1) + 4q(q - 1)i + 4qr(i - 1) : 1 \leq i \leq p - 1\}$
To illustrate the techniques used in this paper, we present an illustration of the different types of cuts of three faces namely front (figures 3(a)), top (figure 3(b)) and side (figure 3(c)) views of $Z(p, q, r)$ crystal of employed in the Zeolite LTA framework to compute the topological indices.

4. Various degree based topological indices of Zeolite LTA

In this section we compute the degree based topological indices listed in table 2 for the Zeolite LTA framework the same manner as in the previous section.

There are $8(pq + qr + pr)$ vertices of degree 3 and $24pq - 8(pq + qr + pr)$ vertices are of degree 4. The edge partitions are presented in table 3.

Theorem 4. For $G = Z(p, q, r), p \leq q \leq r$ we have

1. $R_6(G) = 48(16^a)pq + [8(9^a) + 8(12^a) - 20(16^a)]$
   
   $(pq + qr + pr) + [4(9^a) + 8(12^a) - 12(16^a)](p + q + r) + 48(16^a - 12^a)$

2. $R(G) = \{288\sqrt{3}pq + (96 - 56\sqrt{3})(pq + qr + pr) + (96 - 40\sqrt{3})(p + q + r) - 576 + 288\sqrt{3}/24\sqrt{3} \}

3. $RR(G) = 192pq + (16\sqrt{3} - 56)(pq + qr + pr) + (16\sqrt{3} - 36)(p + q + r) + 192 - 96\sqrt{3}$
Table 2. Degree based topological indices.

| Topological Indices                     | Mathematical Expressions |
|-----------------------------------------|--------------------------|
| Generalized Randić [56]                | $R_1(G) = \sum_{uv \in E(G)} [d(u)d(v)]^4$ |
| Randić [57]                            | $R(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}$ |
| Reciprocal Randić [58]                 | $RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}$ |
| Reduced reciprocal Randić [59]         | $RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u) - 1)(d(v) - 1)}$ |
| First Zagreb [20]                      | $M_1(G) = \sum_{uv \in E(G)} d(u)^2$ |
| Second Zagreb [20]                     | $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$ |
| Reduced Second Zagreb [60]             | $RM_2(G) = \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1)$ |
| Hyper Zagreb [61]                      | $HM(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2$ |
| Augmented Zagreb [62]                  | $AZ(G) = \sum_{uv \in E(G)} \left( \frac{d(u) + d(v)}{2d(u) + d(v) + 1} \right)^3$ |
| Atom bond connectivity [63]            | $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v)}{d(u) + d(v) + 1}}$ |
| Harmonic [64]                          | $H(G) = \sum_{uv \in E(G)} \frac{1}{d(u) + d(v)}$ |
| Sum-connectivity [65]                   | $SC(G) = \sum_{uv \in E(G)} \frac{1}{d(u) + d(v)}$ |
| Geometric arithmetic [66]              | $GA(G) = \sum_{uv \in E(G)} \frac{d(u) + d(v)}{d(u) + d(v) + 1}$ |

4. $RRR(G) = 144pqr + (8\sqrt{6} - 42)(pq + qr + pr) + (8\sqrt{6} - 4)(p + q + r) + 144 - 48\sqrt{6}$.

5. $M_1(G) = 384pqr - 56(pq + qr + pr)$.

6. $M_2(G) = 768pqr - 152(pq + qr + pr) - 60(p + q + r) + 192$. 

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**Table 2. Degree based topological indices.**

| Topological Indices                     | Mathematical Expressions |
|-----------------------------------------|--------------------------|
| Generalized Randić [56]                | $R_1(G) = \sum_{uv \in E(G)} [d(u)d(v)]^4$ |
| Randić [57]                            | $R(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}$ |
| Reciprocal Randić [58]                 | $RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}$ |
| Reduced reciprocal Randić [59]         | $RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u) - 1)(d(v) - 1)}$ |
| First Zagreb [20]                      | $M_1(G) = \sum_{uv \in E(G)} d(u)^2$ |
| Second Zagreb [20]                     | $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$ |
| Reduced Second Zagreb [60]             | $RM_2(G) = \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1)$ |
| Hyper Zagreb [61]                      | $HM(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2$ |
| Augmented Zagreb [62]                  | $AZ(G) = \sum_{uv \in E(G)} \left( \frac{d(u) + d(v)}{2d(u) + d(v) + 1} \right)^3$ |
| Atom bond connectivity [63]            | $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v)}{d(u) + d(v) + 1}}$ |
| Harmonic [64]                          | $H(G) = \sum_{uv \in E(G)} \frac{1}{d(u) + d(v)}$ |
| Sum-connectivity [65]                   | $SC(G) = \sum_{uv \in E(G)} \frac{1}{d(u) + d(v)}$ |
| Geometric arithmetic [66]              | $GA(G) = \sum_{uv \in E(G)} \frac{d(u) + d(v)}{d(u) + d(v) + 1}$ |

4. $RRR(G) = 144pqr + (8\sqrt{6} - 42)(pq + qr + pr) + (8\sqrt{6} - 4)(p + q + r) + 144 - 48\sqrt{6}$.

5. $M_1(G) = 384pqr - 56(pq + qr + pr)$.

6. $M_2(G) = 768pqr - 152(pq + qr + pr) - 60(p + q + r) + 192$. 

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Table 3. The Edge partition of Zeolite graph.

| (d(u), d(v)) | Frequency |
|--------------|-----------|
| (3,3)        | 8(pq + qr + pr) + 4(p + q + r) |
| (3,4)        | 8(pq + qr + pr) + 8(p + q + r) - 48 |
| (4,4)        | 48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48 |

7. \(RM_2(G) = 432pqr - 100(pq + qr + pr) - 44(p + q + r) + 144\).

8. \(HM(G) = 3072pqr - 600(pq + qr + pr) - 232(p + q + r) + 720\).

9. \(AZ(G) = [49152000pqr - 4666532(pq + qr + pr) - 3855657(p + q + r) + 13320192]/54000\).

10. \(ABC(G) = [648 - 12\sqrt{3} + 72\sqrt{5} - 270\sqrt{2})(pq + qr + pr) + (16\sqrt{5} + 72\sqrt{5} - 162\sqrt{2})(p + q + r) + 648\sqrt{2} - 432\sqrt{5}]/18\sqrt{3}.

11. \(H(G) = [252pqr - (pq + qr + pr) + 13(p + q + r) - 361]/21.

12. \(SC(G) = 24\sqrt{14}pqr + (8\sqrt{14} + 16\sqrt{3} - 10\sqrt{42})(pq + qr + pr) + (4\sqrt{14} + 16\sqrt{3} - 6\sqrt{42})(p + q + r) + 24(\sqrt{42} - 2\sqrt{3})\).

13. \(GA(G) = [336pqr + (32\sqrt{3} - 84)(pq + qr + pr) + (32\sqrt{3} - 56)(p + q + r) - 192\sqrt{3} + 336]/7.

Proof.

\[
R_n(G) = \sum_{u,v\in E(G)} [d(u)d(v)]^n
= (3 \times 3)^n(8(pq + qr + pr) + 4(p + q + r)) + (3 \times 4)^n(8(pq + qr + pr) + 8(p + q + r) - 48)
+ (4 \times 4)^n(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48)
= 48(16^n)pqr + 8(9^n) + 8(12^n) - 40\sqrt{3}\frac{p + q + r}{24}.

R(G) = \frac{1}{\sqrt{3 \times 3}}(8(pq + qr + pr) + 4(p + q + r)) + \frac{1}{\sqrt{3 \times 4}}(8(pq + qr + pr) + 8(p + q + r) - 48)
+ \frac{1}{\sqrt{4 \times 4}}(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48)
= 288\sqrt{3}pqr + 96\sqrt{3} \frac{p + q + r}{24}.

RR(G) = \sum_{u,v\in E(G)} (d(u)d(v))
= (3 \times 3)^n(8(pq + qr + pr) + 4(p + q + r)) + (3 \times 4)^n(8(pq + qr + pr) + 8(p + q + r) - 48)
+ (4 \times 4)^n(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48)
= 192pqr + (16\sqrt{3} - 56)(pq + qr + pr) + (16\sqrt{3} - 56)(p + q + r) + 192 - 96\sqrt{3}.

RRR(G) = \sum_{u,v\in E(G)} (\sqrt{d(u)} - 1)(\sqrt{d(v)} - 1)
= (2 \times 2)^n(8(pq + qr + pr) + 4(p + q + r)) + (2 \times 3)^n(8(pq + qr + pr) + 8(p + q + r) - 48)
+ (3 \times 3)^n(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48)
= 144pqr + (8\sqrt{6} - 42)(pq + qr + pr) + (8\sqrt{6} - 4)(p + q + r) + 144 - 48\sqrt{6}.

M_4(G) = \sum_{u\in V(G)} d(u)^2
= (3^n(8(pq + qr + pr)) + 4^2(24pqr - 8(pq + qr + pr))
= 384pqr - 56(pq + qr + pr)
\[ M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \\
= (3 \times 3)(8(pq + qr + pr) + 4(p + q + r)) + (3 \times 4)(8pq + qr + pr + 8(p + q + r) - 48) \\
= + (4 \times 4)(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48) \\
= 768pqr - 152(pq + qr + pr) - 60(p + q + r) + 192 \]

\[ RM_2(G) = \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1) \\
= (2 \times 2)(8(pq + qr + pr) + 4(p + q + r)) + (2 \times 3)(8pq + qr + pr + 8(p + q + r) - 48) \\
= + (3 \times 3)(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48) \\
= 432pqr - 100(pq + qr + pr) - 44(p + q + r) + 144 \]

\[ HM(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2 \\
= (3 + 3)^2(8(pq + qr + pr) + 4(p + q + r)) + (3 + 4)^2(8pq + qr + pr + 8(p + q + r) - 48) \\
= + (4 + 4)^2(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48) \\
= 3072pqr - 600(pq + qr + pr) - 232(p + q + r) + 720 \]

\[ AZ(G) = \sum_{uv \in E(G)} \left( \frac{d(u)d(v)}{d(u) + d(v) - 2} \right)^3 \\
= \left( \frac{3 \times 3}{3 + 3 - 2} \right)^3(8pq + qr + pr + 4(p + q + r)) + \left( \frac{3 \times 4}{3 + 4 - 2} \right)^3(8pq + qr + pr + 8(p + q + r) - 48) \\
= + \left( \frac{4 \times 4}{4 + 4 - 2} \right)^3(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48) \\
= [4915200pqr - 4666532(pq + qr + pr) - 3855657(p + q + r) + 13320192] / 54000 \]

\[ ABCG(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} \\
= \sqrt{\frac{3 + 3 - 2}{3 \times 3}}(8pq + qr + pr + 4(p + q + r)) + \sqrt{\frac{3 + 4 - 2}{3 \times 4}}(8pq + qr + pr + 8(p + q + r) - 48) \\
= + \sqrt{\frac{4 + 4 - 2}{4 \times 4}}(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48) \\
= 648\sqrt{2}pqr + (32\sqrt{3} + 72\sqrt{5} - 270\sqrt{1})pq + qr + pr \\
= +(16\sqrt{3} + 72\sqrt{5} - 162\sqrt{2})(p + q + r) + 648\sqrt{2} - 432\sqrt{5} / 18\sqrt{3} \]

\[ H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)} \\
= \frac{2}{(3 + 3)}(8pq + qr + pr + 4(p + q + r)) + \frac{2}{(3 + 4)}(8pq + qr + pr + 8(p + q + r) - 48) \\
= + \frac{2}{(4 + 4)}(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48) \\
= [252pqr - (pq + qr + pr) + 13(p + q + r) - 36] / 21 \]

\[ SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}} \\
= \frac{1}{\sqrt{3 + 3}}(8pq + qr + pr + 4(p + q + r)) + \frac{1}{\sqrt{3 + 4}}(8pq + qr + pr + 8(p + q + r) - 48) \\
= + \frac{1}{\sqrt{4 + 4}}(48pqr - 20(pq + qr + pr) - 12(p + q + r) + 48) \\
= 24\sqrt{2}pqr + (8\sqrt{14} + 16\sqrt{3} - 10\sqrt{42})(pq + qr + pr) + (4\sqrt{14} + 16\sqrt{3} - \sqrt{42})(p + q + r) \\
= + 24(\sqrt{2} - 2\sqrt{3}) \]
GA(G) = \sum_{\text{arc} \in E(G)} \frac{2(\sqrt{d(u)d(v)})}{d(u) + d(v)} = 2 \left(\frac{\sqrt{3 \times 3}}{3 + 3}\right)(8(pq + qr + pr) + 4(p + q + r)) + 2 \left(\frac{\sqrt{4 \times 4}}{4 + 4}\right)(48pq - 20(pq + qr + pr) - 12(p + q + r) + 48) = [336pq + (32\sqrt{3} - 84)(pq + qr + pr) + (32\sqrt{3} - 56)(p + q + r) - 192\sqrt{3} + 336]/7

5. Conclusion

In this paper we give the exact expression for various distance based topological indices of Zeolite LTA framework works using the well known cut method and also we compute various degree based indices of Zeolite LTA framework works. These indices are under investigation for other variants of β-cage like Sodalite (SOD) and Faujasite (FAU).

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Conflict of interest

The authors declare that they have no conflict of interest.

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