J Math Chem (2018) 56:1493–1510
https://doi.org/10.1007/s10910-018-0881-x

ORIGINAL PAPER

Hyper-Wiener and Wiener polarity indices of silicate and oxide frameworks

Micheal Arockiaraj[1] · S. Ruth Julie Kavitha[1] · Krishnan Balasubramanian[2] · Ivan Gutman[3]

Received: 13 September 2017 / Accepted: 5 February 2018 / Published online: 12 February 2018

Abstract Molecular descriptors are graph invariants representing the chemical structure in graph-theoretical terms. There is a wide range of such descriptors and the computation of these invariants for the various chemical frameworks is a current area of research. Among these the Wiener types of indices have passed through critical tests and emerged as a useful topological index in QSAR, predictive toxicology and computer-assisted drug discovery as a starting point to reduce a large data set of chemicals. However mathematical techniques to compute hyper-Wiener index continues to pose considerable challenges, as they involve long and complex manipulations. In the present study, we develop a new technique based on vertex cut methods to compute the hyper-Wiener indices of complex silicate and oxide frameworks of current interest for the first time and obtain the analytical expressions of Wiener polarity indices for these chemical frameworks based on vertex neighborhood.

Keywords Distance · Hyper-Wiener index · Silicate network · Oxide network

1 Introduction

Graph theory is largely applied to the characterization of chemical structures, thereby enabling the study of quantitative structure activity (QSAR) and property (QSPR)

Dedicated to Ivan Gutman on his 70th birthday.

✉ S. Ruth Julie Kavitha
juliesuresh91@gmail.com

1 Department of Mathematics, Loyola College, Chennai 600034, India

2 School of Molecular Sciences, Arizona State University, Tempe, AZ 85287-1604, USA

3 Faculty of Science, University of Kragujevac, Kragujevac, Serbia

relationships of the molecular structures [19,20,32,53]. The QSAR/QSPR studies are based on the quantification of the chemical frameworks, by means of which the chemical and biological properties of a molecule can be studied with comparison to its molecular structure. One tool used for this purpose are the topological indices. These indices are employed in the process of correlating the chemical structures with various characteristics such as boiling points, molar heats of formation, etc., and thereby exhibiting their significance in the field of biological sciences.

The topological index of a molecule is a single number that quantifies the structure and the branching pattern of that molecule, which helps in exploring the underlying topology of the molecule. A molecular graph is a graph whose vertices represent atoms and whose edges represent the covalent bonds of the molecule, thus representing the chemical constitution of the underlying molecule. Thus, the topological analysis of a molecule involves translating its molecular structure to a molecular graph and then into a characteristic unique number that may be considered as a descriptor of the molecule under examination.

The Wiener index (W) defined by Wiener [54], is the first topological index to be used in mathematical chemistry. It can be correlated with physico-chemical properties of organic compounds. At present, there exists a large number of topological indices which are classified based on the structural properties of the graphs used for their calculation. The main incentive for developing new molecular descriptors was triggered especially by the pharmaceutical industry in its continuous need for improving drug design methods. In order to treat the newly discovered syndromes, more than half a million new substances are synthesized and characterized every year, whereas only some of them are tested biologically which in turn increases the cost of any new medicine. Any method helping investigators to know which structures are worthy of being synthesized and tested and which are not, results in enormous savings. This is one of the significant roles of the topological indices and this explains partly the interest for developing new descriptors during the past recent years.

Wiener in his initial work [54] used a linear formula consisting of W and Wiener polarity index (W_p), for calculating the boiling point of paraffins. After a period of time, the study of W became more popular compared to W_p. In the recent years, the study of W_p has indeed caught the attention of many researchers. Lukovits et al. [45] demonstrated the quantitative structure-property relationships in a series of acyclic and cycle-containing chemical compounds using W_p whereas Hosoya [27] found a physical-chemical interpretation of W_p. A linear time algorithm for the computation of W_p in case of trees were presented in [13] while the generalized version of W_p was presented in [29] along with a linear time algorithm for trees and partial cubes. Very recently, Chen et al. [8] provided a simple general formula for computing W_p of any graph based on vertex neighborhood and also computed the analytical expressions of W_p for various lattice networks. In this paper, we further continue to explore this index by computing it for the two chemically significant networks.

The hyper-Wiener index (WW), originally introduced by Randić [51] for acyclic graphs, is a generalization of the Wiener index, as it includes squares of distance matrix elements, and thus it can be considered as a quantitative measure of expansiveness of a chemical structure. Klein et al. [41] who generalized Randić's definition of WW to all graphs, consider hyper-Wiener index as one of the useful chemical structural

parameters in QSAR, as it measures expansiveness of a molecular structure weighing expansive graphs to a greater extent compared to ordinary Wiener index of a graph. Randić [51] considers WW hyper-Wiener index to be among useful topological indices as the hyper-Wiener index passes several of Randić's critical tests for it to be among useful indices in QSAR studies. Therefore hyper-Wiener indices together with other topological indices that have passed through critical tests can be useful starting point in computer-assisted drug discovery and predictive toxicological studies in providing guidance to reduce the data set of millions of starting chemicals for which higher level ab initio quantum chemical computations and other CPU-intensive techniques such as quantum molecular dynamics, QM/MM, ONIOM and other accurate quantum chemical methods are difficult to apply for such demanding drug-protein interactions. Consequently, there has been considerable interest in obtaining analytical expressions for hyper-Wiener indices over the years. Cash et al. [7] have obtained mathematical expressions for the hyper-Wiener indices of linear phenylenes, cyclic phenylenes, polyazulenes, and several families of periodic hexagonal chains. Likewise Khalifeh et al. [33] have obtained mathematical expressions for the hyper-Wiener indices of C_4 nanotubes, C_4 nanotori and q-multi-walled polyhex nanotori. Xing et al. [55] have obtained the hyper-Wiener indices of unicyclic graphs. Essalih and El Marraki [14] have obtained the hyper-Wiener indices of corona $C_m \circ C_n$. Thus obtaining analytical expressions for the hyper-Wiener indices continues to be an active area of research for mathematicians and mathematical chemists. In the present study, we fill an important gap in this field by obtaining closed mathematical expressions for the hyper-Wiener indices of large inorganic silicate and oxide networks for the first time by developing a new graph cut method.

2 Mathematical preliminaries

Throughout this paper we consider finite, undirected, connected graphs G, without loops and multiple edges. Let $E(G)$ and $V(G)$ denote the edge set and the vertex set of the graph G. By distance between any pair of vertices u, v in a graph G, we mean the number of edges on a shortest path connecting these vertices in G and is usually denoted by $d_G(u, v)$.

A subgraph H of a graph G is said to be a convex subgraph if for any vertices u, v of H, any shortest path between u and v in G lies completely in H. An edge cut F of G is said to be a convex edge cut if the two components of $G - F$ are the convex subgraphs of G. The Hamming distance $H(l(u), l(v))$ between the binary strings $l(u)$ and $l(v)$ is defined as the number of positions in which the two strings differ. A connected graph G is called a partial cube if and only if its vertices are labeled with binary strings of fixed length such that for all vertices $u, v \in G$ we have $H(l(u), l(v)) = d_G(u, v)$.

A convex vertex cut X of G is defined as analogous to the convex edge cut, the only difference being the cut X which comprises of vertices instead of edges. An independent set S of $V(G)$ is defined as a set in which no two vertices are adjacent to each other. A vertex v of G is said to be a corner vertex if it is not the internal vertex in the shortest path between any pair of vertices in G and $\angle_G$ denotes the collection of corner vertices of G.

Definition 1 [54] The Wiener index $W(G)$ is the sum of distances between all pairs of vertices in G,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v).$$

It is the oldest and the most studied graph invariant. There are various algorithms [5,48,57] for the evaluation of this index and a number of papers were devoted to compute the explicit formulae for various classes of graphs [2,11,12,16,42,49].

Definition 2 [54] The Wiener polarity index $W_p(G)$ is defined as the number of unordered pairs of vertices that are at distance 3 in G,

$$W_p(G) = |\{\{u, v\} \subseteq V(G)|d_G(u, v) = 3\}|.$$

In [44], Liu et al. found the bounds of W_p in terms of Zagreb, Wiener, hyper-Wiener indices. The mathematical properties of this index and its applications in chemistry can be found in [9,44] and the references cited therein. Other recent works on W_p are found in [8,28,58].

The hyper-Wiener index WW was introduced by Randić in case of trees [51] and was extended to general graphs by Klein et al. in [41]. According to Randić [51], in the case of trees, WW is equal to the sum of products $n(u)\cdot n(v)$ of all pairs of vertices u, v, where $n(u)$ and $n(v)$ are number of vertices lying on the two sides of the path connecting u and v. This generalizes the earlier result of Wiener [54], according to which the Wiener index of a tree is equal to the sum of products $n(u)\cdot n(v)$ of all pairs of adjacent vertices u, v.

Unfortunately, Randić's original definition of WW is not applicable to cycle-containing graphs. In order to avoid this difficulty, Klein et al. [41] demonstrated that in the case of trees, WW satisfies the right-hand side of Eq. (1). They then proposed that the same expression be used also in the case of cycle-containing graphs, which eventually was universally accepted. Thus we have:

Definition 3 [41] The hyper-Wiener index $WW(G)$ of a graph G is

$$WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G(u, v) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G^2(u, v). \quad (1)$$

Various properties of this index were reported in [30,33,35,43,60] and its bounds were discussed in [15]. It has also been observed that there is a relation between Wiener and hyper-Wiener indices [21,36,59] and they show good correlation with various physico-chemical and biological properties [10,46] of chemical compounds.

A so-called *cut method* (or *orthogonal cut method*) for computing various distance-based topological indices was discovered in [37] and then applied in a long series of papers to benzenoid [1,17,18,22,23,31,38,56] and non-benzenoid chemical species [3,4,24,25,34]. The mathematical details of the cut method are outlined in the survey [39]. In what follows, we describe the version of the cut method, suitable for the calculation of hyper-Wiener indices.

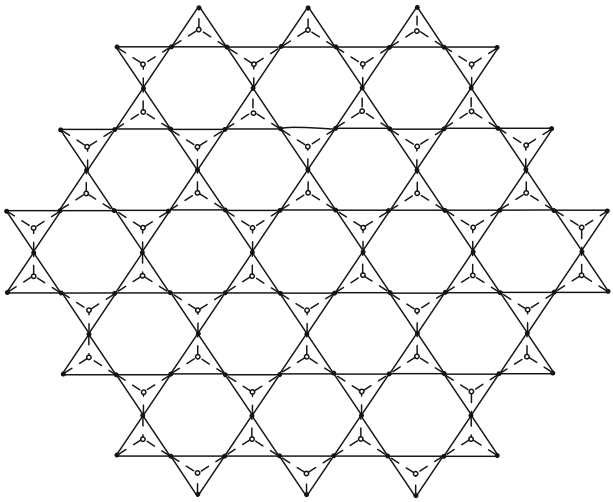

Fig. 1 A three dimensional silicate network and deletion of dotted lines and hollow vertices gives the three dimensional oxide network

Let G be a partial cube embedded into the q-cube and for any $1 \leq i, j \leq q$, let n_{ij}^{01} be the number of vertices of G whose ith and jth co-ordinates are equal to 0 and 1, respectively, and in a similar way we define the terms n_{ij}^{00}, n_{ij}^{10} and n_{ij}^{11}.

Theorem 1 [35] *Let G be a partial cube on n vertices embedded into the q-cube. Then*

$$WW(G) = W(G) + \sum_{i=1}^{q} \sum_{j=i+1}^{q} \left[n_{ij}^{11}\, n_{ij}^{00} + n_{ij}^{01}\, n_{ij}^{10} \right].$$

Based on the above formula, Žigert et al. established general expressions for the hyper-Wiener index of several classes of benzenoid systems [40,60]. Yet, there exist only a limited number of such results, due to computational complexities.

Most of the distance and/or degree-based topological indices [3,26,50], except the Wiener polarity and hyper-Wiener indices, have been computed for the silicate and oxide networks as depicted in Fig. 1 and the method described in Theorem 1 cannot be used to calculate the hyper-Wiener index of these networks. This motivates us to derive a new method for computing the same and is discussed in the next section.

3 Hyper-Wiener index via vertex cut method

In the recent paper [3], the first three authors have developed a method for computing degree and distance-based indices as the sum of the vertex contributions and the advantage of this method is that it can be applied to certain classes of graphs when the usual cut method [39] is not applicable. In this section we derive the formula for

computing the hyper-Wiener index using the vertex cut method and we begin with the concept of betweenness centrality.

The betweenness centrality $B(x)$ of a vertex $x \in V(G)$ is the sum of the fraction of all pairs of shortest paths that pass through the vertex x. Mathematically,

$$B(x) = \sum_{u,v \in V(G)\setminus\{x\}, u \neq v} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}}$$

where $\sigma_{u,v}$ denote the total number of shortest (u, v)-paths in G and $\sigma_{u,v}(x)$ denote the number of shortest (u, v)-paths passing through the vertex x. This centrality index $B(x)$ plays a significant role in decomposing the Wiener index in terms of vertex contributions [3,52]. But an extension of this index is sufficient to decompose the hyper-Wiener index and is described as follows.

The betweenness centrality $B(x, y)$ of two distinct vertices $x, y \in V(G)$ is the sum of the fraction of all pairs of shortest paths that pass through both the vertices x and y. Mathematically,

$$B(x, y) = \sum_{u,v \in V(G)\setminus\{x,y\}, u \neq v} \frac{\sigma_{u,v}(x, y)}{\sigma_{u,v}}$$

where $\sigma_{u,v}(x, y)$ represents the number of shortest (u, v)-paths that pass through the vertices x and y while $\sigma_{u,v}$ denotes the total number of shortest (u, v)-paths in G.

Theorem 2 *Let G be a graph having n vertices. Then*

$$WW(G) = 2W(G) - \binom{n}{2} + \sum_{\{x,y\} \subseteq V(G)} B(x, y). \tag{2}$$

Proof From the definition of $B(x, y)$, we have

$$\begin{aligned}
\sum_{\{x,y\} \subseteq V(G)} B(x, y) &= \sum_{x,y \in V(G), x \neq y} \left(\sum_{u,v \in V(G)\setminus\{x,y\}, u \neq v} \frac{\sigma_{u,v}(x, y)}{\sigma_{u,v}} \right) \\
&= \sum_{u,v \in V(G), u \neq v} \left(\sum_{x,y \in V(G)\setminus\{u,v\}, x \neq y} \frac{\sigma_{u,v}(x, y)}{\sigma_{u,v}} \right) \\
&= \sum_{u,v \in V(G), u \neq v} \binom{d_G(u, v) - 1}{2}.
\end{aligned}$$

In other way, we have

$$2 \sum_{\{x,y\} \subseteq V(G)} B(x, y) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u, v) - 1)(d_G(u, v) - 2). \tag{3}$$

We now algebraically split the term $d_G^2(u, v)$ as,

$$d_G^2(u, v) = d_G(u, v) + [d_G(u, v) - 1][d_G(u, v) - 2] + 2[d_G(u, v) - 1] \quad (4)$$

Obviously the first term on the right-hand side of Eq. (1) is one half of the Wiener index. Now, using Eqs. (3) and (4), we arrive the formula for the hyper-Wiener index as follows.

$$\begin{aligned} WW(G) &= \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G^2(u, v) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} \\ &\quad \times \Big[d_G(u, v) + [d_G(u, v) - 1][d_G(u, v) - 2] + 2[d_G(u, v) - 1]\Big] \\ &= W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} \Big[[d_G(u, v) - 1][d_G(u, v) - 2] + 2[d_G(u, v) - 1]\Big] \\ &= 2W(G) - \binom{n}{2} + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} \Big[[d_G(u, v) - 1][d_G(u, v) - 2]\Big] \\ &= 2W(G) - \binom{n}{2} + \sum_{\{x,y\}\subseteq V(G)} B(x, y) \end{aligned}$$

□

Now we present Theorem 2 in an elegant way to compute $WW(G)$ using vertex cuts with the following notations. Consider the convex vertex cuts in pairs (V_i, V_j), then we arrive any one of the two cases as shown in the Fig. 2. Suppose the cuts are intersecting each other, we denote the number of vertices in the four fragments G_1, G_2, G_3 and G_4 as $n_{11}(V_i, V_j)$, $n_{22}(V_i, V_j)$, $n_{12}(V_i, V_j)$ and $n_{21}(V_i, V_j)$ respectively as depicted in Fig. 2a. On the other side if the cuts are parallel to each other, either $n_{12}(V_i, V_j)$ or $n_{21}(V_i, V_j)$ is zero as shown in Fig. 2b.

Theorem 3 *Let G be a connected graph admitting a vertex partition $\{V_i\}_{i=1}^k \cup \angle_G$ of $V(G)$ such that each V_i is a convex vertex cut and an independent set. Then*

$$\begin{aligned} WW(G) &= 2W(G) - \binom{|V(G)|}{2} + \sum_{i=1}^{k}\sum_{j=i+1}^{k} \\ &\quad \times \Big[n_{11}(V_i, V_j)\, n_{22}(V_i, V_j) + n_{12}(V_i, V_j)\, n_{21}(V_i, V_j)\Big]. \end{aligned} \quad (5)$$

Proof In order to prove the theorem it is enough to show that the term $\sum_{\{x,y\}\subseteq V(G)} B(x, y)$ is equivalent to the last term in Eq. (5). For any two disjoint sets $X, Y \subseteq V(G)$, we have the following notation

$$B(X, Y) = \sum_{\{x,y\}\subseteq V(G), x\in X, y\in Y} B(x, y).$$

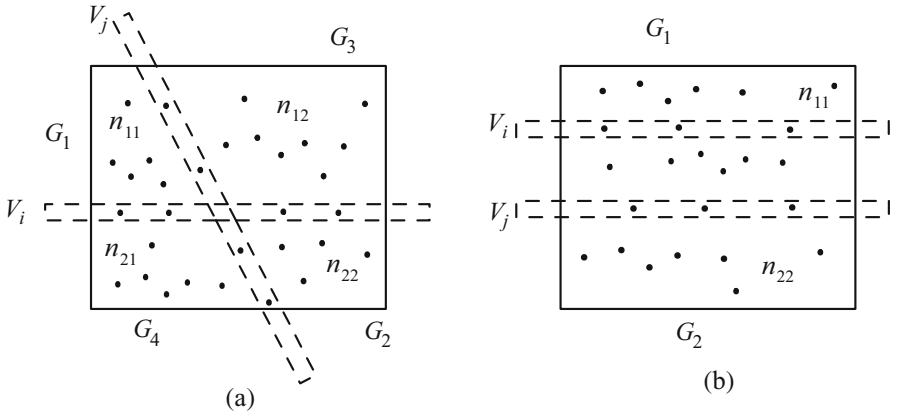

Fig. 2 Different cases of elementary cuts (**a**) intersecting cuts, (**b**) parallel cuts

Thus we have

$$\sum_{\{x,y\}\subseteq V(G)} B(x,y) = \sum_{i=1}^{k}\sum_{j=i+1}^{k} B(V_i,V_j) + \sum_{\{x,y\}\subseteq \angle_G} B(x,y) + \sum_{\{x,y\}\subseteq V(G), x\in V_i, y\in \angle_G} B(x,y).$$

The last two summations in the above equation vanish since there exists no shortest paths passing through the corner vertex.

Suppose V_i and V_j are intersecting cuts. Then $B(V_i, V_j)$ counts the number of pairs of vertices $\{x, y\}$ such that $x \in V(G_1)$ and $y \in V(G_2)$ in addition to the number of pairs of vertices $\{x, y\}$ such that $x \in V(G_3)$ and $y \in V(G_4)$ as depicted in Fig. 2a. Consequently,

$$B(V_i,V_j) = n_{11}(V_i,V_j)\, n_{22}(V_i,V_j) + n_{12}(V_i,V_j)\, n_{21}(V_i,V_j).$$

On the other hand if V_i and V_j are parallel cuts, we have to consider the pairs $\{x, y\}$ such that $x \in V(G_1)$ and $y \in V(G_2)$ as depicted in Fig. 2b. Then either $n_{12}(V_i, V_j)$ or $n_{21}(V_i, V_j)$ becomes zero, and therefore for this case we have,

$$B(V_i,V_j) = n_{11}(V_i,V_j)\, n_{22}(V_i,V_j).$$

Therefore, in general we have the result

$$\sum_{\{x,y\}\subseteq V(G)} B(x,y) = \sum_{i=1}^{k}\sum_{j=i+1}^{k} \Big[n_{11}(V_i,V_j)\, n_{22}(V_i,V_j) + n_{12}(V_i,V_j)\, n_{21}(V_i,V_j) \Big].$$

which gives the required formula (5). □

We now exhibit the significance of the above result by computing the hyper-Wiener indices of two chemically important frameworks such as silicate networks and oxide networks in the following sections.

4 Silicate networks

Silicates are the largest and most important class of rock-forming minerals and make up approximately 90% of the earth's crust. They are classified based on the structure of their silicate groups and are obtained by fusing metal oxides or metal carbonates with sand [47]. A number of research papers were devoted to explore the properties of this chemical network [3,6,26,47,50]. The basic chemical unit of silicate is a (SiO_4) tetrahedron in which the corner vertices represents the oxygen nodes and the central vertex represents the silicon node. These tetrahedra combine in a variety of ways to form three-dimensional networks of silicates. Silicate network of dimension n is denoted by SL_n, where n denotes the order of circumscribing as shown in the Fig. 1. It consists of $15n^2 + 3n$ number of vertices and $36n^2$ number of edges.

Theorem 4 *For a silicate network of dimension n,*

$$WW(SL_n) = \frac{n}{12}\left(2740n^5 + 3858n^4 + 1309n^3 - 228n^2 - 179n - 12\right).$$

Proof Let G denote the silicate network SL_n and let the indexed sets $\{H_p\}$, $\{O_p\}$, $\{A_p\}$ represent the set of all horizontal, obtuse and acute vertex cuts [3] of the silicate network SL_n, where $1 \leq p \leq 2n-1$ and the remaining vertices form a set $\angle_G$ of corner vertices of G. Let $V_i, V_j \in \{\{H_p\}, \{O_p\}, \{A_p\}\}$ and by Theorem 3,

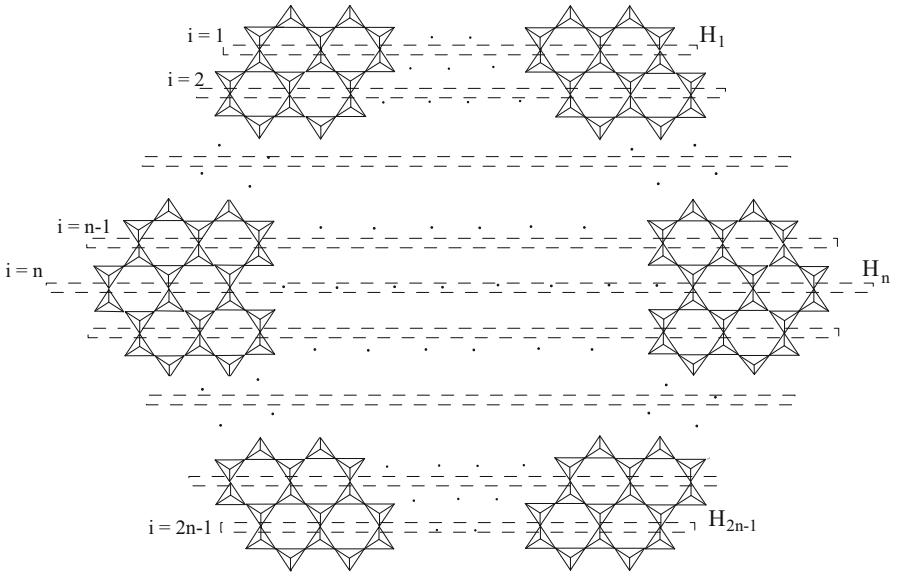

Fig. 3 Convex vertex cuts of type P

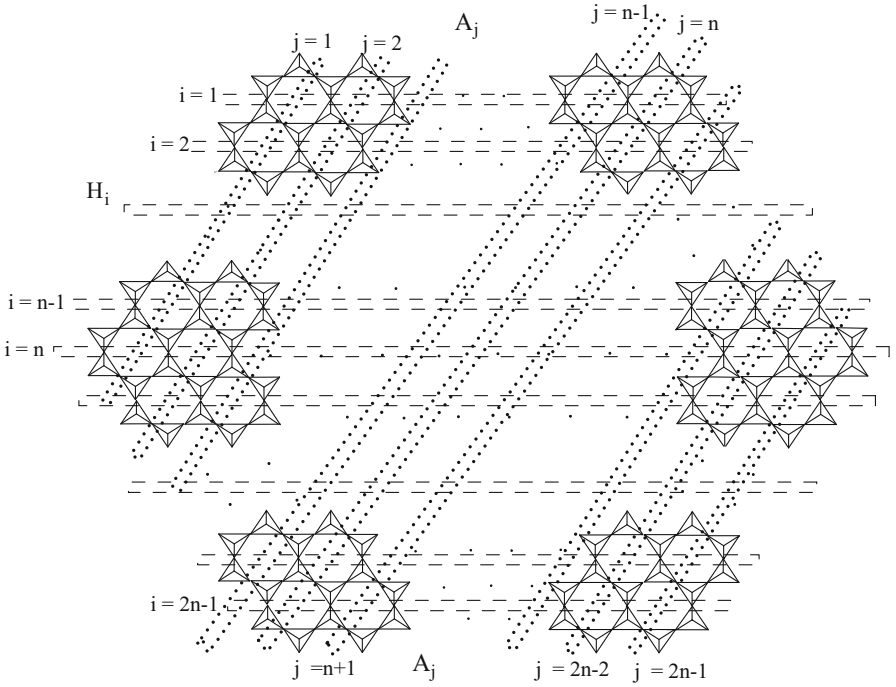

Fig. 4 Convex vertex cuts of type *I*

$$\begin{aligned} WW(G) &= 2W(G) - \binom{|V(G)|}{2} + \sum_{i=1}^{6n-3} \sum_{j=i+1}^{6n-3} \\ &\quad \times \Big[n_{11}(V_i, V_j)\, n_{22}(V_i, V_j) + n_{12}(V_i, V_j)\, n_{21}(V_i, V_j) \Big] \\ &= 2W(G) - \binom{|V(G)|}{2} + WW^*(G) \end{aligned} \tag{6}$$

where

$$WW^*(G) = \sum_{i=1}^{6n-3} \sum_{j=i+1}^{6n-3} \Big[n_{11}(V_i, V_j)\, n_{22}(V_i, V_j) + n_{12}(V_i, V_j)\, n_{21}(V_i, V_j) \Big].$$

The Wiener index of silicate network has been computed in [3] and is given by

$$W(G) = \frac{n}{2}\big(410n^4 + 295n^3 + 18n^2 - 31n - 2\big). \tag{7}$$

We now compute $WW^*(G)$ by considering the vertex cut in pairs. We call the two different types as (1) Type P as shown in Fig. 3, in which the cuts are parallel to each other (2) Type I as shown in Fig. 4, in which the cuts intersect each other.

Table 1 $n_{11}(H_i, H_j)$ and $n_{22}(H_i, H_j)$ for parallel pair of cuts

Range for		$n_{11}(H_i, H_j)$	$n_{22}(H_i, H_j)$
i	j		
$1 \le i \le n-1$	$i+1 \le j \le n-1$	$\sum_{k=1}^{i}\{5(n+k)-2\}$	$\frac{15n^2+5n}{2}+4(n+j)+3$ $+\sum_{k=1}^{n-j-1}\{5(n+j+k)+3\}$
	$n \le j \le 2n-1$		$\sum_{k=1}^{2n-j}\{5(n+k)-2\}$
$n+1 \le i \le 2n-2$	$i+1 \le j \le 2n-1$	$\frac{15n^2+5n}{2}+4(3n-i)+3$ $+\sum_{k=1}^{2n-i-1}\{5(3n-i+k)+3\}$	$\sum_{k=1}^{2n-j}\{5n+5k-2\}$

Table 2 $n_{rs}(H_i, A_j)$, $r, s = 1, 2$ for intersecting pair of cuts

Range for i	Range for j	$n_{11}(H_i, A_j)$	$n_{12}(H_i, A_j)$
		$n_{21}(H_i, A_j)$	$n_{22}(H_i, A_j)$
$1 \le i \le n$	$1 \le j \le n$	$5ij$	$i(5i-10j+10n-1)/2$
		$j(5j-10i+10n-1)/2$	$(30n^2-5a^2+10ai-10an-a-5i^2-10ni-i+2n)/2$
	$n+1 \le j \le n+i-1$	$(j-n+10ij+10jn-5j^2-5n^2)/2$	$(i-j+n)(5i-5j-1+5n)/2$
		$(20jn-n-10ij-5n^2)/2$	$(35n^2-i+n+10ij-10ni-20jn-5i^2)/2$
	$n+i \le j \le 2n-1$	$i(5i+10n+1)/2$	–
		–	$(j-2n)(5j-20n-1)/2$
$n+1 \le i \le 2n-1$	$1 \le j \le i-n$	$j(5j+10n+1)/2$	–
		–	$(i-2n)(5i-20n-1)/2$
	$i-n+1 \le j \le n$	$(10ij-n+i+10ni-5i^2-5n^2)/2$	$(20ni-n-10ij-5n^2)/2$
		$(i-j-n)(5i-5j+1-5n)/2$	$(n-j+10ij-20ni-10jn-5j^2+35n^2)/2$
	$n+1 \le j \le 2n-1$	$(10ij-5i^2+10ni+i-5j^2+10jn+j-10n^2-2n)/2$	$(j-2n)(5j-10i+1)/2$
		$(i-2n)(5i-10j+1)/2$	$5(i-2n)(j-2n)$

Table 3 Partition of the vertex set based on the third neighborhood of vertices of SL_n

i	$\lvert N^3_{SL_n}(v_i)\rvert, v_i \in V_i$	$\lvert V_i\rvert$
1	9	24
2	12	$12(n-2)$
3	11	18
4	14	$12(n-2)$
5	16	$6(n-1)$
6	12	$6(n-1)$
7	18	$6n^2-12n+6$
8	22	$9n^2-21n+12$

By symmetry of G, we have

$$WW^*(G) = 3[WW^*(P) + WW^*(I)] \tag{8}$$

where

$$WW^*(P) = \sum_{i=1}^{2n-1}\sum_{j=i+1}^{2n-1}\Big[n_{11}(H_i, H_j)\, n_{22}(H_i, H_j) + n_{12}(H_i, H_j)\, n_{21}(H_i, H_j)\Big]$$

and

$$WW^*(I) = \sum_{i=1}^{2n-1}\sum_{j=1}^{2n-1}\Big[n_{11}(H_i, A_j)n_{22}(H_i, A_j) + n_{12}(H_i, A_j)n_{21}(H_i, A_j)\Big].$$

We split the proof into three cases: In the first two cases, we compute separately the quantities $WW^*(P)$ and $WW^*(I)$. Finally we compute the hyper-Wiener index by manipulating the computed results.

Case I: $WW^*(P)$

In this case, it is enough to calculate the two quantities $n_{11}(H_i, H_j)$ and $n_{22}(H_i, H_j)$ as shown in Fig. 3. For different values of i and j, the computed values of $n_{11}(H_i, H_j)$ and $n_{22}(H_i, H_j)$ are tabulated in Table 1. Using Table 1, we now compute the value of $WW^*(P)$ as follows.

$$\begin{aligned} WW^*(P) &= \sum_{i=1}^{2n-1}\sum_{j=i+1}^{2n-1} n_{11}(H_i, H_j)\, n_{22}(H_i, H_j) \\ &= \sum_{i=1}^{n}\left[\sum_{j=i+1}^{n-1} n_{11}(H_i, H_j)\, n_{22}(H_i, H_j) + \sum_{j=n}^{2n-1} n_{11}(H_i, H_j)\, n_{22}(H_i, H_j)\right] \end{aligned}$$

$$+\sum_{i=n+1}^{2n-1}\sum_{j=i+1}^{2n-1} n_{11}(H_i, H_j)\, n_{22}(H_i, H_j)$$
$$= \frac{n}{12}(n-1)(375n^4 + 26n^3 - 79n^2 - 22n + 2).$$

Case II: $WW^*(I)$

Now we turn our attention to the pair of vertex cuts that are intersecting each other as shown in Fig. 4. Here we consider all pair of cuts of the form (H_i, A_j) where H_i represents one of the horizontal vertex cuts of G and A_j denotes one of the acute vertex cuts of G. The computed values of the quantities $n_{rs}(H_i, A_j)$, $r, s = 1, 2$ are tabulated in Table 2. For convenience, let us denote $n_{rs}(H_i, A_j)$ $r, s = 1, 2$ as n_{rs}. With all the computed expressions, we now obtain $WW^*(I)$ as

$$\begin{aligned}
WW^*(I) &= \sum_{i=1}^{2n-1}\sum_{j=1}^{2n-1} n_{11}\, n_{22} + n_{12}\, n_{21} \\
&= \sum_{i=1}^{n}\left[\sum_{j=1}^{n} n_{11}\, n_{22} + n_{12}\, n_{21} + \sum_{j=n+1}^{n+i-1} n_{11}\, n_{22} + n_{12}\, n_{21} + \sum_{j=n+i}^{2n-1} n_{11}\, n_{22}\right] \\
&\quad + \sum_{i=n+1}^{2n-1}\left[\sum_{j=1}^{i-n} n_{11}\, n_{22} + \sum_{j=i-n+1}^{n} n_{11}\, n_{22} + n_{12}\, n_{21} + \sum_{j=n+1}^{2n-1} n_{11}\, n_{22} + n_{12}\, n_{21}\right] \\
&= \frac{n^2}{36}\left(1615n^4 - 15n^3 - 566n^2 - 75n + 85\right).
\end{aligned}$$

Case III: $WW(G)$

We now first compute the expression for $WW^*(G)$. By Eq. (8),

$$WW^*(G) = \frac{n}{12}\left(2740n^5 - 1062n^4 - 881n^3 + 96n^2 + 157n - 6\right).$$

Using Theorem 3, we compute the formula for the hyper-Wiener index as follows:

$$WW(G) = 2W(G) - \binom{|V(G)|}{2} + WW^*(G)$$
$$WW(SL_n) = \frac{n}{12}\left(2740n^5 + 3858n^4 + 1309n^3 - 228n^2 - 179n - 12\right).$$

□

5 Oxide networks

Oxide networks are obtained from the silicate networks by omitting the central vertex which means the silicon node as shown in Fig. 1. We denote the oxide network of dimension n as OX_n and the properties of this framework were studied in [3,6,50]. It has a total number of $9n^2 + 3n$ vertices and $18n^2$ edges. Using the similar proof lines of the previous section, we now compute the hyper-Wiener index of oxide framework as follows.

Theorem 5 *For an oxide network of dimension n,*

$$WW(OX_n) = \frac{n}{20}\left(1644n^5 + 2382n^4 + 1055n^3 + 60n^2 - 179n - 42\right).$$

Proof As in Theorem 4, considering the various types of pairs of elementary cuts, we have computed the expression for $WW^*(OX_n)$ as

$$\begin{aligned} WW^*(OX_n) &= 3\left[WW^*(P) + WW^*(I)\right] \\ &= \frac{n^2}{20}\left(1644n^4 - 570n^3 - 595n^2 + 121\right). \end{aligned}$$

The Wiener index of OX_n [3] is given as

$$W(OX_n) = \frac{3n}{10}\left(246n^4 + 205n^3 + 50n^2 - 25n - 6\right).$$

By using Theorem 3, the formula for the hyper-Wiener index of oxide network is given as

$$\begin{aligned} WW(OX_n) &= 2W(OX_n) - \binom{|V(G)|}{2} + WW^*(OX_n) \\ &= \frac{n}{20}\left(1644n^5 + 2382n^4 + 1055n^3 + 60n^2 - 179n - 42\right). \end{aligned}$$

□

6 Wiener polarity index of silicate and oxide networks

In this section, we compute the Wiener polarity indices of the silicate and oxide frameworks based on vertex neighborhood which is defined as follows: For any integer i, let $N_G^i(v)$ denote the ith neighborhood of a vertex v and symbolically

$$N_G^i(v) = \{u \in V(G) | d_G(u, v) = i\}.$$

The following lemma gives a simple general formula for computing W_p in terms of third neighborhood.

Lemma 1 [8] *For any graph G, the Wiener polarity index $W_p(G)$ can be expressed as,*

$$W_p(G) = \frac{1}{2}\sum_{v \in V(G)} |N_G^3(v)|.$$

Theorem 6 *For a silicate network of dimension n,*

$$W_p(SL_n) = 153n^2 - 99n - 3.$$

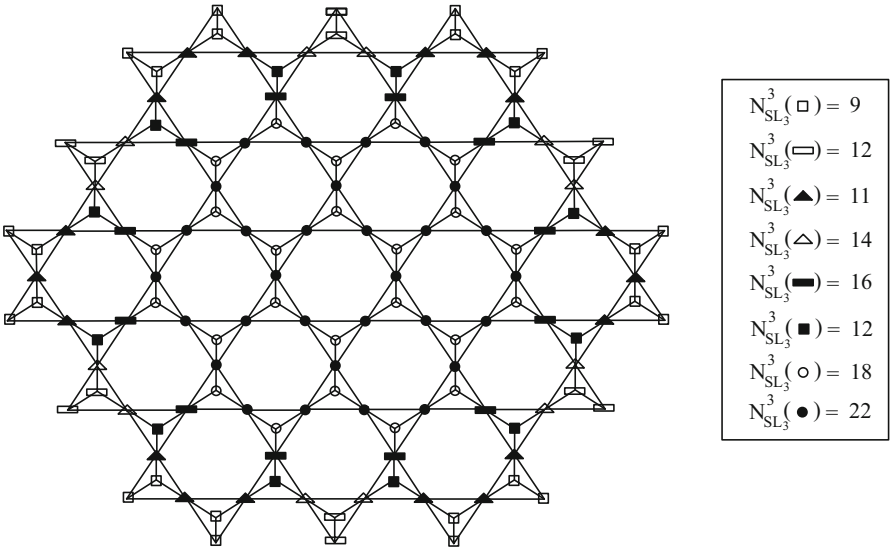

Fig. 5 Vertex partition of SL_3 based on third neighborhood $N^3_{SL_3}(v)$

Proof We first split the vertex set $V(SL_n)$ into eight disjoint sets based on $|N^3_{SL_n}(v)|$ as shown in Table 3 and Fig. 5. Using Lemma 1, we compute $W_p(SL_n)$ as follows.

$$\begin{aligned} W_p(SL_n) &= \frac{1}{2}\sum_{v\in V(SL_n)} |N^3_{SL_n}(v)| \\ &= \frac{1}{2}\sum_{i=1}^{8} |V_i||N^3_{SL_n}(v_i)| \\ &= 153n^2 - 99n - 3. \end{aligned}$$

□

Theorem 7 *For an oxide network of dimension n,*

$$W_p(OX_n) = 63n^2 - 39n - 3.$$

Proof In OX_n the vertex set is decomposed into six sets based on $|N^3_{OX_n}(v)|$ and are tabulated in Table 4. By Lemma 1, we have,

$$\begin{aligned} W_p(OX_n) &= \frac{1}{2}\sum_{v\in V(OX_n)} |N^3_{OX_n}(v)| \\ &= \frac{1}{2}\sum_{i=1}^{6} |V_i||N^3_{OX_n}(v_i)| \\ &= 63n^2 - 39n - 3. \end{aligned}$$

□

Table 4 Partition of the vertex set based on the third neighborhood of vertices of OX_n

i	$\lvert N^3_{OX_n}(v_i)\rvert$, $v_i \in V_i$	$\lvert V_i\rvert$
1	6	12
2	8	$6(n-2)$
3	7	18
4	9	$12(n-2)$
5	10	$6(n-1)$
6	14	$9n^2-21n+12$

7 Concluding remarks

In this paper, we have presented the vertex version formula for computing the hyper-Wiener index WW, and thereby calculated expressions for WW for two chemically significant metal organic frameworks. In earlier literature, this index has been studied only for a limited number of graphs, due to its complicated computing procedures, which in turn signifies the work of the present paper. Furthermore, we have computed the Wiener polarity index W_p of these complex chemical frameworks based on its chemical significance. Since we dealt with chemical graphs, the results obtained here will be of much use in QSAR/QSPR studies, as well as for analyzing properties of chemical compounds.

Acknowledgements M. Arockiaraj is supported by Project No. SB/FTP/MS-004/2014, Science and Engineering Research Board, New Delhi, India.

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