On certain topological indices of octahedral and icosahedral networks

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Abstract: The authors have computed topological indices of two metal–organic frameworks of considerable interest in reticular chemistry, namely octahedral and icosahedral networks. The topological indices of these metal–organic frameworks are extremely useful not only in the characterisation of these complex networks but also in obtaining correlation relationships of a number of their properties. In this study, they have obtained exact analytical expressions for a large number of topological indices such as the Randić index, Zagreb index, harmonic index, sum–connectivity index, atom–bond connectivity index, geometric–arithmetic index and their corresponding variants for the two newly constructed networks. Furthermore, they have used the recently introduced partition method by the transitive closure of Djoković–Winkler relation to obtain the Wiener indices for the chain and even cyclic octahedral and icosahedral frameworks with an observation that this method is not successful in computing the Wiener index of these two networks and they pose an open problem for the same.

1 Introduction

Topological indices of large chemical structures such as metal–organic frameworks can be extremely useful in both characterisation of structures and computing their physico–chemical properties that are otherwise difficult to compute for such large networks of importance in reticular chemistry. Synthesis of novel reticular metal–organic frameworks and networks in which covalent fibres are woven into crystals are becoming increasingly important in recent years [1, 2]. Topological indices numerically represent the structural characteristics of molecules that are obtained by the use of graph theoretical concepts applied to these large networks of interest in reticular chemistry. These descriptors play a significant role in the fields of control theory and mathematical chemistry, especially in the quantitative structure–activity relationships. The topological descriptors are of great importance, as they deal with topological characterisations of the molecules. In general, it acts like advanced models in the chemical and control field of applications and thereby play a vital role in controlling quantum phenomena which has been an implicit goal of much quantum physics and chemistry research. In addition, the mathematical techniques comprising of group theory and graph theory have found several applications to signal and image processing [5–8].

Topological indices are invariant to not only different labellings of the various atoms in the network but also to different displays of the networks that are topologically equivalent. These indices characterise the underlying connectivity relationships among the vertices and thus they are important structural invariants that correlate with both chemical reactivity and biological activity. Therefore, the topological analysis of a metal–organic framework comprised of transforming its underlying connectivity into a unique number that represents a descriptor of the metal–organic framework under consideration.

The concept of topological index originated from the pioneering work of Wiener [9] while he was attempting to find structural relationships to boiling points of paraffins. There are a large number of topological indices which are classified based on the structural properties of the graphs used for their calculations. In general, they are classified into distance-based topological indices, degree-based topological indices and counting related indices of graphs. These classes of topological indices are of great importance and play a vital role in chemical characterisation. A large number of degree-based indices have been proposed and the computation of these indices for various chemical networks is an active area of research in both chemical and mathematical literatures [9–25].

The Wiener index is the oldest and the most studied topological index, having a wide range of applications [10, 11]. Randić index [12] is one of the most widely used degree-based index for a number of chemical properties. It has been observed that there is a good correlation between the Randić index and several physico–chemical properties of alkanes such as boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapour pressure, surface areas and so on. Moreover, numerous applications of this index were reported, most of them dealt with medicinal and pharmacological applications of these indices. Zagreb indices [13] and Estrada’s atom–bond connectivity (ABC) indices [14] are yet another set of degree-based topological indices, which have reliable predicting power and thus they have been employed in deriving multi-linear regression models for statistical correlation of properties. The topological indices such as atom–bond connectivity and geometric–arithmetic are also used to predict the bio-activity of the chemical compounds [15]. Comparative studies of the chemical applicability of these indices were recently reported in [16, 17]. Consequently, generation of a varied set of topological indices can be extremely useful as such indices constitute a variable platform for correlating with different properties for which a single index approach may not be the most suitable. Thus in the current study, we have obtained exact analytical expressions for a large number of topological indices of both networks comprised of octahedra and icosahedra for the first time, and we anticipate these indices provide significant contribution to control problems in network science and also play a major role in the fields of reticular chemistry.

2 Mathematical preliminaries

Let \( G \) be a simple and connected graph with vertex set \( V(G) \) and edge set \( E(G) \). The distance between two vertices \( u \) and \( v \) of a graph \( G \), denoted by \( d_G(u, v) \), is the number of edges in the shortest
A network is simply a connected graph having no multiple edges.

A vertex-weighted graph \( (G,w) \) is a graph \( G \) together with the weight function \( w: V(G) \rightarrow \mathbb{R}^+ \). The Wiener index of a vertex-weighted graph \( W(G,w) \) is defined [23] as

\[
W(G,w) = \sum_{u,v \in V(G)} w(u)w(v)d_G(u,v)
\]

It is obvious that when \( w(u) = 1 \) for all \( u \in V(G) \), \( W(G,w) \) reduces to \( W(G) \). The Djkovik-Winkler relation \( \Theta \) is defined as follows: two edges \( a = xy \) and \( b = uv \) of a graph \( G \) are said to be \( \Theta \) related if \( d(x,y) + d(y,v) \neq d(x,v) + d(y,u) \). This relation \( \Theta \) is reflexive and symmetric but not transitive, in general, and hence its transitive closure \( \Theta^* \) is an equivalence relation. The \( \Theta^* \) relation induces a \( \Theta^* \) partition, which decomposes the edge set \( E(G) \) into \( \Theta^* \) classes. A partition \( \Psi = \{E_1, E_2, \ldots, E_k\} \) is said to be coarser than \( \Theta^* \) partition if each set \( E_i \) is the union of one or more \( \Theta^* \) classes of \( G \).

**Theorem 1 [10]:** Let \( (G,w) \) be a connected, weighted graph and let \( \Psi = \{E_1, E_2, \ldots, E_k\} \) be a partition of \( E(G) \) coarser than the \( \Theta^* \) partition. Then

\[
W(G,w) = \sum_{i=1}^{k} W(G/E_i, w_i)
\]

where \( w_i: V(G/E_i) \rightarrow \mathbb{R}^+ \) is defined by \( w_i(C) = \sum_{x \in E} w(x) \), for all connected components \( C \) of \( G/E_i \).

The rest of this paper is organised as follows: using \( \Theta \)-partition technique, we compute the Wiener indices for chain and even cyclic octahedral frameworks in Section 3 and we compute the same for chain and even cyclic isocahedra frameworks in Section 4. We introduce two types of chemical networks based on octahedra and isocahedra in Sections 5 and 6, respectively, and discuss a large number of topological indices for both the networks. Finally, we conclude the study in Section 7.

### 3 Chain and cyclic octahedral frameworks

An octahedron graph shown in Fig. 1 is a polyhedral graph corresponding to the skeleton of a Platonic solid. This Platonic graph consists of 6 vertices and 12 edges. The analogues of this structure play a vital role in the fields of reticular chemistry, which deals with the synthesis and properties of metal–organic frameworks [26, 27]. The different types of octahedral structures arise from the ways these octahedra can be connected.

A chain octahedral structure of dimension \( n \) denoted as \( \text{CHO}_n \) is obtained by arranging \( n \) octahedra linearly as shown in Fig. 2. The number of vertices and edges of \( \text{CHO}_n \) are \( 5n+1 \) and \( 12n \), respectively. We compute the exact formula for the Wiener index of chain octahedral structure as follows.

**Theorem 2:** Let \( G \) denote the chain octahedral structure \( \text{CHO}_n \), \( n \geq 1 \). Then

\[
W(G) = n(25n^2 + 105n - 22)/6.
\]

**Proof:** Let \( \{E_1, 1 \leq i \leq n\} \) be the \( \Theta^* \) partition of the edge set \( E(G) \), where each \( E_i \) comprises of edges of the \( i \)th octahedron of \( G \). The decomposed graph for each \( \Theta^* \) class and its corresponding weighted quotient graph are shown in Fig. 3.

For each \( E_i \), the weighted quotient graph \( (G/E_i, w) \) is the same for all \( i \) except the fact that the weights of the two vertices at the bottom of the octahedron. Let \( w(a_i) \) and \( w(b_i) \) be the weights of the two vertices at the bottom of the octahedron in \( (G/E_i, w) \). It is to be noted that the weights of all other vertices are the same and is equal to 1 in \( (G/E_i, w) \) as shown in Fig. 3b. For each \( E_i \), we have

![Fig. 1 Structure of an octahedron](image1)

![Fig. 2 Chain octahedral structure CHOₙ](image2)
The Wiener index of the weighted quotient graph \( W(G) \) is given as

\[
W(G) = \sum_{i=1}^{n} W(G/E_i, w)
\]

\[
= \sum_{i=1}^{n} \{w(a_i)w(b_i) + 5(w(a_i) + w(b_i)) + 7\}
\]

\[
= n(25n^2 + 105n - 22)/6.
\]

\[\square\]

The cyclic octahedral structure of dimension \( n \) is denoted by \( CYO_n \), is obtained by arranging \( n \) octahedra in cyclic order, as shown in Fig. 4. For \( n \geq 3 \), \( CYO_n \) consists of \( 5n \) number of vertices and \( 12n \) number of edges.

**Theorem 3:** Let \( G \) denote the cyclic octahedral structure \( CYO_n \), \( n \geq 4 \) and \( n \) is even. Then

\[
W(G) = n(25n^2 + 120n - 64)/8.
\]

**Proof:** Let \( \{E_i, 1 \leq i \leq n/2\} \) be the \( \Theta^\ast \) partition of the edge set \( E(G) \). Here, each \( E_i \) comprises of edges of diametrically opposite pairs of octahedra. The decomposed graph for each \( \Theta^\ast \) class and its corresponding weighted quotient graph \( (G/E_i, w) \) are shown in Fig. 5. For each \( E_i \), the weighted quotient graph \( (G/E_i, w) \) is the same for all \( i \) including the weights of all the vertices due to symmetry. Except the central two vertices, all other vertices have equal weight as 1 in \( (G/E_i, w) \) as shown in Fig. 5. The two central vertices have the same weight as \((5n-8)/2\).

For \( 1 \leq i \leq n/2 \), \( W(G/E_i, w) = i^2 + 20i + 48 \) where \( i = (5n-8)/2 \).

By Theorem 1, we have

\[
W(G) = \sum_{i=1}^{n/2} W(G/E_i, w) = n(25n^2 + 120n - 64)/8. \square
\]

It is to be noted that for odd-dimensional cyclic structures, the \( \Theta^\ast \)-partition technique contains exactly one \( \Theta^\ast \) class as the entire edge set. Hence, this technique does not work for odd dimension because the quotient graph is the original graph.

### 4 Chain and cyclic icosahedral frameworks

An icosahedron graph is also a Platonic graph, having 12 vertices and 30 edges as shown in Fig. 6. The analogues of the frameworks considered here are also the backbones of recent materials of reticular chemistry [1, 2, 28]. We obtain the Wiener indices of chain and cyclic icosahedral frameworks in a similar way to that of octahedral frameworks. The chain icosahedral framework of dimension \( n \) is denoted by \( CHI_n \) and is shown in Fig. 7. It has \( 11n + 1 \) number of vertices and 30n number of edges.

**Theorem 4:** Let \( G \) denote the chain icosahedral structure \( CHI_n \), \( n \geq 1 \). Then

\[
W(G) = n(121n^2 + 825n - 298)/6.
\]

**Proof:** Let \( \{E_i, 1 \leq i \leq n\} \) be the \( \Theta^\ast \) partition of the edge set \( E(G) \) where each \( E_i \) comprises of edges of the \( i \)th icosahedron of \( CHI_n \), as shown in Fig. 8.

Following the proof lines of Theorem 2, we have:

\[
w(a_i) = 11(i - 1) + 1
\]

\[
w(b_i) = 11(n - i) + 1
\]

The Wiener index of the weighted quotient graph \( (G/E_i, w) \), \( 1 \leq i \leq n \), is computed as

\[
W(G/E_i, w) = w(a_i)w(b_i) + 17(w(a_i) + w(b_i)) + 73
\]

Using Theorem 1, we arrive that
Let \( \Theta \) denote the cyclic icosahedral structure CYI, \( n \geq 4 \) and \( n \) is even. Then

\[
W(G) = n(121n^2 + 1056n - 544)/8.
\]

**Proof:** Let \( \{E_i, 1 \leq i \leq n/2\} \) be the \( \Theta \) partition of the edge set \( E(G) \). In this case, each \( E_i \) consists of edges of diametrically opposite pairs of icosahedra. In Fig. 9, we have shown the decomposed graph for each \( \Theta \) class and its corresponding weighted quotient graph.

Similar to the proof lines of Theorem 3, we have \( \sum \) (11n - 20)/2. The Wiener index of the weighted quotient graph \( (G/E_i, w) \), \( 1 \leq i \leq n/2 \), is obtained as

\[
W(G/E_i, w) = i^2 + 68t + 444.
\]

By Theorem 1, we get

\[
W(G) = \sum_{i=1}^{n/2} W(G/E_i, w) = n(121n^2 + 1056n - 544)/8. \quad \Box
\]

## 5 Octahedral networks

An octahedral sheet-like structure is a ring of octahedral structures, which are linked to other rings by sharing corner vertices in a two-dimensional plane. An octahedral network of dimension \( n \) is denoted by \( OT_n \), where \( n \) is the order of circumscribing, as shown in Fig. 10.

Number of vertices and edges in \( OT_n \) with \( n \geq 1 \) are \( 27n^2 + 3n \) and \( 72n^2 \), respectively. We study the degree-based topological indices such as Randić index, Zagreb index, atom–bond connectivity index, geometric–arithmetic index and their corresponding variants, harmonic and sum–connectivity indices for the octahedral network as follows.

**Theorem 6:** Let \( G \) be the octahedral network \( OT_n \), \( n \geq 2 \). Then

1. \( R_d(G) = 18n(16\alpha^2 + 32\beta^2 + 64^\alpha) + 12n(16^\alpha - 64^\beta) \)
2. \( R(G) = 3n(9n + 6\sqrt{2n} + 2)/4 \)
3. \( R_{\alpha, \beta}(G) = 9n(9n + 2)/32 \)
4. \( RR(G) = 24n(9n + 6\sqrt{2n} - 2) \)
5. \( RR(R) = 12n(15n + 3\sqrt{27n} - 4) \)
6. \( M_1(G) = 96n(9n - 1) \)
7. \( M_2(G) = 288n(9n - 2) \)
8. \( NK(G) = e^{\alpha+3\alpha} \)
9. \( \alpha(G) = 2e^{12\alpha^2 + 6\alpha} \)
10. \( \alpha(G) = 2e^{12\alpha^2 - 2e^{12\alpha^2}} \)
11. \( \alpha(G) = e^{12\alpha^2 - 2e^{12\alpha^2}} \)
12. \( \alpha(G) = 120n(15n - 4) \)
13. \( HM(G) = 576n(9n - 4) \)
14. \( AZ(G) = 1024n(1221153n - 346250)/385875 \)
15. \( ABC(G) = \) \( (((9\sqrt{6})^2 + (9\sqrt{14}/4 + 9\sqrt{5}))/4 \)
16. \( H(G) = 3n(17n + 2)/4 \)
17. \( SC(G) = 3n(3n + 3\sqrt{2n} + 4\sqrt{3n} + 2\sqrt{2} + 2)/2 \)
18. \( GA(G) = 12n(2\sqrt{2} + 3) \)

**Proof:** The octahedral network \( OT_n \) has \( 18n^2 + 6n \) vertices of degree 4 and \( 9n^2 - 3n \) vertices of degree 8. The edge set of \( OT_n \) is partitioned into three sets based on the degrees of end vertices of each edge as given in Table 2. By simplification we get the required proof. \( \Box \)
Table 3  Edge set partition of the octahedral networks based on end-vertex degree sum neighbours of edges

| l  | (S_v, S_e), where (u, v) ∈ E(G) | Number of edges | |E_i(G)| |
|---|---|---|---|
| 1 | (20, 20) | 6n |
| 2 | (20, 24) | 24n |
| 3 | (20, 40) | 12 |
| 4 | (20, 44) | 12(n - 1) |
| 5 | (24, 24) | 18(n - 1) |
| 6 | (24, 40) | 24 |
| 7 | (24, 44) | 48(n - 1) |
| 8 | (24, 48) | 36n^2 - 60n + 24 |
| 9 | (40, 44) | 12 |
| 10 | (44, 48) | 12n - 18 |
| 11 | (44, 44) | 12n - 18 |
| 12 | (48, 48) | 18(n - 1)^2 |

Table 11  Icosahedral network IS

Theorem 7: Let G be the octahedral network OT_n, n ≥ 2. Then

(i) ABC_i(G) = \frac{3}{4} \left( \frac{47}{\sqrt{2}} - \frac{3}{5} \right) - 12 + \frac{186}{\sqrt{3}} - \frac{9}{11} \frac{43}{\sqrt{2}}
+ \sqrt{35} + \frac{3}{2} \frac{29}{5} + \sqrt{5} \frac{41}{\sqrt{2}} - 3 \frac{15}{22}
+ \frac{19}{5} \frac{3}{2} \frac{7}{7} + 3 \frac{37}{4} \frac{7}{2} + \frac{3}{2} \frac{73}{5} + 3 \frac{62}{55} + 3 \frac{86}{41}
+ \sqrt{22} + 5 \frac{3}{2} \frac{12}{2} + 12)n + \left( \frac{3}{4} \frac{47}{\sqrt{2}} + \frac{3}{2} \frac{47}{\sqrt{2}} + 3 \frac{23}{2} \right)^2.

(ii) GA_i(G) = (36 + 24\sqrt{2})n^2 + \left( \frac{3}{5} \frac{35}{2} + \frac{48}{5} \frac{30}{11} + \frac{96}{66} \frac{66}{17} \right)
+ \frac{48}{5} \frac{33}{23} - 40\sqrt{2} - 36)n + \frac{3}{5} \frac{45}{2} + 6\sqrt{15}
+ \sqrt{110} - 96n\frac{66}{17} - 48\frac{33}{23} + 24\sqrt{2}.

Proof: The edge set of OT_n is partitioned into 12 sets E_i(OT_n), 1 ≤ i ≤ 12, based on the degree sum of the neighbours of end vertices of each edge, as given in Table 3. The proof follows from Table 3 by simplification. □

6  Icosahedral networks

In this section, we introduce another new network based on icosahedron. Icosahedral network is obtained from the octahedral network by replacing all the octahedra with the icosahedral. An n-dimensional icosahedral network is denoted by IS_n is shown in Fig. 11.

It has 63n^2 + 3n number of vertices and 180n^2 number of edges. We discuss the degree-based indices of this network as follows.

Theorem 8: Let G be the icosahedral network IS_n, n ≥ 2. Then

(i) \( R_s(G) = 18n(25\sqrt{5}(6) + 50\sqrt{3}(3) + 100\sqrt{5})(3) - 50^{\sqrt{5}} - 100(22) \),

(ii) \( R_s(G) = 3n(39n + 9\sqrt{2}n - \sqrt{2} + 4)/5, \)

(iii) \( R_s(G) = 3n(93n + 8)/50, \)

(iv) \( R_s(G) = 30n(24n + 9\sqrt{2}n - \sqrt{5} - 1), \)

(v) \( R_s(G) = 18n(51n - 4), \)

(vi) \( M_2(G) = 150(n(15n - 1), \)

(vii) \( M_2(G) = 150n(48n - 7), \)

(viii) \( NK(G) = 2^{30} - 3n \cdot 2^{9}n^{2}, \)

(ix) \( x_n(G) = 2^{3}n - m \cdot 2^{2}n^{2}, \)

(x) \( x_n(G) = 2^{5} - 3n \cdot 2^{3}n^{2}, \)

(x) \( x_n(G) = 2^{5} - 3n \cdot 2^{3}n^{2}, \)

(xii) \( R_s(G) = 90n(57n - 10), \)

(xiii) \( HM(G) = 150(m(201n - 29), \)

(xiv) \( AZ(G) = 15625n(82, 699, 620n - 16, 178, 969)/136, 670, 976, \)

(xv) \( ABC(G) = 3\frac{28n(81n + 9\sqrt{13n - \sqrt{3}} + 6)}/5, \)

(xvi) \( H(G) = n(153n + 8)/5 \) and

(xvii) \( GA(G) = 2n(63n + 18\sqrt{2}n - 2\sqrt{2} + 3), \)

(xviii) \( SC(G) = 9n\sqrt{9n + 54\sqrt{10}n + 18\sqrt{15n - 6\sqrt{5}}, \}

+ 9\sqrt{10} - 2\sqrt{15}/5 \)

(xix) \( ABC(G) = \left( 6 \frac{318}{5} + 18\sqrt{6}/5 + 72\sqrt{3}/5 + 18\sqrt{5}/35 \right) \)

\( + \frac{3}{5} \frac{42^2}{4} + 18\sqrt{206}/35 + 9\sqrt{13}/35 \)^2,

\( + \frac{2}{5} \frac{48}{5} + 2\frac{3}{5} \frac{318}{5} - 4\sqrt{2} + 48\sqrt{3}/25 + 6\sqrt{6}/5 - 6\sqrt{5}/35 \)

\( + 18\sqrt{2} \frac{62}{5} + 48\sqrt{14}/14 + 6\sqrt{206}/65 + 96\sqrt{5}/11 \)

\( + \frac{6}{5} \frac{38}{35} - \frac{18\sqrt{138}}{35} \) \( + \frac{2}{5}\sqrt{2} \frac{42}{5} + 8\sqrt{11} \)

\( + 12\frac{31}{5} + 12\sqrt{206}/35 - 18\sqrt{6}/5 + 48\sqrt{14}/13 \)

\( + \frac{9\sqrt{138}}{35} + 6\frac{41}{13} + 6\frac{38}{13} - 144\sqrt{2}/25 \).

(xx) \( GA(G) = \left( 72\frac{242}{13} + 3\sqrt{35} + 72\frac{30}{11} + 18\sqrt{21}/5 + 24\sqrt{5} \)

+ 36n^2 + \left( \frac{24}{5} \frac{30}{11} - 24\sqrt{47}/13 - \sqrt{35} + 24\sqrt{6}/5 \right)

\( + 72\frac{375}{19} + 8\sqrt{182}/9 - 6\sqrt{21} - 40\sqrt{2})n - 24\sqrt{5}/5 \)

\( + 32\sqrt{5} + 708\sqrt{21}/95 + 72\sqrt{375}/19 + 8\sqrt{182}/9 + 48\sqrt{39}/25 \).

Proof: The icosahedral network IS_n has 54n^2 + 6n vertices of degree 5 and 9n^2 - 3n vertices of degree 10. The edge set of IS_n is partitioned into three sets as in Table 4 based on the degrees of end
Table 4  Edge set partition of the icosahedral networks based on end-vertex degree of edges

<table>
<thead>
<tr>
<th>(d_i, d_j), where u ∈ E(G)</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5, 5)</td>
<td>108n^2 + 18n</td>
</tr>
<tr>
<td>(5, 10)</td>
<td>54n^2 - 6n</td>
</tr>
<tr>
<td>(10, 10)</td>
<td>18n^2 - 12n</td>
</tr>
</tbody>
</table>

Table 5  Edge set partition of the icosahedral networks based on end-vertex degree sum neighbors of edges

| l   | (S_i, S_j), where u ∈ E(G) | Number of edges | |E|(G) |
|-----|-----------------------------|-----------------|------|
| 1   | (25, 35)                    | 18n^2 - 6n      |      |
| 2   | (25, 30)                    | 36n^2 + 12n     |      |
| 3   | (25, 25)                    | 18n^2 + 12n     |      |
| 4   | (30, 35)                    | 36n^2 - 12n     |      |
| 5   | (30, 30)                    | 12n             |      |
| 6   | (30, 60)                    | 24              |      |
| 7   | (30, 65)                    | 36(n - 1)       |      |
| 8   | (30, 70)                    | 18n^2 - 30n + 12|      |
| 9   | (35, 65)                    | 48(n - 1)       |      |
| 10  | (35, 60)                    | 24              |      |
| 11  | (35, 70)                    | 36n^2 - 60n + 24|      |
| 12  | (60, 65)                    | 12              |      |
| 13  | (65, 65)                    | 12n - 18        |      |
| 14  | (65, 70)                    | 12(n - 1)       |      |
| 15  | (70, 70)                    | 18(n - 1)^2     |      |

vertices of each edge and the same is partitioned into 15 sets as in Table 5 based on the degree sum of the neighbours of end vertices of each edge. The proof is similar to Theorems 6 and 7.

7 Concluding remarks

In this paper, we have designed two interesting chemical frameworks and the analytical closed formulae of degree-based indices for these networks were manifested, which will help the researchers working in network science and control problems to understand and explore the underlying topologies of these frameworks. It provides partial controlling methods in the area of modifying and upgrading the chemical and physical targets, and thereby helps in analysing the significant properties of the given networks.

We have also computed the Wiener index for cyclic octahedral as well as icosahedral structures which help in finding out the Wiener indices of the octahedral and icosahedral tube structures, using the formula for Cartesian product of graphs [25]. On the other side, when we apply the Θ’ partition for the octahedral and icosahedral networks, it is possible to find the weighted quotient graphs. However, computing the Wiener index of weighted quotient graphs is not that much efficient which requires a new method for computing the same. For instance, the weighted quotient graphs for octahedral network of dimension two are shown in Fig. 12. There are totally four Θ’ classes, indeed for any dimension, out of which three of them are isomorphic to Fig. 12h. Computing the Wiener indices of these quotient graphs will not be efficient when n is large.

8 References