Transmission in H-Naphtalenic Nanosheet

Jane Olive Sharon [1]   T.M. Rajalaxmi [2,*]   Sandi Klavžar [3,4,5]
R. Sundara Rajan [6]   Indra Rajasingh [7]

[1]Department of Computer Science, Sri Sivasubramaniya Nadar College of Engineering,
Chennai 603 110, India
janeolivesharon@gmail.com

[2] Department of Mathematics, Sri Sivasubramaniya Nadar College of Engineering,
Chennai
603 110, India
laxmi.raji18@gmail.com

[3] Faculty of Mathematics and Physics, University of Ljubljana, Slovenia
[4] Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia
[5] Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia
sandi.klavzar@fmf.uni-lj.si

[6] Department of Mathematics, Hindustan Institute of Technology and Science, Padur,
Chennai 603 103, India
vprsundar@gmail.com

[7] School of Advanced Sciences, Vellore Institute of Technology, Chennai, India, 600 127
indrarajasingh@yahoo.com

Abstract

In network analysis, centrality measures identify the most important vertices within a graph. In a connected graph, the transmission of a vertex u is the sum of the lengths of the shortest paths between the node and all other nodes in the graph. In this paper, we discuss a method to uniquely identify a vertex in a plane nanosheet. Using this approach, we compute the transmission of every vertex in H-naphtalenic nanosheets.

Keywords: vertex transmission; nano-network; H-naphtalenic nonosheet; coordinatization; edge cut

AMS Subj. Class. (2020): 05C09, 05C12, 05C92

---

[*] To whom correspondence should be addressed.

1   Introduction

The advent of social networks, big data, and e-commerce has emphasized the importance of analyzing a unique type of data structure called a graph or a network, which depicts relationships among its entities. In network analysis, centrality measures identify the most important vertices within a graph. Applications include identifying the most influential person in a social network, key infrastructure nodes in the internet or urban networks, and super-spreaders of a disease [9].

The transmission of a vertex u in a graph G, also called the total distance, farness, and the vertex Wiener value in the literature, is the sum of the lengths of shortest paths between u and all other vertices in G [1, 18, 24, 27, 31, 26, 34]. Using transmission, the celebrated Wiener index can be described as one half of the sum of the transmissions of its vertices. Moreover, the Wiener complexity is defined as the number of different transmissions of its vertices, [2, 3, 17].

The transmission is also closely related to other topological indices [32], describes median vertices, and characterizes the distance-balanced property and the opportunity index, see [7, 10]. In a connected graph, closeness centrality of a node is a measure of centrality, calculated as the reciprocal of the sum of the lengths of the shortest paths between the node and all other nodes in the graph. Graphs in which all its vertices have pairwise different transmissions are called transmission irregular graphs [3]. This class of graphs received a lot of attention, see [4, 14, 15, 16].

A nano-network is a set of inter-connected nanomachines, which are able to perform simple tasks such as computing, data storing, sensing and actuation. Two-dimensional nanosheets have shown great potential for separation applications because of their exceptional molecular transport properties. Nanosheet materials such as graphene oxides, metal-organic frameworks, and covalent organic frameworks display unique, precise, and fast molecular transport through nanopores and nanochannels [21].

Among two-dimensional nanosheets, naphtalenic nanosheets play an important role, cf. [29] and references therein. In this paper we are interested in the H-naphtalenic nanosheets, whose mathematical properties have been earlier studied in [6, 19, 20]. Here we compute the transmission of every vertex in a H-naphtalenic nanosheet and proceed as follows. In the next section we give necessary definitions, discuss a general framework for coordinatizations of graph vertices, and introduce the two-parametric family $HN(m,n)$ of H-naphtalenic nanosheets. In Section 3 we make a closer look to the structure of these nanosheets and prove a couple of preliminary counting results. In Section 4 we define a coordinatization of H-naphtalenic nanosheets and, using it, derive expressions for the transmission of each of its vertices.

2 Preliminaries

If $G = (V(G), E(G))$ is a graph, then the usual shortest-path distance between vertices $u, v \in V(G)$ is denoted by $d(u, v)$. The *transmission* $T(u)$ of $u \in V(G)$ is defined as $T(u) = \Sigma_{v \in V(G)} d(u, v)$. A subgraph H of G is *convex* if given any two vertices u and v in H, every (u, v)-shortest path in G lies lies entirely in H. A *convex cut* of G is a set of edges $F \subseteq E(G)$ such that $G - F$ consists of two components, each of them being a convex subgraph of G. If a partition of the edge set of G is such that every member of the partition is convex, then we speak of a *convex edge partition* of G.

If a graph G admits a convex edge partition, then it can be used to determine distance based topological indices of G. The seminal paper on this important approach [23] led to wide developments. The progress up to 2015 is surveyed in [25], to check the up-to-date investigations the reader can start with [28, 33] and references therein.

A weaker version of the convex edge partition was introduced in [31] as follows. Let G be a graph and $u \in V(G)$. Then a partition $\{S_1, \ldots, S_k\}$ of $E(G)$ into edge cuts S_i, $i \in [k] = \{1, \ldots, k\}$, is a *u-transmission partition* if for every i, every shortest path from u to any other vertex passes through at most one edge of S_i. In our computations of the transmission of H-naphtalenic nanosheets, the following result from [31] will be useful.

Theorem 2.1. (Transmission Lemma) *Let G be a graph, $u \in V(G)$, and let $\{S_1, \ldots, S_k\}$ be a u-transmission partition. If G_i, $i \in [k]$, is the component of $G \backslash S_i$ which contains u, then $T(u) = \Sigma_{i=1}^{k}(|V(G)| - |V(G_i)|)$.*

2.1 Coordinatizations

In euclidean geometry, we fix the frames of references as the X-axis and the Y-axis and uniquely determine the location of any point in the plane with respect to these coordinate axes. Extending this idea, we define a k-tuple coordinate to every point in the plane of a nanosheet which uniquely determines the location of every vertex in the nanosheet. This will simplify the computation of transmission distances of vertices. Moreover, it can also aid us in computing certain centrality measures in social networks and distance based topological indices in chemical graphs. We next present a general frame for such coordinatizations.

Let G be a (connected) graph and let $\{F_1, \ldots, F_k\}$ be a partition of $E(G)$ into edge sets F_i, where F_i is a union of one or more edge cuts, satisfying the property that if $xy \in F_i$ then x and y lie in different components of $G - F_i$. Let j_i be the number of components of $G - F_i$. Labeling these components by the first j_i positive integers, we can define a mapping

$$\ell : V(G) \to [j_1] \times \cdots \times [j_k]$$

by setting $\ell(x) = (x_1, \ldots, x_k)$, where x_i is the component of $G - F_i$ in which u lies. Such a labeling is a *coordinatization*, if the function ℓ is injective. In a coordinatization, vertices of G thus receive unique labels.

3

There are several useful coordinatizations known from the literature. Hypercubes of dimension n and their (isometric) subgraphs can be naturally coordinatized by binary n-tuples, which was in [13] used for the first time to compute the Wiener index of partial cubes without computing the distances between pairs of vertices. Using coordinatization with three coordinates, the Wiener index of benzenoid systems can be computed in linear time [12, 23]. For a general framework where coordinatizations with respect to canonical metric representations are used see [22]. In this paper we introduce a coordinatization of H-naphtalenic nanosheets and demonstrate how to use it to compute the transmissions of of its vertices.

2.2 H-naphtalenic nanosheets

Metal Organic Framework (MOF) nanosheets are being used extensively due to their mechanical flexibility and optical transparency. Its edges can be partitioned into obtuse and acute cuts, see Fig. 1(a). Whereas the edge set of the triangular benzenoid nanosheet can be partitioned into horizontal, acute and obtuse cuts, see Fig. 1(b). As a further example consider a Type II C_4 C_8 (R) nanosheet, which is a trivalent decoration made by alternating squares C_4 and octagons C_8, its edge set can be partitioned into horizontal, vertical, acute, and obtuse cuts, see Fig. 1(c).

We define a subgraph induced by the set of vertices between two consecutive cuts of the same type α as an α-channel, where α may be horizontal, vertical, acute or obtuse. Any vertex v in the nanosheet, is assigned the coordinate tuple whose first entry i represents the ith horizontal-channel, the second entry j represents the jth vertical-channel, the third entry k represents the kth acute-channel, and the fourth entry l represents the lth obtuse-channel in which v lies. This uniquely determines the location of v in the nanosheet.

The H-naphtalenic nanosheet $HN(m,n)$ is constructed with the basic block B of two hexagons sharing an edge. $HN(m,n)$ has m row-blocks, each row-block comprising of n number of B-blocks bound sequentially by two horizontal edges called column-binding edges between two B-blocks and n column-blocks, each column-block comprising of m number of B-blocks bound sequentially by vertical edges called row-binding edges as shown in Fig. 2(a). $HN(m,n)$ has $10mn$ vertices and $15mn - 2m - 2n$ edges.

3 Channels in $HN(m,n)$

We now proceed to give a partition of the edge set of $HN(m,n)$ as follows:

- horizontal cuts $H_1, \ldots, H_{2m-1}$ as in Fig. 2(a).

- vertical cuts $C_1, \ldots, C_{n-1}$ as in Fig. 2(a).

- acute cuts $A_1, \ldots, A_{m+2n-1}$ as in Fig. 2(b).

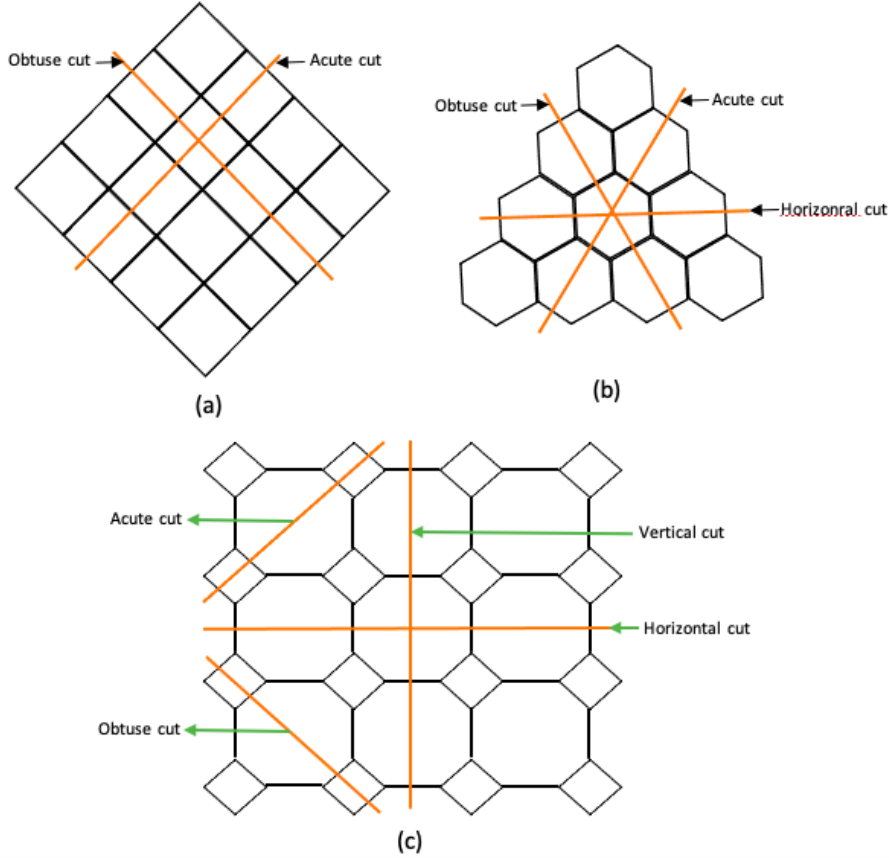- obtuse cuts $O_1, \ldots, O_{m+2n-1}$ as in Fig. 2(a).

Figure 1: a) Metal Organic Framework, b) Triangular benzenoid, c) Type II $C_4C_8(R)$ - $T^2[p,q]$

We note that $\{A_1, \ldots, A_{m+2n-1}, O_1, \ldots, O_{m+2n-1}, H_1, \ldots, H_{2m-1}, C_1, \ldots, C_{n-1}\}$ is an edge partition of $HN(m,n)$, such that each set is an edge cut whose removal partitions $HN(m,n)$ into two components and for any vertex u in $HN(m,n)$, the condition of the Transmission Lemma is satisfied.

We define channels arising out of acute cuts, denoted by a-channel as follows. The acute cut A_1 partitions $HN(m,n)$ into two components with one of the components inducing a path of length 2. We call this subgraph a-channel 1. The subgraph induced by vertices that fall between cuts A_{k-1} and A_k is called a-channel k, $2 \leq k \leq m + 2n - 1$. The acute cut A_{m+2n-1} partitions $HN(m,n)$ into two components with one of the components inducing a path of length 2, which we call a-channel $(m + 2n)$. We note that a-channel k and a-channel $(m + 2n - (k - 1))$ are isomorphic for $k \in [[\lceil \frac{m+2n}{2} \rceil]]$. Similarly, we define channels arising out of obtuse cuts and call then o-channel l, $l \in [m + 2n]$.

Lemma 3.1. *In $HN(m,n)$, let s_k^a be the number of vertices in a-channel k, $k \in [[\lceil \frac{m+2n}{2} \rceil]]$.*
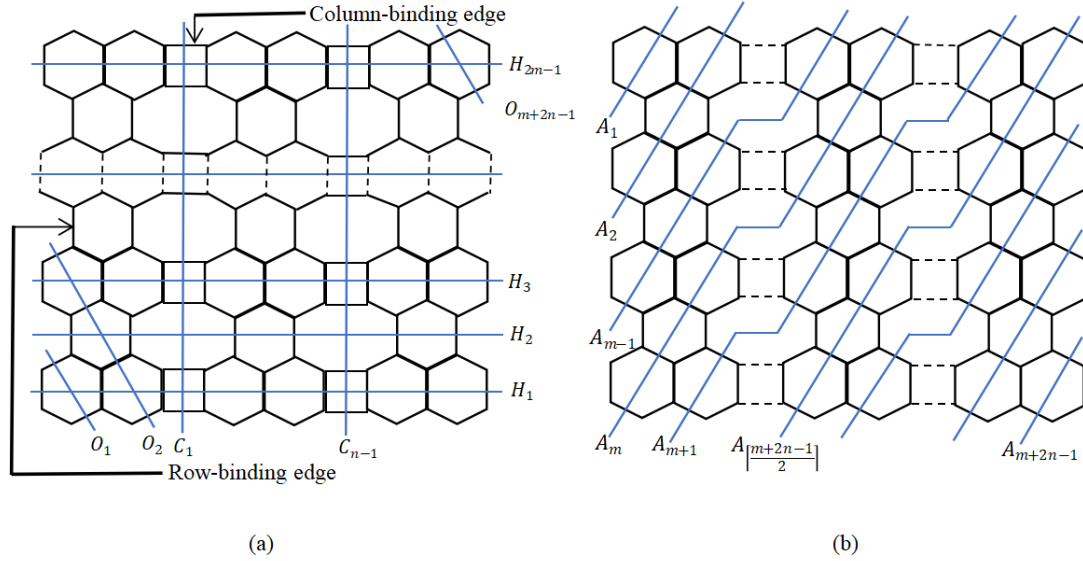
5

Figure 2: (a) Horizontal, vertical and obtuse cuts (b) Acute cuts

If $k \in [m]$, then

$$s_k^a = \begin{cases} 5k - 2; & k \text{ odd,} \\ 5k - 3; & k \text{ even,} \end{cases}$$

and if $m + 1 \le k \le \lceil \frac{m+2n}{2} \rceil$, then

$$s_k^a = \begin{cases} 5m; & m \text{ even,} \\ 5m - 1; & m \text{ odd, } k \text{ even,} \\ 5m + 1; & m \text{ odd, } k \text{ odd.} \end{cases}$$

Proof. For $k \in [m]$, the a-channel k contains k terms in the summation beginning with 3, followed by an alternating sequence of numbers 4 and 6. This readily gives

$$s_k^a = \begin{cases} 3 + \frac{k-1}{2}(4+6); & k \text{ odd,} \\ 3 + \frac{k-2}{2}(4+6) + 4; & k \text{ even.} \end{cases}$$

For $m + 1 \le k \le \lceil \frac{m+2n}{2} \rceil$, the a-channel k contains m terms in the summation with an alternating sequence of numbers 4 and 6, beginning with 4 if $k = m + j$, j odd; and beginning with 6 if $k = m + j$, j even. Therefore,

$$s_k^a = \begin{cases} \frac{m}{2} \times 10 = 5m; & m \text{ even,} \\ \frac{m-1}{2} \times 10 + 4 = 5m - 1; & m \text{ odd, } k \text{ even,} \\ \frac{m-1}{2} \times 10 + 6 = 5m + 1; & m \text{ odd, } k \text{ odd,} \end{cases}$$

6

and we are done. $\qquad\square$

Lemma 3.2. *In $HN(m,n)$, let $S_k^a = s_1^a + \cdots + s_k^a$, $k \in [\lceil \frac{m+2n}{2} \rceil]$. If $k \in [m]$, then*

$$S_k^a = \begin{cases} \frac{5k^2}{2}; & k \text{ even,} \\ \frac{5k^2}{2} + \frac{1}{2}; & k \text{ odd,} \end{cases}$$

and if $m + 1 \le k \le \lceil \frac{m+2n}{2} \rceil$, then

$$S_k^a = \begin{cases} 5mk - \frac{5m^2}{2}; & m \text{ even,} \\ 5mk - \frac{5m^2-1}{2}; & m \text{ odd, } k \text{ odd,} \\ 5mk - \frac{5m^2+1}{2}; & m \text{ odd, } k \text{ even.} \end{cases}$$

Proof. If $k \in [m]$ is even, then

$$S_k^a = 3 + (3+4) + (3+4+6) + \cdots + (3 + \frac{k-2}{2}(4+6) + 4) = \frac{5k^2}{2}$$

and if k is odd, then

$$S_k^a = 3 + (3+4) + (3+4+6) + \cdots + (3 + \frac{k-1}{2}(4+6)) = \frac{5k^2}{2} + \frac{1}{2}.$$

Let m be even. Then for $m + 1 \le k \le \lceil \frac{m+2n}{2} \rceil$, every a-channel k consists of $5m$ vertices and hence $s_k^a = \frac{5m^2}{2} + 5m(k-m) = 5mk - \frac{5m^2}{2}$.

Let m be odd. Then alternate a-channels beginning with a-channel $(m+1)$ consist of $5m - 1$ and $5m + 1$ vertices, respectively. For $m + 1 \le k \le \lceil \frac{m+2n}{2} \rceil$, k odd implies $(k - m)$ is even. Then $s_k^a = \frac{5m^2}{2} + \frac{1}{2} + 5m(k-m) = 5mk - (\frac{5m^2-1}{2})$. On the other hand, k even implies $(k-m)$ is odd. Then $s_k^a = \frac{5m^2}{2} + \frac{1}{2} + 5m(k-m-1) + (5m-1) = 5mk - (\frac{5m^2+1}{2})$. $\qquad\square$

4 Coordinatization of vertices in $HN(m,n)$ and their transmissions

A unique 4-tuple representation for any vertex u in $HN(m,n)$ helps to locate the position of u in the nanosheet. In order to achieve this representation, every row-block is split into 2 rows. The horizontal cut H_{2i-1} splits the ith row-block into two horizontal paths. The rows, the column-blocks, the a-channels and the o-channels determine the 4-tuple representation of any vertex in the nanosheet. In this way every vertex u of $HN(m,n)$ is uniquely represented as $u \equiv (i, j, k, l)$, where, i represents the row, j represents the column-block, k represents the a-channel, and l represents the o-channel in which u lies. See Fig. 3.

The following lemmas determine the contribution of the horizontal, vertical, acute and obtuse cuts to the transmission $T(u)$ of vertices u of $HN(m,n)$. If u is represented as (i, j, k, l), then the coordinates are from the ranges $i \in [2m]$, $j \in [n]$, and $k, l \in [m + 2n]$.
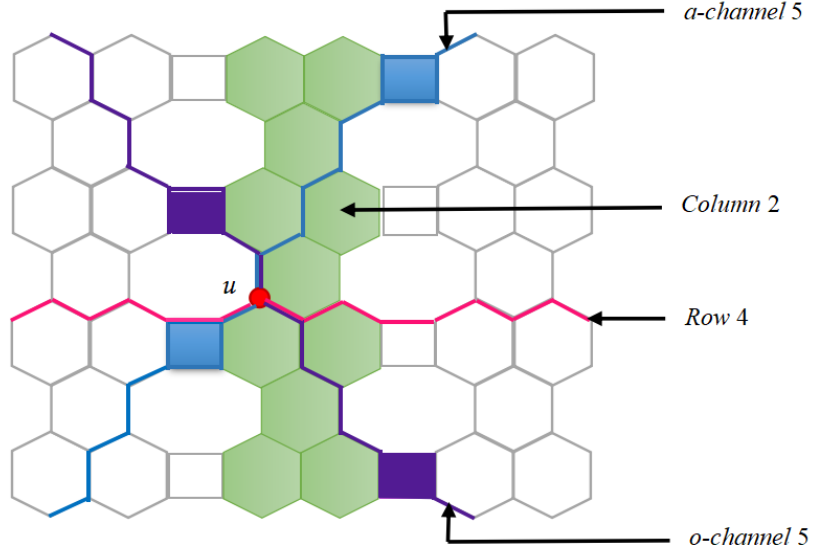
7

Figure 3: In $HN(4,3)$, $u \equiv (4,2,5,5)$

Lemma 4.1. *If $u \equiv (i,j,k,l)$ is a vertex of $HN(m,n)$, then the contribution to $T(u)$ by the horizontal cuts is given by*

$$T_h(u) = 5n(i^2 + (2m+1)(m-i)).$$

Proof. Each row in $HN(m,n)$ contains $5n$ vertices. Therefore, by the Transmission Lemma,

$$
\begin{aligned}
T_h(u) &= ((1 \times 5n) + (2 \times 5n) + \cdots + (i-1)5n) \\
&\quad + ((2m-i)5n + (2m-(i+1))5n + \cdots + (2m-(2m-1))5n) \\
&= 5n \left(\frac{(i-1)i}{2} + \frac{(2m-i)(2m-i+1)}{2} \right) \\
&= 5n(i^2 + (2m+1)(m-i)).
\end{aligned}
$$

$\square$

Lemma 4.2. *If $u \equiv (i,j,k,l)$ is a vertex of $HN(m,n)$, then the contribution to $T(u)$ by the vertical cuts is given by*

$$T_V(u) = 10m \left(\frac{n(n+1)}{2} + j(j-1-n) \right).$$

8

Proof. Each column-block in $HN(m,n)$ contains $10m$ vertices. Therefore, by the Transmission Lemma,

$$T_V(u) = ((1 \times 10m) + (2 \times 10m) + \cdots + (j-1)10m) + ((n-j)10m$$
$$+ (n-(j+1))10m + \cdots + (n-(n-1))10m)$$
$$= 10m\left(\frac{n(n+1)}{2} + j(j-1-n)\right).$$

$\square$

Lemma 4.3. *Let* $R_k^a = \Sigma_{i=1}^k S_i^a$, $k \in [\lceil \frac{m+2n}{2} \rceil]$. *If* $k \in [m]$, *then*

$$R_k^a = \begin{cases} \frac{5}{12}\ k\ (k+1)(2k+1) + \frac{k+1}{4}; & k\ odd, \\ \frac{5}{12}\ k\ (k+1)(2k+1) + \frac{k}{4}; & k\ even, \end{cases}$$

and if $m+1 \le k \le \lceil \frac{m+2n}{2} \rceil$, *then*

$$R_k^a = \begin{cases} R_m^a + \frac{5m(k-m)(k+1)}{2}; & m\ even\ or\ m\ odd\ and\ k\ even, \\ R_m^a + \frac{5m(k-m)(k+1)+1}{2}; & m\ odd\ and\ k\ even. \end{cases}$$

Proof. If $k \le m$, then by Lemma 3.2,

$$R_k^a = \begin{cases} \Sigma_{i=1}^k \frac{5i^2}{2} + \left(\frac{k+1}{2}\right)\frac{1}{2}; & k\ odd, \\ \Sigma_{i=1}^k \frac{5i^2}{2} + \left(\frac{k}{2}\right)\frac{1}{2}; & k\ even, \end{cases}$$

and the result follows.

Let next $m+1 \le k \le \lceil \frac{m+2n}{2} \rceil$. If m is even, or if both m and k are odd, then

$$R_k^a - R_m^a = \Sigma_{i=m+1}^k (5mi - \frac{5m^2}{2})$$
$$= 5m((k-m)m + \frac{(k-m)(k-m+1)}{2}) - (k-m)\frac{5m^2}{2}$$
$$= \frac{5m(k-m)(k+1)}{2}.$$

And if m is odd and k is even, then

$$R_k^a - R_m^a = \frac{5m(k-m)(k+1)+1}{2}.$$

$\square$

Lemma 4.4. *If $u \equiv (i, j, k, l)$ is a vertex of $HN(m,n)$, then the contribution $T_a(u)$ to $T(u)$ by the acute cuts is given by*

$$
T_a(u) = \begin{cases}
\frac{5}{6} (k-1)k(2k-1) + \lfloor \frac{k}{2} \rfloor + 5mn(m+2n+1-2k); \\
\qquad\qquad k \leq m+1, \\
\frac{5}{6} (m+1)m(2m+1) + \lfloor \frac{m}{2} \rfloor + 5m(k-m-1)k + 5mn(m+2n+1-2k); \\
\qquad\qquad k > m+1, \ m \text{ even or } m \text{ odd and } k \text{ odd}, \\
\frac{5}{6} (m+1)m(2m+1) + \lceil \frac{m}{2} \rceil + 5m(k-m-1)k + 5mn(m+2n+1-2k); \\
\qquad\qquad k > m+1, \ m \text{ odd and } k \text{ even}.
\end{cases}
$$

Proof. For convenience, we drop the superfix a in the following derivation, as we are dealing only with acute cuts. Further, the Transmission Lemma is used for every acute cut A_k, $1 \leq k \leq \lceil \frac{m+2n}{2} \rceil$.

Case 1: m even.
In this case we compute as follows:

$$
\begin{aligned}
T_a(u) &= R_{k-1} + (S_{\frac{m+2n}{2}} - S_k) + (S_{\frac{m+2n}{2}} - S_{k+1}) + \cdots + \\
&\quad (S_{\frac{m+2n}{2}} - S_{\frac{m+2n}{2}-1}) + (\frac{m+2n}{2} - k) \, S_{\frac{m+2n}{2}} + R_{\frac{m+2n}{2}} \\
&= R_{k-1} + 2(\frac{m+2n}{2} - k) \, S_{\frac{m+2n}{2}} + R_{\frac{m+2n}{2}} - (S_k + S_{k+1} + \cdots + S_{\frac{m+2n}{2}-1}) \\
&= R_{k-1} + 2(\frac{m+2n}{2} - k) \, S_{\frac{m+2n}{2}} + R_{\frac{m+2n}{2}} \\
&\quad - (R_{\frac{m+2n}{2}} - (S_1 + S_2 + \cdots + S_{k-1}) - S_{\frac{m+2n}{2}}) \\
&= 2R_{k-1} + 2(\frac{m+2n}{2} - k) \, S_{\frac{m+2n}{2}} + S_{\frac{m+2n}{2}} \\
&= 2R_{k-1} + (m+2n-2k+1)S_{\frac{m+2n}{2}}
\end{aligned}
$$

By Lemma 4.3, if $k-1 \leq m$, then

$$
2R_{k-1} = \frac{5}{6} (k-1)k(2k-1) + \lfloor \frac{k}{2} \rfloor
$$

and if $k-1 \geq m+1$, then

$$
\begin{aligned}
2R_{k-1} &= 2R_m + 5m(k-m-1)k \\
&= \frac{5}{6} (m+1)m(2m+1) + \frac{m}{2} + 5m(k-m-1)k
\end{aligned}
$$

By Lemma 3.2, $S_{\frac{m+2n}{2}} = 5m \left(\frac{m+2n}{2} \right) - \frac{5m^2}{2} = 5mn$.

Therefore

$$
T_a(u) = \begin{cases}
\frac{5}{6}\,(k-1)k(2k-1) + \lfloor \frac{k}{2} \rfloor + 5mn(m+2n+1-2k); \\
\qquad\qquad k \le m+1, \\
\frac{5}{6}\,(m+1)m(2m+1) + \lfloor \frac{m}{2} \rfloor + 5m(k-m-1)k + 5mn(m+2n+1-2k); \\
\qquad\qquad k > m+1.
\end{cases}
$$

Case 2: m odd.
Now we compute as follows:

$$
\begin{aligned}
T_a(u) &= R_{k-1} + (S_{\lceil \frac{m+2n}{2} \rceil} - S_k) + (S_{\lceil \frac{m+2n}{2} \rceil} - S_{k+1}) + \cdots + \\
&\quad (S_{\lceil \frac{m+2n}{2} \rceil} - S_{\lceil \frac{m+2n}{2} \rceil - 1}) + (\lceil \frac{m+2n}{2} \rceil - k)\, S_{\lceil \frac{m+2n}{2} \rceil} + R_{\lceil \frac{m+2n}{2} \rceil - 1} \\
&= R_{k-1} + (\lceil \frac{m+2n}{2} \rceil - k)\,(S_{\lceil \frac{m+2n}{2} \rceil - 1} + S_{\lceil \frac{m+2n}{2} \rceil}) + R_{\lceil \frac{m+2n}{2} \rceil - 1} \\
&\quad - (S_k + S_{k+1} + \cdots + S_{\lceil \frac{m+2n}{2} \rceil - 1}) \\
&= 2R_{k-1} + (\lceil \frac{m+2n}{2} \rceil - k)\,(S_{\lceil \frac{m+2n}{2} \rceil - 1} + S_{\lceil \frac{m+2n}{2} \rceil}) \\
&= 2R_{k-1} + (\frac{m+2n+1}{2} - k)\,(S_{\lceil \frac{m+2n}{2} \rceil - 1} + S_{\lceil \frac{m+2n}{2} \rceil}).
\end{aligned}
$$

By Lemma 4.3, if $k-1 \le m$, then

$$
2R_{k-1} = \frac{5}{6}\,(k-1)k(2k-1) + \left\lfloor \frac{k}{2} \right\rfloor,
$$

and if $k-1 \ge m+1$, then

$$
2R_{k-1} = 2R_m + 2R_{k-m-1}.
$$

Hence

$$
T_a(u) = \begin{cases}
\frac{5}{6}\,(m+1)m(2m+1) + \lfloor \frac{m}{2} \rfloor + 5m(k-m-1)k; \\
\qquad m \text{ even, or } m \text{ odd and } k \text{ odd}, \\
\frac{5}{6}\,(m+1)m(2m+1) + \lceil \frac{m}{2} \rceil + 5m(k-m-1)k; \\
\qquad m \text{ odd and } k \text{ even}.
\end{cases}
$$

Note that $S_{\lceil \frac{m+2n}{2} \rceil - 1} + S_{\lceil \frac{m+2n}{2} \rceil} = S_{\frac{m+2n-1}{2}} + S_{\frac{m+2n+1}{2}}$. If $\frac{m+2n-1}{2}$ is even, then $\frac{m+2n+1}{2}$ is odd. Therefore,

$$
\begin{aligned}
S_{\frac{m+2n-1}{2}} + S_{\frac{m+2n+1}{2}} &= 5m\left(\frac{m+2n-1}{2}\right) - \left(\frac{5m^2+1}{2}\right) + 5m\left(\frac{m+2n+1}{2}\right) - \left(\frac{5m^2-1}{2}\right) \\
&= 5m(m+2n) - 5m^2 = 10mn.
\end{aligned}
$$

On the other hand, if $\frac{m+2n-1}{2}$ is odd, then $\frac{m+2n+1}{2}$ is even and therefore,

$$S_{\frac{m+2n-1}{2}} + S_{\frac{m+2n+1}{2}} = 5m(\frac{m+2n-1}{2}) - (\frac{5m^2-1}{2}) + 5m(\frac{m+2n+1}{2}) - (\frac{5m^2+1}{2})$$
$$= 5m(m+2n) - 5m^2 = 10mn.$$

In either case, $S_{\lceil\frac{m+2n}{2}\rceil-1} + S_{\lceil\frac{m+2n}{2}\rceil} = 10mn$.
Thus,

$$T_a(u) = \begin{cases} \frac{5}{6}(k-1)k(2k-1) + \lfloor\frac{k}{2}\rfloor + 5mn(m+2n+1-2k); \\ \qquad\qquad k \le m+1, \\ \frac{5}{6}(m+1)m(2m+1) + \lfloor\frac{m}{2}\rfloor + 5m(k-m-1)k + 5mn(m+2n+1-2k); \\ \qquad\qquad m+1 < k \le \lceil\frac{m+2n}{2}\rceil, \ m \text{ even, or } m \text{ odd and } k \text{ odd,} \\ \frac{5}{6}(m+1)m(2m+1) + \lceil\frac{m}{2}\rceil + 5m(k-m-1)k + 5mn(m+2n+1-2k); \\ \qquad\qquad m+1 < k \le \lceil\frac{m+2n}{2}\rceil, \ m \text{ odd and } k \text{ even.} \end{cases}$$

$\square$

The symmetric nature of the structure of $HN(m,n)$ implies that the role played by the acute cuts is the same as those of the obtuse cuts. Hence the contribution $T_o(u)$ of the obtuse cuts to $T(u)$ is obtained by replacing k by l in $T_a(u)$. All is now prepared to formulate the main result of this paper.

Theorem 4.5. *If $u \equiv (i,j,k,l)$ is a vertex of $HN(m,n)$, then the transmission of u in $HN(m,n)$ is given by*

$$T(u) = T_h(u) + T_V(u) + T_a(u) + T_o(u),$$

where,

$$T_h(u) = 5n(i^2 + (2m+1)(m-i)), \ i \in [2m],$$

$$T_V(u) = 10m(\frac{n(n+1)}{2} + j(j-1-n)), \ j \in [n],$$

$$T_a(u) = \begin{cases} \frac{5}{6}(k-1)k(2k-1) + \lfloor\frac{k}{2}\rfloor + 5mn(m+2n+1-2k); \\ \qquad\qquad k \le m+1, \\ \frac{5}{6}(m+1)m(2m+1) + \lfloor\frac{m}{2}\rfloor + 5m(k-m-1)k + 5mn(m+2n+1-2k); \\ \qquad\qquad m+1 < k \le \lceil\frac{m+2n}{2}\rceil, \ m \text{ even, or } m \text{ odd and } k \text{ odd,} \\ \frac{5}{6}(m+1)m(2m+1) + \lceil\frac{m}{2}\rceil + 5m(k-m-1)k + 5mn(m+2n+1-2k); \\ \qquad\qquad m+1 < k \le \lceil\frac{m+2n}{2}\rceil, \ m \text{ odd and } k \text{ even,} \end{cases}$$

12

and

$$T_o(u) = \begin{cases} \frac{5}{6}(l-1)l(2l-1) + \lfloor\frac{l}{2}\rfloor + 5mn(m+2n+1-2l); \\ \qquad\qquad l \le m+1, \\ \frac{5}{6}(m+1)m(2m+1) + \lfloor\frac{m}{2}\rfloor + 5m(l-m-1)l + 5mn(m+2n+1-2l); \\ \qquad\qquad m+1 < l \le \lceil\frac{m+2n}{2}\rceil, \ m \text{ even, or } m \text{ odd and } l \text{ odd}, \\ \frac{5}{6}(m+1)m(2m+1) + \lceil\frac{m}{2}\rceil + 5m(l-m-1)l + 5mn(m+2n+1-2l); \\ \qquad\qquad m+1 < l \le \lceil\frac{m+2n}{2}\rceil, \ m \text{ odd and } l \text{ even}. \end{cases}$$

In Theorem 4.5, the transmission of the vertices $u \equiv (i, j, k, l)$, where $i \in [2m]$, $j \in [n]$, and $k, l \in [\lceil (m+2n)/2\rceil]]$ have been determined. Hence the vertices $u \equiv (i, j, k, l)$ for which $\lceil\frac{m+2n}{2}\rceil < k, l \le m + 2n$ have not been considered. But the symmetric nature of $HN(m, n)$ implies that

$$T(2m+1-i, n+1-j, m+2n+1-k, m+2n+1-l) = T(i, j, k, l).$$

For example, $T(2m, n, 2n+1, m+2n) = T(1, 1, m, 1)$. Thus Theorem 4.5 is sufficient to determine $T(u)$ of every vertex u in $HN(m, n)$.

5   Conclusions

In this paper, a coordinate system has been defined to uniquely identify the location of a vertex in $HN(m, n)$. This coordinate system together with the Transmission Lemma has led to a challenging computational procedure to arrive at the transmission of every vertex in $HN(m, n)$. Closeness centrality measure is an easy consequence of the study on transmission of vertices. This paper throws light on determining transmission of vertices in several other nanosheets.

References

[1] A. Abiad, B. Brimkov, A. Erey, L. Leshock, X. Martnez-Rivera, Suil O., S.Y. Song, J. Williford, On the Wiener index, distance cospectrality and transmission-regular graphs, Discrete Appl. Math. 230 (2017) 1–10.

[2] Y. Alizadeh, V. Andova, S. Klavžar, R. Škrekovski, Wiener dimension: fundamental properties and (5,0)-nanotubical fullerenes, MATCH Commun. Math. Comput. Chem. 72 (2014) 279–294.

[3] Y. Alizadeh, S. Klavžar, On graphs whose Wiener complexity equals their order and on Wiener index of asymmetric graphs, Appl. Math. Comput. 328 (2018) 113–118.

[4] S. Al-Yakoob, D. Stevanović, On transmission irregular starlike trees, Appl. Math. Comput. 380 (2020) Article 125257.

[5] M. Arockiaraj, A.J. Shalini, Extended cut method for edge Wiener, Schultz and Gutman indices with applications, MATCH Commun. Math. Comput. Chem. 76 (2016) 233–250.

[6] A. Bahrami, M. Alaeiyan, Fifth geometric-arithmetic index of H-naphtalenic nanosheet $[4n, 2m]$, J. Comput. Theoret. Nanosci. 12 (2015) 689–690.

[7] K. Balakrishnan, B. Brešsar, M. Changat, S. Klavžar, A. Vesel, P. Žigert Pleteršek, Equal opportunity networks, distance-balanced graphs, and Wiener game, Discrete Optim. 12 (2014) 150–154.

[8] A. Bonato, N. Hadi, P. Horn, P. Prałat, C. Wang, Models of online social networks, Internet Math. 6 (2009) 285–313.

[9] B. Buechel, V. Buskens, The dynamics of closeness and betweenness, J. Math. Sociol. 37 (2013) 159–191.

[10] M. Cavaleri, A. Donno, A. Scozzari, Total distance, Wiener index and opportunity index in wreath products of star graphs, Electron. J. Combin. 26 (2019) Article 1.21.

[11] M.S. Chen, K.G. Shin, D.D. Kandlur, Addressing, routing, and broadcasting in hexagonal mesh multiprocessors, IEEE Trans. Comput. 39 (1990) 10–18.

[12] V. Chepoi, S. Klavžar, The Wiener index and the Szeged index of benzenoid systems in linear time, J. Chem. Inf. Comput. Sci. 37 (1997) 752–755.

[13] M. Črepnjak, N. Tratnik, The Szeged index and the Wiener index of partial cubes with applications to chemical graphs, Appl. Math. Comput. 309 (2017) 324–333.

[14] A. A. Dobrynin, Infinite family of transmission irregular trees of even order, Discrete Math. 342 (2019) 74–77.

[15] A. A. Dobrynin, Infinite family of 3-connected cubic transmission irregular graphs, Discrete Appl. Math. 257 (2019) 151–157.

[16] A. A. Dobrynin, R. Sharafdini, Stepwise transmission irregular graphs, Appl. Math. Comput. 371 (2020) Article 124949.

[17] A.A. Dobrynin, A.Y. Vesnin, On the Wiener complexity and the Wiener index of fullerene graphs, Mathematics 7 (2019) Article 1071.

[18] H. Hua, On the total distance and diameter of graphs, Bull. Aust. Math. Soc. 98 (2018) 14–17.

[19] N. Idrees, M.J. Saif, A. Sadiq, A. Rauf, F. Hussain, Topological indices of H-naphtalenic nanosheet, Open Chem. 16 (2018) 1184–1188.

[20] Z. Iqbal, M. Ishaq, A. Aslam, M. Aamir, W. Gao, The measure of irregularities of nanosheets, Open Phys. 18 (2020) 419–431.

[21] S. Kim, H. Wang, Y.M. Lee, 2D Nanosheets and Their Composite Membranes for Water, Gas, and Ion Separation, Angew. Chem. Int. Ed. 58 (2019) 17512–17527.

[22] S. Klavžar, On the canonical metric representation, average distance, and partial Hamming graphs, European J. Combin. 27 (2006) 68–73.

[23] S. Klavžar, I. Gutman, B. Mohar, Labeling of benzenoid systems which reflects the vertex-distance relations, J. Chem. Inf. Comput. Sci. 35 (1995) 590–593.

[24] S. Klavžar, D.A. Jemilet, I. Rajasingh, P. Manuel, N. Parthiban, General transmission lemma and Wiener complexity of triangular grids, Appl. Math. Comput. 338 (2018) 115–122.

[25] S. Klavžar, M.J. Nadjafi-Arani, Cut method: Update and recent developments and equivalence of independent approaches, Curr. Org. Chem. 19 (2015) 348–358.

[26] M. Knor, R. Škrekovski, A. Tepeh, On the difference between Wiener index and GraovacPisanski index, MATCH Commun. Math. Comput. Chem. 83 (2020) 109–120.

[27] M. Krnc, R. Škrekovski, Centralization of transmission in networks, Discrete Math. 338 (2015) 2412–2420.

[28] K.P. Narayankar, A.T. Kahsay, S. Klavžar, On peripheral Wiener index: line graphs, Zagreb index, and cut method, MATCH Commun. Math. Comput. Chem. 83 (2020) 129–141.

[29] M. Pandeeswar, T. Govindaraju, Green-fluorescent naphthalene diimide: conducting layered hierarchical 2D nanosheets and reversible probe for detection of aromatic solvents, RSC Adv. 3 (2013) 11459–11462.

[30] I. Rajasingh, R. Bharati, A. Muthumalai, A.S. Shanthi, On excessive index of certain networks, Theoret. Comput. Sci. 501 (2013) 34–40.

[31] I. Rajasingh, P. Manuel, N. Parthiban, D.A. Jemilet, R.S. Rajan, Transmission in butterfly networks, Comput. J. 59 (2016) 1174–1179.

[32] R. Sharafdini, T. Réti, On the transmission-based graph topological indices, Kragujevac J. Math. 44 (2020) 41–63.

[33] N. Tratnik, Generalized cut method for computing the edge-Wiener index, Discrete Appl. Math. 282 (2020) 222–233.

[34] K. Xu, K.Ch. Das, S. Klavžar, H. Li, Comparison of Wiener index and Zagreb eccentricity indices, MATCH Commun. Math. Comput. Chem. 84 (2020) 595–610.