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Minimum eccentric connectivity index for graphs with fixed order and fixed number of pending vertices

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Abstract: The eccentric connectivity index of a connected graph G is the sum over all vertices v of the product $d_G(v)e_G(v)$, where $d_G(v)$ is the degree of v in G and $e_G(v)$ is the maximum distance between v and any other vertex of G. This index is helpful for the prediction of biological activities of diverse nature, a molecule being modeled as a graph where atoms are represented by vertices and chemical bonds by edges. We characterize those graphs which have the smallest eccentric connectivity index among all connected graphs of a given order n. Also, given two integers n and p with $p \leq n-1$, we characterize those graphs which have the smallest eccentric connectivity index among all connected graphs of order n with p pending vertices.

Keywords: Eccentric connectivity index, extremal graph theory

1 Introduction

A chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory where atoms are represented by vertices and chemical bonds by edges. Arthur Cayley [1] was probably the first to publish results that consider chemical graphs. In an attempt to analyze the chemical properties of alkanes, Wiener [11] has introcuced the *path number index*, nowadays called *Wiener index*, which is defined as the sum of the lengths of the shortest paths between all pairs of vertices. Mathematical properties and chemical applications of this distance-based index have been widely researched.

Numerous other topological indices are used for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies that help to describe and understand the structure of molecules [10, 6], among which the *eccentric connectivity index* which can be defined as follows. Let $G = (V, E)$ be a simple connected undirected graph. The *distance* $dist_G(u, v)$ between two vertices u and v in G is the number of edges of a shortest path in G connecting u and v. The *eccentricity* $e_G(v)$ of a vertex v is the maximum distance between v and any other vertex, that is $\max\{dist_G(v, w) \mid w \in V\}$. The *eccentric connectivity index* $\xi^c(G)$ of G is defined by

$$\xi^c(G) = \sum_{v \in V} d_G(v) e_G(v).$$

This index was introduced by Sharma et al. in [9] and successfully used for mathematical models of biological activities of diverse nature [2, 3, 7, 8, 5]. Recently, Hauweele et al. [4] have characterized those graphs which have the largest eccentric connectivity index among all connected graphs of given order n. These results are summarized in Table 1, where

- K_n is the complete graph of order n;
- P_n is the path of order n;
- W_n is the wheel of order n, i.e., the graph obtained by joining a vertex to all vertices of a cycle of order $n - 1$;
- M_n is the graph obtained from K_n by removing a maximum matching and, if n is odd, an additional edge adjacent to the unique vertex that still degree $n - 1$;
- $\mathsf{E}_{n,D}$ is the graph constructed from a path $u_0 - u_1 - \ldots - u_D$ by joining each vertex of a clique K_{n-D-1} to u_0, u_1 and u_2.

Table 1: Largest eccentric connectivity index for a fixed order n

n	optimal graphs
1	K_1
2	K_2
3	K_3 and P_3
4	M_4
5	M_5 and W_5
6	M_6
7	M_7
8	M_8 and $\mathsf{E}_{8,4}$
≥ 9	$\mathsf{E}_{n,\lceil \frac{n+1}{3} \rceil + 1}$

In addition to the above-mentioned graphs, we will also consider the following ones:

- C_n is the chordless cycle of order n;
- $\mathsf{S}_{n,x}$ is the graph of order n obtained by linking all vertices of a stable set of $n - x$ vertices with all vertices of a clique K_x. The graph $\mathsf{S}_{n,1}$ is called a *star*.

Also, for $n \geq 4$ and $p \leq n - 3$, let $\mathsf{H}_{n,p}$ be the graph of order n obtained by adding a dominating vertex (i.e., a vertex linked to all other vertices) to the graph or order $n - 1$ having p vertices of degree 0, and

- $n - 1 - p$ vertices of degree 1 if $n - p$ is odd;
- $n - 2 - p$ vertices of degree 1 and one vertex of degree 2 if $n - p$ is even.

For illustration, $\mathsf{H}_{8,3}$ and $\mathsf{H}_{9,3}$ are drawn on Figure 1. Note that $\mathsf{H}_{4,0} \simeq \mathsf{S}_{4,2}$. Moreover, $\mathsf{H}_{4,0}$ has two dominating vertices while $\mathsf{H}_{4,1}$ and $\mathsf{H}_{n,p}$ have exactly one dominating vertex for all $n \geq 5$ and $p \leq n-3$.

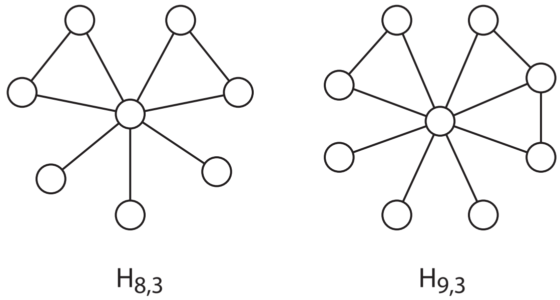

Figure 1: Two graphs with $p = 3$ pending vertices

In this paper, we first give an alternative proof to a result of Zhou and Du [12] showing that the stars are the only graphs with smallest eccentric connectivity index among all connected graphs of given order $n \geq 4$. These graphs have $n-1$ pending vertices (i.e., vertices of degree 1). We then consider all pairs (n,p) of integers with $p \leq n-1$ and characterize the graphs with smallest eccentric connectivity index among all connected graphs of order n with p pending vertices.

2 Minimizing ξ^c for graphs with fixed order

K_1 and K_2 are the only connected graphs with 1 and 2 vertices, respectively, while K_3 and P_3 are the only connected graphs with 3 vertices. Since $\xi^c(\mathsf{K}_3) = \xi^c(\mathsf{P}_3) = 6$, all connected graphs of given order $n \leq 3$ have the same eccentric connectivity index. From now on, we therefore only consider connected graphs with fixed order $n \geq 4$. A proof of the following theorem was already given by Zhou and Du in [12]. Ours is slightly different.

Theorem 1 *Let G be a connected graph of order $n \geq 4$. Then $\xi^c(G) \geq 3(n-1)$, with equality if and only if $G \simeq \mathsf{S}_{n,1}$.*

Proof. Let x be the number of dominating vertices (i.e., vertices of degree $n-1$) in G. We distinguish three cases.

- If $x = 1$, then let u be the dominating vertex in G. Clearly, $e_G(u) = 1$ and $d_G(u) = n-1$. All vertices $v \neq u$ have eccentricity $e_G(v) = 2$, while their degree is at least 1 (since G is connected). Hence, $\xi^c(G) \geq (n-1) + 2(n-1) = 3(n-1)$, with equality if and only if all $v \neq u$ have degree 1, i.e., $G \simeq \mathsf{S}_{n,1}$.
- If $x > 1$, then all dominating vertices u have $d_G(u)e_G(u) = n-1$, while all non-dominating vertices v have $d_G(v) \geq x \geq 2$ and $e_G(v) \geq 2$, which implies $d_G(u)e_G(u) \geq 4$. If $n = 4$, we therefore have $\xi^c(G) \geq 3n > 3(n-1)$, while if $n > 4$, we have $\xi^c(G) \geq 2(n-1) + 4(n-2) = 6n - 10 > 3(n-1)$.
- If $x = 0$, then every pending vertex v has $e_G(v) \geq 3$ since its only neighbor is a non-dominating vertex. Since the eccentricity of the non-pending vertices is at least two, we have $d_G(v)e_G(v) \geq 3$ for all vertices v in G, which implies $\xi^c(G) \geq 3n > 3(n-1)$.

□

Stars have $n-1$ pending vertices. As will be shown in the next section, a similar result is more challenging when the total number of pending vertices is fixed to a value strictly smaller than $n-2$.

3 Minimizing ξ^c for graphs with fixed order and fixed number of pending vertices

Let G be a connected graph of order $n \geq 4$ with p pending vertices. Clearly, $p \leq n-1$, and $G \simeq \mathsf{S}_{n,1}$ if $p = n-1$. For $p = n-2$, let u and v be the two non-pending vertices. Note that u is adjacent to v since G is connected. Clearly, G is obtained by linking $x \leq n-3$ vertices of a stable set S of $n-2$ vertices to u, and the $n-2-x$ other vertices of S to v. The $n-2$ pending vertices w have $d_G(w) = 1$ and $e_G(w) = 3$, while $e_G(u) = e_G(v) = 2$ and $d_G(u) + d_G(v) = n$. Hence $\xi^c(G) = 3(n-2) + 2n = 5n-6$ for all graphs of order n with $n-2$ pending vertices.

The above observations show that all graphs of order n with a fixed number $p \geq n-2$ of pending vertices have the same eccentric connectivity index. As will be shown, this is not the case when $n \geq 4$ and $p \leq n-3$. We will prove that $\mathsf{H}_{n,p}$ is almost always the unique graph minimizing the eccentric connectivity index. Note that

$$\xi^c(\mathsf{H}_{n,p}) = \begin{cases} n-1+2p+4(n-p-1) = 5n-2p-5 & \text{if } n-p \text{ is odd} \\ n-1+2p+4(n-p-2)+6 = 5n-2p-3 & \text{if } n-p \text{ is even.} \end{cases}$$

Theorem 2 *Let G be a connected graph of order $n \geq 4$ with $p \leq n-3$ pending vertices and one dominating vertex. Then $\xi^c(G) \geq \xi^c(\mathsf{H}_{n,p})$, with equality if and only if $G \simeq \mathsf{H}_{n,p}$.*

Proof. The dominating vertex u in G has $d_G(u)e_G(u) = n-1$, the pending vertices v have $d_G(v)e_G(v) = 2$, and the other vertices w have $e_G(w) = 2$ and $d_G(w) \geq 2$. Hence, $\xi^c(G)$ is minimized if all non-pending and non-dominating vertices have degree 2, except one that has degree 3 if $n-p-1$ is odd. In other words, $\xi^c(G)$ is minimized if and only if $G \simeq \mathsf{H}_{n,p}$. □

Theorem 3 *Let G be a connected graph of order $n \geq 4$, with at least two dominating vertices.*

- *If $n = 4$ then $\xi^c(G) \geq 12$, with equality if and only if $G \simeq \mathsf{K}_4$.*
- *If $n = 5$ then $\xi^c(G) \geq 20$, with equality if and only if $G \simeq \mathsf{S}_{5,2}$ or $G \simeq \mathsf{K}_5$.*
- *If $n \geq 6$ then $\xi^c(G) \geq 6n-10$, with equality if and only if $G \simeq \mathsf{S}_{n,2}$.*

Proof. Let x be the number of dominating vertices in G. Then $d_G(u)e_G(u) = n-1$ for all dominating vertices u, while $e_G(v) = 2$ and $d_G(v) \geq x$ for all other vertices v. Hence, $\xi^c(G) \geq -2x^2 + x(3n-1)$.

- If $n = 4$ then $\xi^c(G) \geq f(x) = -2x^2 + 11x$. Since $2 \leq x \leq 4$, $f(2) = 14, f(3) = 15$, and $f(4) = 12$, we conclude that $\xi^c(G) \geq 12$, with equality if and only if $x = 4$, which is the case when $G \simeq \mathsf{K}_4$.
- If $n = 5$ then $\xi^c(G) \geq f(x) = -2x^2 + 14x$. Since $2 \leq x \leq 5$, $f(2) = f(5) = 20$ and $f(3) = f(4) = 24$, we conclude that $\xi^c(G) \geq 20$, with equality if and only if $x = 2$ or 5, which is the case when $G \simeq \mathsf{S}_{5,2}$ or $G \simeq \mathsf{K}_5$.
- If $n \geq 6$ then $-2x^2 + x(3n-1)$ is minimized for $x = 2$, which is the case when $G \simeq \mathsf{S}_{n,2}$.

□

Theorem 4 *Let G be a connected graph of order $n \geq 4$, with $p \leq n-3$ pending vertices and no dominating vertex. Then $\xi^c(G) > \xi^c(\mathsf{H}_{n,p})$ unless $n = 5$, $p = 0$ and $G \simeq \mathsf{C}_5$, in which case $\xi^c(G) = \xi^c(\mathsf{H}_{n,0}) = 20$.*

Proof. Let U be the subset of vertices u in G such that $d_G(u) = e_G(u) = 2$. If U is empty, then all non-pending vertices v in G have $d_G(v) \geq 2$ and $e_G(v) \geq 2$ (since G has no dominating vertex), and at least one of these two inequalities is strict, which implies $d_G(u)e_G(u) \geq 6$. Also, every pending vertex w has $e_G(w) \geq 3$ since their only neighbor is not dominant. Hence, $\xi^c(G) \geq 6(n-p) + 3p = 6n-3p$. Since $p \leq n-3$, we have $\xi^c(G) \geq 5n-2p+3 > \xi^c(\mathsf{H}_{n,p})$.

So, assume $U \neq \emptyset$. Let u be a vertex in U, and let v, w be its two neighbors. Also, let $A = N(v) \setminus (N(w) \cup \{w\})$, $B = (N(v) \cup N(w)) \setminus \{u\}$, and $C = N(w) \setminus (N(v) \cup \{v\})$. Since $e_G(u) = 2$, all vertices of G belong to $A \cup B \cup C \cup \{u, v, w\}$. We finally define B' as the subset of B that contains all vertices b of B with $d_G(b) = 2$ (i.e., their only neighbors are v and w).

Case 1: v is adjacent to w.

$A \neq \emptyset$ else w is a dominating vertex, and $C \neq \emptyset$ else v is dominating. Let G' be the graph obtained from G by replacing every edge linking v to a vertex $a \in A$ with an edge linking w to a, and by removing all edges linking v to a vertex of $B \setminus B'$. Clearly, G' is also a connected graph of order n with p pending vertices, and w is the only dominating vertex in G'. It follows from Theorem 2 that $\xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$. Also,

- $d_G(u) = d_{G'}(u)$ and $e_G(u) = e_{G'}(u)$;
- $d_G(x) = d_{G'}(x)$ and $e_G(x) \geq e_{G'}(x)$ for all $x \in A \cup C$;
- $d_G(x) = d_{G'}(x)$ and $e_G(x) = e_{G'}(x)$ for all $x \in B'$;
- $d_G(x) > d_{G'}(x)$ and $e_G(x) = e_{G'}(x)$ for all $x \in B \setminus B'$.

Hence,

$$\sum_{x \in A\cup B\cup C\cup\{u\}} d_G(x)e_G(x) \geq \sum_{x \in A\cup B\cup C\cup\{u\}} d_{G'}(x)e_{G'}(x).$$

Moreover,

- $d_G(v)e_G(v) + d_G(w)e_G(w) = 2(|A| + |B| + 2) + 2(|C| + |B| + 2) = 2|A| + 4|B| + 2|C| + 8$;
- $d_{G'}(v)e_{G'}(v) + d_{G'}(w)e_{G'}(w) = 2(|B'| + 2) + |A| + |B| + |C| + 2$.

We therefore have

$$\begin{aligned}
\xi^c(G) - \xi^c(G') &= \sum_{x \in A\cup B\cup C\cup\{u\}} d_G(x)e_G(x) + (d_G(v)e_G(v) + d_G(w)e_G(w)) \\
&\quad - \sum_{x \in A\cup B\cup C\cup\{u\}} d_{G'}(x)e_{G'}(x) - (d_{G'}(v)e_{G'}(v) + d_{G'}(w)e_{G'}(w)) \\
&\geq (2|A| + 4|B| + 2|C| + 8) - (2(|B'| + 2) + |A| + |B| + |C| + 2) \\
&= |A| + |C| + 3(|B'| + |B \setminus B'|) - 2|B'| + 2 \\
&= |A| + |C| + |B'| + 3|B \setminus B'| + 2 > 0
\end{aligned}$$

This implies $\xi^c(G) > \xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$.

Case 2: v is not adjacent to w, and both $A \cup (B \setminus B')$ and $C \cup (B \setminus B')$ are nonempty.

Let G' be the graph obtained from G by adding an edge linking v to w, by replacing every edge linking v to a vertex $a \in A$ with an edge linking w to a, and by removing all edges linking v to a vertex of $B \setminus B'$. Clearly, G' is also a connected graph of order n with p pending vertices. As in the previous case, we have

$$\sum_{x \in A\cup B\cup C\cup\{u\}} d_G(x)e_G(x) \geq \sum_{x \in A\cup B\cup C\cup\{u\}} d_{G'}(x)e_{G'}(x).$$

Moreover, $e_G(v) \geq 2$ and $e_G(w) \geq 2$, while $e_{G'}(v) \leq 2$ and $e_{G'}(w) = 1$, which implies

- $d_G(v)e_G(v) + d_G(w)e_G(w) \geq 2(|A| + |B| + 1) + 2(|C| + |B| + 1) = 2|A| + 4|B| + 2|C| + 4$;
- $d_{G'}(v)e_{G'}(v) + d_{G'}(w)e_{G'}(w) \leq 2(|B'| + 2) + |A| + |B| + |C| + 2$.

We therefore have

$$\begin{aligned}
\xi^c(G) - \xi^c(G') &\geq (2|A| + 4|B| + 2|C| + 4) - (2(|B'| + 2) + |A| + |B| + |C| + 2) \\
&= |A| + |C| + |B'| + 3|B \setminus B'| - 2.
\end{aligned}$$

If $B \setminus B' \neq \emptyset$, w is the only dominating vertex in G', and $\xi^c(G) - \xi^c(G') > 0$. It then follows from Theorem 2 that $\xi^c(G) > \xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$. So assume $B \setminus B' = \emptyset$. Since $A \cup (B \setminus B') \neq \emptyset$, and $C \cup (B \setminus B') \neq \emptyset$, we have $A \neq \emptyset$ and $C \neq \emptyset$. Hence, once again, w is the only dominating vertex in G', and we know from Theorem 2 that $\xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$.

- If $|B'| \geq 1$, $|A| \geq 2$ or $|C| \geq 2$, then $\xi^c(G) > \xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$.
- If $|B'| = 0$ and $|A| = |C| = 1$, there are two possible cases:

– if the vertex in A is not adjacent to the vertex in C, then $n = 5$, $p = 2$, $G \simeq \mathsf{P}_5$ and $G' \simeq \mathsf{H}_{5,2}$. Hence, $\xi^c(G) = 24 > 16 = \xi^c(\mathsf{H}_{n,p})$;

– if the vertex in A is adjacent to the vertex in C, then $n = 5$, $p = 0$, $G \simeq \mathsf{C}_5$ and $G' \simeq \mathsf{H}_{5,2}$. Hence, $\xi^c(G) = \xi^c(\mathsf{H}_{n,p}) = 20$;

Case 3: v is not adjacent to w, and at least one of $A \cup (B \setminus B')$ and $C \cup (B \setminus B')$ is empty.

Without loss of generality, suppose $A \cup (B \setminus B') = \emptyset$. We distinguish two subcases.

Case 3.1: $B' = \emptyset$.

Since $n \geq 4$, $C \neq \emptyset$. Also, since $p \leq n-3$, there is a non-pending vertex $r \in C$. Let G' be the graph obtained from G by removing the edge linking u and v and by linking v to w and to r. Note that G' is a connected graph of order n with p pending vertices : while v was pending in G, but not u, the situation is the opposite in G'. Note also that Theorem 2 implies $\xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$ since w is the only dominating vertex in G'. We then have:

- $d_G(u)=2$, $d_{G'}(u)=1$ and $e_G(u)=e_{G'}(u)=2$, which gives $d_G(u)e_G(u) - d_{G'}(u)e_{G'}(u) = 2$;
- $d_G(v)=1$, $d_{G'}(v)=2$ $e_G(v)=3$ and $e_{G'}(v)=2$, which gives $d_G(v)e_G(v) - d_{G'}(v)e_{G'}(v) = -1$;
- $d_G(w)=n-2$, $d_{G'}(w)=n-1$ $e_G(w)=2$ and $e_{G'}(w)=1$, which gives $d_G(w)e_G(w) - d_{G'}(w)e_{G'}(w) = n-3$;
- $d_{G'}(r)=d_G(r)+1$, $e_G(r)=3$ and $e_{G'}(w)=2$, which gives $d_G(r)e_G(r) - d_{G'}(r)e_{G'}(r) = d_G(r) - 2$;
- $d_{G'}(c)=d_G(c)$ and $e_G(c) > e_{G'}(c)$ for all $c \in (C \setminus \{r\})$. Since r has a neighbor in C of degree at least 2, we have $\sum_{c \in C \setminus \{r\}}(d_G(c)e_G(c) - d_{G'}(c)e_{G'}(c) \geq 2)$.

Hence, $\xi^c(G) - \xi^c(G') \geq 2 - 1 + \underbrace{n-3}_{>0} + \underbrace{d_G(r) - 2}_{\geq 0} + 2 > 0$, which implies $\xi^c(G) > \xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$.

Case 3.2: $B' \neq \emptyset$.

Let $b_1, \ldots, b_{|B'|}$ be the vertices in B'. Remember that the unique neighbors of these vertices are v and w. Let G' be the graph obtained from G as follows. We first add an edge linking v to w. Then, for every odd $i < |B'|$, we add an edge linking b_i to b_{i+1} and remove the edges linking v to b_i and to b_{i+1}. We then have

- $d_G(x) = d_{G'}(x)$ and $e_G(x) = e_{G'}(x)$ for all $x \in B' \cup C \cup \{u\}$;
- $d_G(v) = |B'| + 1$, $d_{G'}(v) \leq 3$, $e_G(v) \geq 2$, and $e_{G'}(v) \leq 2$;
- $d_G(w) = |B'| + |C| + 1$, $d_{G'}(w) = |B'| + |C| + 2$, $e_G(w) = 2$, and $e_{G'}(w) = 1$.

Hence,

$$\begin{array}{rcl} \xi^c(G) - \xi^c(G') & = & d_G(v)e_G(v) + d_G(w)e_G(w) - d_{G'}(v)e_{G'}(v) + d_{G'}(w)e_{G'}(w) \\ & \geq & 2(|B'| + 1) + 2(|B'| + |C| + 1) - 6 - (|B'| + |C| + 2) \\ & = & 3|B'| + |C| - 4. \end{array}$$

IF $|B'| \geq 2$ or $|C| \geq 2$, then $\xi^c(G) - \xi^c(G') > 0$, and since w is then the only dominating vertex in G', we know from Theorem 2 that $\xi^c(G) > \xi^c(G') \geq \xi^c(\mathsf{H}_{n,p})$. So, assume $|B'| = 1$ and $|C| \leq 1$:

- if $|C| = 0$ then $n = 4$, $p = 0$, $G \simeq \mathsf{C}_4$ and $G' \simeq \mathsf{H}_{4,0}$ which implies $\xi^c(G) = 16 > 14 = \xi^c(\mathsf{H}_{n,p})$;
- if $|C| = 1$ then $n = 5$, $p = 1$, $\xi^c(G) = 23$ and $G' \simeq \mathsf{H}_{5,1}$ which implies $\xi^c(G) > 20 = \xi^c(\mathsf{H}_{n,p})$.

□

We can now combine these results as follows. Assume G is a connected graph of order n with p pending vertices. If $p \geq 1$, then G has at most one dominating vertex, and it follows from Theorems 2 and 4 that $\mathsf{H}_{n,p}$ is the only graph with maximum eccentric connectivity index. If $p = 0$ and $n = 4$, then G cannot contain exactly one dominating vertex, and Theorems 3 and 4 show that K_4 is the only graph with maximum eccentric connectivity index. If $p = 0$ and $n = 5$, Theorems 2, 3 and 4 show that $\mathsf{H}_{5,0}$, $\mathsf{S}_{5,2}$, K_5 and

C_5 are the only candidates to minimize the eccentric connectivity index, and since $\xi^c(\mathsf{H}_{5,0}) = \xi^c(\mathsf{S}_{5,2}) = \xi^c(\mathsf{K}_5) = \xi^c(\mathsf{C}_5) = 20$, the four graphs are the optimal ones. If $p = 0$ and $n \geq 6$ then we know from Theorems 2, 3 and 4 that $\mathsf{S}_{n,2}$ and $\mathsf{H}_{n,0}$ are the only candidates to minimize the eccentric connectivity index. Since $\xi^c(\mathsf{S}_{6,2}) = 26 < 27 = \xi^c(\mathsf{H}_{6,0})$, $\xi^c(\mathsf{S}_{7,2}) = 32 > 30 = \xi^c(\mathsf{H}_{7,0})$ and $\xi^c(\mathsf{S}_{n,2}) = 6n-10 > 5n-3 \geq \xi^c(\mathsf{H}_{n,0})$ for $n \geq 8$, we deduce that $\mathsf{S}_{6,2}$ is the only graph with maximum eccentric connectivity index when $n = 6$ and $p = 0$, while $\mathsf{H}_{n,0}$ is the only optimal graph when $n \geq 7$ and $p = 0$. This is summarized in the following Corollary.

Corollary 1 *Let G be a connected graph of order $n \geq 4$ with $p \leq n-3$ pending vertices.*

- *If $p \geq 1$ then $\xi^c(G) \geq \xi^c(\mathsf{H}_{n,p})$, with equality if and only if $G \simeq \mathsf{H}_{n,p}$;*
- *If $p = 0$ then*
  - *if $n = 4$ then $\xi^c(G) \geq 12$, with equality if and only if $G \simeq \mathsf{K}_4$;*
  - *if $n = 5$ then $\xi^c(G) \geq 20$, with equality if and only if $G \simeq \mathsf{H}_{5,0}$, $\mathsf{S}_{5,2}$, K_5 or C_5;*
  - *if $n = 6$ then $\xi^c(G) \geq 26$, with equality if and only if $G \simeq \mathsf{S}_{6,2}$;*
  - *if $n \geq 7$ then $\xi^c(G) \geq \xi^c(\mathsf{H}_{n,0})$, with equality if and only if $G \simeq \mathsf{H}_{n,0}$.*

4 Conclusion

We have characterized the graphs with smallest eccentric connectivity index among those of fixed order n and fixed or non-fixed number of pending vertices. Such a characterization for graphs with a fixed order n and a fixed size m was given in [12]. It reads as follows.

Theorem 5 *Let G be a connected graph of order n with m edges, where $n-1 \leq m < \binom{n}{2}$. Also, let*

$$k = \left\lfloor \frac{2n-1-\sqrt{(2n-1)^2-8m}}{2} \right\rfloor.$$

Then $\xi^c(G) \geq 4m - k(n-1)$, with equality if and only if G has k dominating vertices and $n-k$ vertices of eccentricity 2.

It is, however, an open question to characterize the graphs with largest eccentric connectivity index among those of fixed order n and fixed size m. The following conjecture appears in [4], where $\mathsf{E}_{n,D,k}$ is the graph of order n constructed from a path $u_0 - u_1 - \ldots - u_D$ by joining each vertex of a clique K_{n-D-1} to u_0 and u_1, and k vertices of the clique to u_2.

Conjecture 1 *Let G be a connected graph of order n with m edges, where $n-1 \leq m \leq \binom{n-1}{2}$. Also, let*

$$D = \left\lfloor \frac{2n+1-\sqrt{17+8(m-n)}}{2} \right\rfloor \text{ and } k = m - \binom{n-D+1}{2} - D + 1.$$

Then $\xi^c(G) \leq \xi^c(\mathsf{E}_{n,D,k})$, with equality if and only if $G \simeq \mathsf{E}_{n,D,k}$ or $D = 3$, $k = n-4$ and G is the graph constructed from a path $u_0 - u_1 - u_2 - u_3$, by joining $1 \leq i \leq n-3$ vertices of a clique K_{n-4} to u_0, u_1, u_2 and the $n-4-i$ other vertices of K_{n-4} to u_1, u_2, u_3.

References

[1] Cayley, A. On the mathematical theory of isomers. Philosophical Magazine, Series 5, 47 (1874), 444–446.

[2] Dureja, H., Gupta, S., and Madan, A. Predicting anti-hiv-1 activity of 6-arylbenzonitriles: Computational approach using superaugmented eccentric connectivity topochemical indices. Journal of Molecular Graphics and Modelling 26, 6 (2008), 1020–1029.

[3] Gupta, S., Singh, M., and Madan, A. Eccentric distance sum: A novel graph invariant for predicting biological and physical properties. Journal of Mathematical Analysis and Applications 275, 1 (2002), 386–401.

[4] Hauweele, P., Hertz, A., Mélot, H., Ries, B., and Devillez, G. Maximum eccentric connectivity index of graphs with given diameter. ArXiv e-print 1808.10203 (2018).

[5] Ilić, A., and Gutman, I. Eccentric connectivity index of chemical trees. MATCH Commun. Math. Comput. Chem. 65 (2011).

[6] Karelson, M. Molecular descriptors in QSAR/QSPR. Wiley-Interscience. 2000.

[7] Kumar, V., Sardana, S., and Madan, A. K. Predicting anti-hiv activity of 2,3-diaryl-1,3-thiazolidin-4-ones: computational approach using reformed eccentric connectivity index. Journal of Molecular Modeling 10, 5 (Dec 2004), 399–407.

[8] Sardana, S., and Madan, A. Application of graph theory: Relationship of molecular connectivity index, wiener's index and eccentric connectivity index with diuretic activity. MATCH Commun. Math. Comput. Chem. 43 (03 2001).

[9] Sharma, V., Goswani, R., and Madan, A.K. Eccentric Connectivity Index: A Novel Highly Discriminating Topological Descriptor for Structure Property and Structure Activity Studies. J. Chem. Inf. Comput. Sci. 37 (1997), 273–282.

[10] Todeschini, R., and Consonni, V. Handbook of molecular descriptors. Wiley-VCH, Weinheim, vol. 11. 01 2000.

[11] Wiener, H. Structural determination of paraffin boiling points. Journal of the American Chemical Society 69, 1 (1947), 17–20.

[12] Zhou, B., and Du, Z. On eccenctric connectivity index. MATCH Commun. Math. Comput. Chem. 63 (2010), 181–198.