Yugoslav Journal of Operations Research 29 (2019), Number 2, 193–202 DOI: https://doi.org/10.2298/YJOR181115010D

MINIMUM ECCENTRIC CONNECTIVITY INDEX FOR GRAPHS WITH FIXED ORDER AND FIXED NUMBER OF PENDANT **VERTICES**

Gauvain DEVILLEZ

Computer Science Department, University of Mons, Mons, Belgium gauvain.devillez@umons.ac.be

Alain HERTZ

Department of Mathematics and Industrial Engineering, Polytechnique Moontréal, Montréal, Canada alain.hertz@gerad.ca

Hadrien MELOT ´ Computer Science Department, University of Mons, Mons, Belgium hadrien.melot@umons.ac.be

Pierre HAUWEELE Computer Science Department, University of Mons, Mons, Belgium pierre.hauweele@umons.ac.be

Received: November 2018 / Accepted: April 2019

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 . We characterize, with a new elegant proof, those graphs which have the smallest eccentric connectivity index among all connected graphs of a given order n . Then, 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 pendant vertices.

Keywords: Extremal Graph Theory, Eccentric Connectivity Index, Pendant Vertices. MSC: 05C35, 05C40.

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 [\[1\]](#page-9-5) was probably the first to publish results that consider chemical graphs. In an attempt to analyze the chemical properties of alkanes, Wiener [\[12\]](#page-9-2) has introduced 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 to help describe and understand the structure of molecules [\[11,](#page-9-6) [7\]](#page-9-8) by means of studies on quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR). Among these indices, the eccentric connectivity index 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 degree $d_G(v)$ of a vertex v in G is the number of edges incident to v, while the *eccentricity* $e_G(v)$ of v is the maximum distance between v and any other vertex in G, 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 [\[10\]](#page-9-4) and successfully used for mathematical models of biological activities of diverse nature [\[2,](#page-9-0) [3,](#page-9-9) [8,](#page-9-3) [9,](#page-9-7) [6\]](#page-9-10). Recently, Hauweele et al. [\[5\]](#page-9-1) have characterized those graphs which have the largest eccentric connectivity index among all connected graphs of a given order n . These results are summarized in Table [1,](#page-2-0) 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 .

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

- C_n is the chordless cycle of order *n*;
- $S_{n,x}$ 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.

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

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 of 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, $H_{8,3}$ and $H_{9,3}$ are drawn on Figure [1.](#page-2-1) Note that $H_{4,0} \simeq S_{4,2}$. Moreover, $H_{4,0}$ has two dominating vertices while $H_{4,1}$ and $H_{n,p}$ have exactly one dominating vertex for all $n \geq 5$ and $p \leq n-3$.

Figure 1: Two graphs with $p = 3$ pendant vertices .

In this paper, we first give an alternative proof to a result of Zhou and Du [\[13\]](#page-9-11) showing that the stars are the only graphs with smallest eccentric connectivity index among all connected graphs of a given order $n \geq 4$. These graphs have $n-1$ pendant 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 pendant vertices. A similar study appears in [\[4\]](#page-9-12) where bounds on the Randić index are given for graphs with fixed order and fixed number of pendant vertices.

196 G. Devillez, et al. / Minimum Eccentric Connectivity Index

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 K₃ and P₃ are the only connected graphs with 3 vertices. Since ξ^c (K₃) = $\xi^{c}(\mathsf{P}_{3})=6$, 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 [13]. 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 $\xi^{c}(G) \ge 2(n-1) + 4(n-2) = 6n - 10 > 3(n-1)$.
- If $x = 0$, then every pendant vertex v has $e_G(v) \geq 3$ since its only neighbor is a non-dominating vertex. Since the eccentricity of the non-pendant vertices is at least two, we have $d_G(v)e_G(v) \geq 3$ for all vertices v in G, which implies $\xi^{c}(G) \geq 3n > 3(n-1).$

 \Box

The above theorem states that the stars are the only graphs with smallest eccentric connectivity index among all connected graphs of a given order $n \geq 4$. All these extremal graphs have $n - 1$ pendant vertices. In the next section, we give a similar characterization for graphs with a fixed order n and a fixed number p of pendant vertices, where p is possibly strictly smaller than $n-1$.

3. MINIMIZING ξ^c for graphs with fixed order and FIXED NUMBER OF PENDANT VERTICES

Let G be a connected graph of order $n \geq 4$ with p pendant vertices. Clearly, $p \leq n-1$, and $G \simeq S_{n,1}$ if $p = n-1$. For $p = n-2$, let u and v be the two non-pendant 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 $n-2$ pendant 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 $n-2$ pendant vertices.

The above observations show that all graphs of order n with a fixed number $p \geq n-2$ of pendant 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 $p \leq n-3$ pendant vertices and one dominating vertex. Then $\xi^c(G) \geq \xi^c(H_{n,p})$, with equality if and only if $G \simeq H_{n,p}$.

Proof. The dominating vertex u in G has $d_G(u)e_G(u) = n-1$, the pendant 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-pendant 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 $G \simeq \mathsf{H}_{n,p}$. \Box

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

- If $n = 4$ then $\xi^c(G) \ge 12$, with equality if and only if $G \simeq K_4$.
- If $n = 5$ then $\xi^c(G) \ge 20$, 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 $\xi^{c}(G) \ge f(x) = -2x^{2} + 11x$. Since $2 \le x \le 4$, $f(2) =$ $14, f(3) = 15$, 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 $\xi^{c}(G) \ge f(x) = -2x^2 + 14x$. Since $2 \le x \le 5$, $f(2) = f(5) = 20$ 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 $p \leq n-3$ pendant 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-pendant 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 pendant 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 $p \le n - 3$, we have $\xi^{c}(G) \ge 5n - 2p + 3 > \xi^{c}(\mathsf{H}_{n,p})$.

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 pendant vertices, and w is the only dominating vertex in G' . It follows from Theorem [2](#page-4-0) 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,

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

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

$$
\xi^{c}(G) - \xi^{c}(G') = \sum_{x \in A \cup B \cup C \cup \{u\}} d_{G}(x)e_{G}(x) + (d_{G}(v)e_{G}(v) + d_{G}(w)e_{G}(w))
$$

\n
$$
- \sum_{x \in A \cup B \cup C \cup \{u\}} d_{G'}(x)e_{G'}(x) - (d_{G'}(v)e_{G'}(v) + d_{G'}(w)e_{G'}(w))
$$

\n
$$
\geq (2|A| + 4|B| + 2|C| + 8) - (2(|B'| + 2) + |A| + |B| + |C| + 2)
$$

\n
$$
= |A| + |C| + 3(|B'| + |B \setminus B'|) - 2|B'| + 2
$$

\n
$$
= |A| + |C| + |B'| + 3|B \setminus B'| + 2 > 0
$$

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

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 pendant vertices. As in the previous case, we have

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

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

$$
\xi^{c}(G) - \xi^{c}(G') \geq (2|A| + 4|B| + 2|C| + 4) - (2(|B'| + 2) + |A| + |B| + |C| + 2)
$$

= |A| + |C| + |B'| + 3|B \setminus B'| - 2.

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 $\xi^c(G) > \xi^c(G') \geq \xi^c(H_{n,p})$. 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 $|B'| \ge 1, |A| \ge 2$ or $|C| \ge 2$, then $\xi^c(G) > \xi^c(G') \ge \xi^c(H_{n,p})$.
- 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 $n > 4$, $C \neq \emptyset$. Also, since $p \leq n-3$, there is a non-pendant 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 pendant vertices : while v was pendant in G , but not u, the situation is the opposite in G'. Note also that Theorem 2 implies $\xi^c(G') \geq \xi^c(H_{n,p})$ 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 $\sum_{c \in C \setminus \{r\}} (d_G(c)e_G(c) - d_{G'}(c)e_{G'}(c) \ge 2)$.

Hence, $\xi^{c}(G) - \xi^{c}(G') \geq 2 - 1 + n - 3$ $\sum_{>0}$ $+ d_G(r) - 2$ $\sum_{\geq 0}$ $+2$ > 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 $\xi^c(G) > \xi^c(G') \geq \xi^c(H_{n,p})$. So, assume $|B'| = 1$ and $|C| \leq 1$:

- if $|C| = 0$ then $n = 4$, $p = 0$, $G \simeq C_4$ and $G' \simeq H_{4,0}$, 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 $G' \simeq H_{5,1}$, 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 pendant vertices. If $p \geq 1$, then G has at most one dominating vertex, and it follows from Theorems 2 and [4](#page-4-2) that $H_{n,p}$ 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](#page-4-1) 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 $H_{5,0}$, $S_{5,2}$, K_5 , and C_5 are the only candidates to minimize the

 \Box

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 $\xi^c(S_{6,2}) = 26 < 27 = \xi^c(H_{6,0}), \xi^c(S_{7,2}) = 32 >$ $30 = \xi^{c}(\mathsf{H}_{7,0})$ 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 $S_{6,2}$ is the only graph with maximum eccentric connectivity index when $n = 6$ and $p = 0$, while $H_{n,0}$ is the only optimal graph when $n \ge 7$ and $p = 0$. This is summarized in the following Corollary.

Corollary 5. Let G be a connected graph of order $n > 4$ with $p \leq n-3$ pendant vertices.

- If $p \geq 1$ then $\xi^c(G) \geq \xi^c(H_{n,p})$, with equality if and only if $G \simeq H_{n,p}$;
- If $p = 0$ then
	- $-$ if $n = 4$ then $\xi^c(G) \ge 12$, with equality if and only if $G \simeq K_4$;
	- $-$ 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 $\xi^c(G) \geq \xi^c(H_{n,0}),$ with equality if and only if $G \simeq H_{n,0}.$

4. CONCLUSION

We have given a new elegant proof for characterizing the connected graphs of fixed order that have the smallest eccentric connectivity index. We have then characterized those graphs which have the minimum eccentric connectivity index among all connected graphs with a fixed order n and a fixed number p of pendant vertices. Such a characterization for graphs with a fixed order n and a fixed size m was given in [13]. It reads as follows.

Theorem 6. 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 [5], where $E_{n,D,k}$ 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 7. Let G be a connected graph of order n with m edges, where $n-1 ≤$ $m \leq {n-1 \choose 2}$. 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, F.R.S., "On the mathematical theory of isomers", The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 47 (314) (1874) 444–447.
- [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] Hansen, P., and Mélot, H., "Variable neighborhood search for extremal graphs 6. analyzing bounds for the connectivity index", Journal of Chemical Information and Computer Sciences, 43 (1) (2003) 1–14.
- [5] Hauweele, P., Hertz, A., Mélot, H., Ries, B., and Devillez, G., "Maximum eccentric connectivity index for graphs with given diameter", $arXiv$ preprint $arXiv:1808.10203$, to appear in Discrete Applied Mathematics (2018).
- [6] Ilić, A., and Gutman, I., "Eccentric connectivity index of chemical trees", MATCH, Communications in Mathematical and in Computer Chemistry, 65 (3) (2011) 731–744.
- Karelson, M., Molecular Descriptors in QSAR/QSPR, Wiley-Interscience, 2000.
- [8] 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 (2004) 399–407.
- [9] Sardana, S., and Madan, A. K., "Application of graph theory: relationship of molecular connectivity index, Wiener's index and eccentric connectivity index with diuretic activity", Match. Communications in Mathematical and in Computer Chemistry, 43 (2001) 85–98.
- [10] Sharma, V., Goswami, R., and Madan, A., "Eccentric connectivity index: a novel highly discriminating topological descriptor for structure property and structure activity studies", Journal of chemical information and computer sciences, 37 (2) (1997) 273–282.
- [11] Todeschini, R., and Consonni, V., Handbook of molecular descriptors, Wiley-VCH, 2008.
- [12] Wiener, H., "Structural determination of paraffin boiling points", Journal of the American Chemical Society, 69 (1) (1947) 17–20.
- [13] Zhou, B., and Du, Z., "On eccentric connectivity index", MATCH. Communications in Mathematical and in Computer Chemistry, 63 (1) (2010) 181–198.