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Research Article

The Sombor index of trees and unicyclic graphs with given maximum degree

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Abstract

Let $d_G(v)$ be the degree of the vertex v in a graph G. The Sombor index of G is defined as $SO(G) = \sum_{uv\in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}$, which is a new vertex-degree-based topological index introduced by Gutman. Let $\mathscr{T}_{n,\Delta}$ and $\mathscr{U}_{n,\Delta}$ be the sets of trees and unicyclic graphs, respectively, with n vertices and maximum degree Δ. In this paper, the tree and the unicyclic graph with the minimum Sombor index from the sets $\mathscr{T}_{n,\Delta}$ and $\mathscr{U}_{n,\Delta}$, respectively, are characterized.

Keywords: Sombor index; tree; unicyclic graph; degree.

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1. Introduction

Let G be a simple undirected graph with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, $N_G(v)$ denotes the set of all neighbors of v, and $d_G(v) = |N_G(v)|$ denotes the degree of the vertex v in G. Denote by $\Delta(G)$ (or Δ) the maximum degree of G. A d-vertex of G is a vertex of degree d. In particular, 1-vertex is called the pendant vertex or the leaf. Denote by S_n, P_n and C_n the star, path and cycle with n vertices, respectively. Let $l(P_n) = |E(P_n)|$ and $l(C_n) = |E(C_n)|$ be the lengths of P_n and C_n, respectively. Let $T_{n,\Delta}$, shown in Figure 1, be the tree obtained by attaching a pendant edge to each of certain $n-\Delta-1$ non-central vertices of S_Δ, and let $U_{n,\Delta}$, shown in Figure 1, be the unicyclic graph obtained by attaching $2\Delta-n+1$ pendant vertices and $n-\Delta-1$ paths P_2 to one vertex of the cycle C_3.

A spider is a tree with at most one vertex of degree more than two and the unique vertex of degree more than two is called the hub of the spider. A leg of a spider is a path from the hub to one of the leaves. Let $S(a_1, a_2, \ldots, a_k)$ be a spider with k legs $P^1, P^2, \ldots, P^k$ for which the lengths $l(P^i) = a_i$ for $1 \le i \le k$. Note that $T_{n,\Delta}$ is also a spider. For convenience, denote by T_Δ the spider whose lengths of all Δ legs are greater than 2 (see Figure 1). Let U_Δ be a unicyclic graph obtained by attaching $\Delta-2$ paths of length at least 2 to a cycle (see Figure 1).

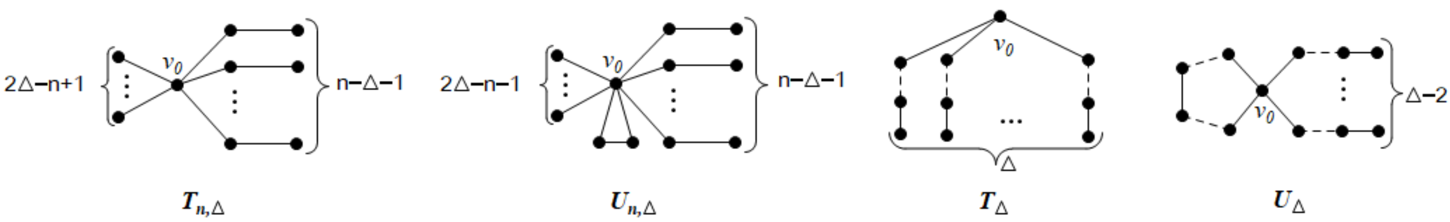

Figure 1: The graphs $T_{n,\Delta}$, $U_{n,\Delta}$, T_Δ, and U_Δ.

The Sombor index of a graph G is defined as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_G^2(u) + d_G^2(v)},$$

which is a novel vertex-degree-based topological index proposed by Gutman [6]. This new topological index immediately arises scholars' extensive attention. Deng et al. [4] showed that the Sombor index can help to predict these physico-chemical properties of octane isomers and confirmed suitability of the Sombor index in QSPR analysis. Redžepović [15] showed that the Sombor index may be used successfully on modeling thermodynamic properties of compounds due to the fact that the

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Sombor index has satisfactory prediction potential in modeling entropy and enthalpy of vaporization of alkanes. Das et al. [2] and Wang et al. [17] obtained the relations between the Sombor index and some other well-known vertex-degree-based topological index, such as the first Zagreb index, the second Zagreb index, the forgotten topological index and so on. For other related results, one may refer to [5, 7, 8, 10, 11, 14] and the references therein.

The extremal value problem of the topological index is of interest in graph theory and mathematical chemistry. The study of extremal value of the Sombor index of graphs has received much attention. Gutman [6] obtained extremal values of the Sombor index among the set of (connected) graphs and the set of trees. Cruz et al. [1] studied the Sombor index of chemical graphs, and characterized the graphs extremal with respect to the Sombor index over the following sets: chemical graphs, chemical trees, and hexagonal systems. Deng et al. [4] obtained a sharp upper bound for the Sombor index among all molecular trees with fixed numbers of vertices, and characterized those molecular trees achieving the extremal value. Liu [13] determined the first fourteen minimum chemical trees, the first four minimum chemical unicyclic graphs, the first three minimum chemical bicyclic graphs, the first seven minimum chemical tricyclic graphs. Réti et al. [16] characterized graphs with the maximum Sombor index in the classes of all connected unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic graphs of a fixed order. Das et al. [3] showed that the graph constructed from the star S_n by adding c edge(s) has the maximum Sombor index among all connected c-cyclic graphs of order n for $5 \le c \le n-2$, which confirms that the conjecture of Réti et al. [16] is true. Zhou et al. [18] determined the tree and the unicyclic graph with the maximum Sombor index among the set of trees and the set of unicyclic graphs with given matching number. Lin et al. [12] obtained lower and upper bounds on the spectral radius, energy and Estrada index of the Sombor matrix of graphs, and characterized the respective extremal graphs.

The purpose of this paper is to study the extremal value problem of Sombor index of trees and unicyclic graphs with given maximum degree. The following theorems are shown.

Theorem 1.1. *Let $n \ge 7$ and $T \in \mathscr{T}_{n,\Delta}$, where $3 \le \Delta \le n-2$.*

(i). *If $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$, then*

$$SO(T) \ge \Delta\sqrt{\Delta^2+4} + 2\sqrt{2}(n-2\Delta-1) + \sqrt{5}\Delta$$

with equality if and only if $T \cong T_\Delta$.

(ii). *If $\lfloor \frac{n-1}{2} \rfloor < \Delta \le n-2$, then*

$$SO(T) \ge (n-\Delta-1)\sqrt{\Delta^2+4} + (2\Delta-n+1)\sqrt{\Delta^2+1} + \sqrt{5}(n-\Delta-1)$$

with equality if and only if $T \cong T_{n,\Delta}$.

Corollary 1.1. *Let T be a chemical tree with $n \ge 9$ vertices. If $\Delta = 3$ or 4, then*

$$SO(T) \ge 2\sqrt{2}n + 3\sqrt{13} + 3\sqrt{5} - 14\sqrt{2} \quad \text{or} \quad SO(T) \ge 2\sqrt{2}n + 12\sqrt{5} - 18\sqrt{2}$$

with equality if and only if $T \cong T_3$ or $T \cong T_4$.

Theorem 1.2. *Let $n \ge 5$ and $U \in \mathscr{U}_{n,\Delta}$, where $3 \le \Delta \le n-2$.*

(i). *If $3 \le \Delta \le \lfloor \frac{n+1}{2} \rfloor$, then*

$$SO(U) \ge \Delta\sqrt{\Delta^2+4} + 2\sqrt{2}(n-2\Delta+2) + \sqrt{5}(\Delta-2)$$

with equality if and only if $U \cong U_\Delta$.

(ii). *If $\lfloor \frac{n+1}{2} \rfloor < \Delta \le n-2$, then*

$$SO(U) \ge (n-\Delta+1)\sqrt{\Delta^2+4} + (2\Delta-n-1)\sqrt{\Delta^2+1} + \sqrt{5}(n-\Delta-1) + 2\sqrt{2}$$

with equality if and only if $U \cong U_{n,\Delta}$.

Corollary 1.2. *Let U be a chemical unicyclic graph with $n \ge 7$ vertices. If $\Delta = 3$ or 4, then*

$$SO(U) \ge 2\sqrt{2}n + 3\sqrt{13} + \sqrt{5} - 8\sqrt{2} \quad \text{or} \quad SO(U) \ge 2\sqrt{2}n + 10\sqrt{5} - 12\sqrt{2}$$

with equality if and only if $U \cong U_3$ or $U \cong U_4$.

2. Preliminaries

The distance between two vertices $u, v \in V(G)$, denoted by $d_G(u, v)$, is defined as the length of a shortest path between u and v. Denote by $\overline{G}$ the complement of G and by P_{uv} the path between vertices u and v. Let $G - u$ denote the graph that arises from a graph G by deleting the vertex $u \in V(G)$ and all the edges incident with u. Let $G - uv$ denote the graph that arises from G by deleting the edge $uv \in E(G)$. Similarly, $G + uv$ is the graph that arises from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$.

Lemma 2.1. [9] *Let $U \subseteq \mathbb{R}$ be an open interval and $f : U \to U$ a convex function. Let $a_1 \geq a_2 \geq \ldots \geq a_n$ and $b_1 \geq b_2 \geq \ldots \geq b_n$ be such elements in U that inequalities $a_1 + a_2 + \ldots + a_n \geq b_1 + b_2 + \ldots + b_i$ hold for every $i \in \{1, 2, \ldots, n\}$ and equality holds for $i = n$. Then*

$$f(a_1) + f(a_2) + \cdots + f(a_n) \geq f(b_1) + f(b_2) + \cdots + f(b_n).$$

Lemma 2.2. *For w_0, $x_0 \in V(G)$ (where w_0, x_0 are not necessarily distinct), suppose that $w_1 w_2 \ldots w_k$, $x_1 x_2 \ldots x_h$ are two path components in $G - w_0$ and $G - x_0$, respectively, where $k, h \geq 1$ and w_k, x_h are pendant vertices of G. If $d_G(x_0) = s \geq 3$, $N_G(x_0) = \{x_1, v_1, v_2, \ldots, v_{s-1}\}$, $d_G(v_i) \geq 1$ for $1 \leq i \leq s-1$, let G' be a new graph with vertex set $V(G') = V(G)$ and edge set $E(G') = G - x_0x_1 + w_kx_1$, see Figure 2. When $w_0 = x_0$, G' is said to be obtained by running graph transformation $\mathbf{A}_1$ of G; when $w_0 \neq x_0$, G' is said to be obtained by running graph transformation $\mathbf{A}_2$ of G. Then $SO(G) > SO(G')$.*

Figure 2: An illustration of Lemma 2.2.

Proof. From given conditions, $d_G(x_0) = s$, $d_{G'}(x_0) = s - 1$, $d_G(w_k) = 1$, $d_{G'}(w_k) = 2$ and for any $v \in V(G) \setminus \{x_0, w_k\}$, $d_G(v) = d_{G'}(v)$. Since $d_G(x_0) = s \geq 3$, by Lemma 2.1, we have

$$\begin{aligned} SO(G) - SO(G') &= \sum_{uv \in E(G)} \sqrt{d_G^2(u) + d_G^2(v)} - \sum_{uv \in E(G')} \sqrt{d_{G'}^2(u) + d_{G'}^2(v)} \\ &= \sum_{i=1}^{s-1} \left[\sqrt{d_G^2(x_0) + d_G^2(v_i)} - \sqrt{d_{G'}^2(x_0) + d_G^2(v_i)}\right] + \sqrt{d_G^2(x_0) + d_G^2(x_1)} \\ &\quad + \sqrt{d_G^2(w_{k-1}) + d_G^2(w_k)} - \sqrt{d_{G'}^2(w_{k-1}) + d_{G'}^2(w_k)} - \sqrt{d_{G'}^2(w_k) + d_{G'}^2(x_1)}. \end{aligned}$$

(i) If $w_0 = x_0$, $k = h = 1$, and $x_1 = v_{s-1}$, then

$$\begin{aligned} SO(G) - SO(G') &= \sum_{i=1}^{s-2} \left[\sqrt{s^2 + d_G^2(v_i)} - \sqrt{(s-1)^2 + d_G^2(v_i)}\right] + 2\sqrt{s^2 + 1} - \sqrt{(s-1)^2 + 4} - \sqrt{5} \\ &> 2\sqrt{s^2 + 1} - \sqrt{(s-1)^2 + 4} - \sqrt{5} \\ &> 0. \end{aligned}$$

(ii) If $w_0 \neq x_0$ and $k = h = 1$, then

$$\begin{aligned} SO(G) - SO(G') &= \sum_{i=1}^{s-1} \left[\sqrt{s^2 + d_G^2(v_i)} - \sqrt{(s-1)^2 + d_G^2(v_i)}\right] + \sqrt{s^2 + 1} + \sqrt{d_G^2(w_0) + 1} - \sqrt{d_G^2(w_0) + 4} - \sqrt{5} \\ &> \sqrt{s^2 + 1} + \sqrt{d_G^2(w_0) + 1} - \sqrt{d_G^2(w_0) + 4} - \sqrt{5} \\ &> 0. \end{aligned}$$

(iii) If $k \geq 2$, $h = 1$, then

$$SO(G) - SO(G') = \sum_{i=1}^{s-1} \left[\sqrt{s^2 + d_G^2(v_i)} - \sqrt{(s-1)^2 + d_G^2(v_i)}\right] + \sqrt{s^2 + 1} + \sqrt{5} - \sqrt{8} - \sqrt{5} > \sqrt{s^2 + 1} - \sqrt{8} > 0.$$

(iv) If $k, h \geq 2$, then

$$\begin{aligned} SO(G) - SO(G') &= \sum_{i=1}^{s-1} \left[\sqrt{s^2 + d_G^2(v_i)} - \sqrt{(s-1)^2 + d_G^2(v_i)} \right] + \sqrt{s^2+4} + \sqrt{5} - 2\sqrt{8} \\ &> \sqrt{s^2+4} + \sqrt{5} - 2\sqrt{8} \\ &> \sqrt{13} + \sqrt{5} - 2\sqrt{8} \\ &> 0. \end{aligned}$$

Combining the above arguments, we have the proof. □

3. The proof of Theorem 1.1

In this section, we determine the tree with the minimum Sombor index among trees with n vertices and maximum degree Δ. If $\Delta = 2$, then $\mathscr{T}_{n,\Delta} = \{P_n\}$. If $\Delta = n-1$, then $\mathscr{T}_{n,\Delta} = \{S_n\}$. From now on, we assume that $3 \leq \Delta \leq n-2$.

Proof of Theorem 1.1. Let T be a tree with n vertices and maximum degree Δ that minimize the Sombor index and let v_0 be a Δ-vertex of T. We will show the following Claims 1-3, which, put together, will get our proof.

Claim 1. T is a spider.

Proof. Suppose T is not a spider. There exists $v \in V(T) \setminus \{v_0\}$, such that $d_T(v) \geq 3$. Then we can get a new tree $T_1 \in \mathscr{T}_{n,\Delta}$ by running graph transformation $\mathbf{A}_1$ on v. By Lemma 2.2, $SO(T_1) < SO(T)$, which contradicts the choice of T. Thus T is a spider. □

Let $T = S(a_1, a_2, \ldots, a_\Delta)$ with Δ legs $P^1, P^2, \ldots, P^\Delta$, and the lengths $l(P^i) = a_i$ for $1 \leq i \leq \Delta$. Without loss of generality, we assume that $a_1 \geq a_2 \geq \ldots \geq a_\Delta$.

Claim 2. If $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$, then $a_\Delta \geq 2$.

Proof. Suppose $a_\Delta = 1$. Since $n - 1 \geq 2\Delta$, we have $a_1 \geq 3$. Let $P^1 = v_0 v_1^1 v_2^1 \ldots v_s^1$ where $s \geq 3$ and $P_\Delta = v_0 v_\Delta$. Let $T_2 = T - v_{s-1}^1 v_s^1 + v_\Delta v_s^1$, by Lemma 2.2, we have $SO(T) - SO(T_2) = \sqrt{\Delta^2+1} + \sqrt{8} - \sqrt{\Delta^2+4} - \sqrt{5} > 0$, which contradicts the choice of T. Thus $a_\Delta \geq 2$, that is, $T \cong T_\Delta$. □

Claim 3. If $\lfloor \frac{n-1}{2} \rfloor < \Delta \leq n-2$, then $a_1 \leq 2$.

Proof. Suppose $a_1 \geq 3$. Since $n - 1 < 2\Delta$, we have $a_\Delta = 1$. Let $P^1 = v_0 v_1^1 v_2^1 \ldots v_s^1$ where $s \geq 3$ and $P_\Delta = v_0 v_\Delta$. Similar to the proof of Claim 2, let $T_3 = T - v_{s-1}^1 v_s^1 + v_\Delta v_s^1$, then $SO(T) > SO(T_3)$, which contradicts the choice of T. Thus $a_1 \leq 2$, that is, $T \cong T_{n,\Delta}$. □

By direct calculations, we get $SO(T_\Delta) = \Delta\sqrt{\Delta^2+4} + \sqrt{8}(n - 2\Delta - 1) + \sqrt{5}\Delta$ and

$$SO(T_{n,\Delta}) = (n - \Delta - 1)\sqrt{\Delta^2+4} + (2\Delta - n + 1)\sqrt{\Delta^2+1} + \sqrt{5}(n - \Delta - 1).$$

This completes the proof of Theorem 1.1. □

4. The proof of Theorem 1.2

In this section, we determine the unicyclic graph with the minimum Sombor index among unicyclic graphs with n vertices and maximum degree Δ. If $\Delta = 2$, then $\mathscr{U}_{n,\Delta} = \{C_n\}$. If $\Delta = n-1$, then $\mathscr{U}_{n,\Delta} = \{S_n + e\}$, where e is a edge in $\overline{S}_n$. Next, we assume that $3 \leq \Delta \leq n-2$.

Proof of Theorem 1.2. Let U be a unicyclic graph with n vertices and maximum degree Δ that minimize the Sombor index. Suppose C is the unique cycle of U. If there exist a Δ-vertex on C, then we chose it and denote by v_0; otherwise, chose any Δ-vertex, also denote by v_0. First, we assume that $v_0 \notin V(C)$. Then there is a vertex $v \in V(C)$ such that $d_U(v, v_0) = \min\{d_U(u, v_0) \mid u \in V(C)\}$, clearly, $d_U(v) \geq 3$. We will show the following Claims 1-5, which, put together, will get our proof.

Claim 1. For any $u \in V(U) \setminus \{v_0, v\}$, $d_U(u) \leq 2$.

Proof. If the claim is not true, there are three cases:

Case i. there exists $u \in V(U) \setminus (V(C) \cup P_{vv_0})$ such that $d_U(u) \geq 3$. Then we can get a new unicyclic graph $U_1 \in \mathscr{U}_{n,\Delta}$ by running graph transformation $\mathbf{A}_1$ on u. By Lemma 2.2, $SO(U) > SO(U_1)$, which contradicts the choice of U.

Case ii. there exists $u \in (V(C) \cup P_{vv_0}) \setminus \{v, v_0\}$ such that $d_U(u) \geq 4$. There are at least two paths starting from u to pendant vertices of U, then by running transformation $\mathbf{A}_1$ on u, we can get a contradiction.

Case iii. there exists $u \in (V(C) \cup P_{vv_0}) \setminus \{v, v_0\}$ such that $d_U(u) = 3$. Let $uu_1u_2 \ldots u_s$ be the path from u to pendant vertex u_s, where $s \geq 1$ and $d_U(u_i) = 2$ for $1 \leq i \leq s-1$. And let $v_0v_1v_2 \ldots v_t$ be one of the paths from v_0 to a pendant vertex v_t, where $t \geq 1$ and $d_U(v_i) = 2$ for $1 \leq i \leq t-1$. Let $U_2 = U - uu_1 + v_su_1$, then U_2 is obtained by running transformation $\mathbf{A}_2$ from U and $U_2 \in \mathscr{U}_{n,\Delta}$. By Lemma 2.2, we have $SO(U) > SO(U_2)$, which contradicts the choice of U.

Combining the above cases, we have $d_U(u) \leq 2$ for any $u \in V(U) \setminus \{v_0, v\}$. □

Claim 2. $d_U(v) \leq 3$.

Proof. If $d_U(v) \geq 5$, there are at least two paths starting from v to pendant vertices of U, similarly, by running transformation $\mathbf{A}_1$, we can get a contradiction. If $d_U(v) = 4$, by running transformation $\mathbf{A}_2$, we can also get a contradiction. □

Denote by $v_1, v_2, \ldots, v_\Delta$ the neighbors of v_0, where $v_1 \in V(P_{vv_0})$.

Claim 3. $v = v_0$, that is to say, there must be $v_0 \in V(C)$.

Proof. For otherwise, we can get a new unicyclic graph $U_3 = U - \{v_0v_i \mid 2 \leq i \leq \Delta-2\} + \{vv_i \mid 2 \leq i \leq \Delta-2\}$ and $U_3 \in \mathscr{U}_{n,\Delta}$. For $\Delta - 1 \leq i \leq \Delta$, $d_U(v_i) \leq 2$, we have

$$\begin{aligned} SO(U) - SO(U_3) &= 2\sqrt{3^2+2^2} + \sum_{i=\Delta-1}^{\Delta} \sqrt{\Delta^2 + d_U^2(v_i)} - 2\sqrt{\Delta^2+2^2} - \sum_{i=\Delta-1}^{\Delta} \sqrt{3^2 + d_U^2(v_i)} \\ &= \left[2\sqrt{3^2+2^2} - \sum_{i=\Delta-1}^{\Delta} \sqrt{3^2 + d_U^2(v_i)}\right] - \left[2\sqrt{\Delta^2+2^2} - \sum_{i=\Delta-1}^{\Delta} \sqrt{\Delta^2 + d_U^2(v_i)}\right] \\ &\geq 0. \end{aligned}$$

We have now in U_3, $d_{U_3}(v) = \Delta$ and $d_{U_3}(v_0) = 3$, then there are at least two paths starting from v_0 to pendant vertices of U_3, similarly, by running transformation $\mathbf{A}_1$ on v_0, we can get a contradiction, which contradicts the choice of U. Thus $v_0 \in V(C)$. □

By Claims 1-3, U is a unicyclic graph obtained by attaching $\Delta - 2$ paths to the vertex v_0 of cycle C. Let $v_1, v_2 \in V(C)$. Similar to the proof of Theorem 1.1, denote by P^i the path from v_0 to a pendant vertex of U and $v_i \in P^i$, where $3 \leq i \leq \Delta$. Without loss of generality, we can assume that $l(P^3) \geq l(P^4) \geq \ldots \geq l(P^\Delta)$.

Claim 4. If $3 \leq \Delta \leq \lfloor \frac{n+1}{2} \rfloor$, then $l(P^\Delta) \geq 2$.

Proof. Suppose that $l(P^\Delta) = 1$. Since $n - 3 \geq 2(\Delta - 2)$, we have the following two cases:

Case i. $l(P^3) \geq 3$. Let $P^\Delta = v_0v_\Delta$ and $P^3 = v_0v_3v_2^3 \ldots v_s^3$, where $s \geq 3$. Let $U_4 = U - v_{s-1}^3v_s^3 + v^\Delta v_s^3$, by Lemma 2.2, we have $SO(U) - SO(U_4) = \sqrt{\Delta^2+1} + \sqrt{8} - \sqrt{\Delta^2+4} - \sqrt{5} > 0$, which contradicts the choice of U.

Case ii. $l(P^3) = 2$ and $|E(C)| \geq 4$. Let x, y, z be three vertices on C different from v_0 such that $xy, yz \in E(C)$. Let $U_5 = U - xy - yz + xz + v_\Delta y$, we have $SO(U) - SO(U_5) = \sqrt{\Delta^2+1} + \sqrt{8} - \sqrt{\Delta^2+4} - \sqrt{5} > 0$, which contradicts the choice of U.

Thus, $l(P^\Delta) \geq 2$, that is, $U \cong U_\Delta$. □

Claim 5. If $\lfloor \frac{n+1}{2} \rfloor < \Delta \leq n-2$, then $l(P^3) \leq 2$ and $|E(C)| = 3$.

Proof. Note that $n - 3 < 2(\Delta - 2)$. If $l(P^3) \geq 3$ or $|E(C)| \geq 4$, then $l(P^\Delta) = 1$. Similar to the proof of Claim 4, we can get a contradiction. Thus $l(P^3) \leq 2$ and $|E(C)| = 3$, that is, $U \cong U_{n,\Delta}$. □

By direct calculations, we get $SO(U_\Delta) = \Delta\sqrt{\Delta^2+4} + \sqrt{8}(n - 2\Delta + 2) + \sqrt{5}(\Delta - 2)$ and

$$SO(U_{n,\Delta}) = (n - \Delta + 1)\sqrt{\Delta^2+4} + (2\Delta - n - 1)\sqrt{\Delta^2+1} + \sqrt{5}(n - \Delta - 1) + \sqrt{8}.$$

This completes the proof of Theorem 1.2. □

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