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On four Sombor-index-like graph invariants of chemical graphs with a given order, number of edges and pendent vertices

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Abstract. Recently, Gutman constructed six novel graph invariants in view of geometric arguments and defined them as Sombor-index-like graph invariants, denoted by $SO_1, SO_2, \cdots, SO_6$. Compared with some popular and commonly used indices, nearly all these six graph invariants have high accuracy in predicting physical and chemical properties. Therefore, in this article, we obtain a lower bound on four Sombor-index-like graph invariants (SO_1, SO_2, SO_5 and SO_6) for all chemical (n, m, k)-graphs (chemical graphs of order n having m edges and k pendent vertices), and characterize those chemical (n, m, k)-graphs achieving the extremal value.

1. Introduction

The topological indices of graphs are useful tools to characterize the chemical or physical properties of compounds[7, 8]. So many topological indices have been proposed and investigated, especially the topological indices which are defined via end-vertices' degrees of edges of the considered chemical graph. Lately in [5], Gutman proposed six new graph invariants by using geometric arguments and called them Sombor-index-like graph invariants. For a graph G, these Sombor-index-like graph invariants, denoted by SO_i $(i = 1, 2, \cdots, 6)$, are defined as

$$SO_1(G) = \frac{1}{2} \sum_{uv \in E(G)} |deg_G^2(u) - deg_G^2(v)|, \tag{1}$$

$$SO_2(G) = \sum_{uv \in E(G)} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)}, \tag{2}$$

$$SO_3(G) = \sum_{uv \in E(G)} \sqrt{2}\frac{deg_G^2(u) + deg_G^2(v)}{deg_G(u) + deg_G(v)}\pi,$$

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$$SO_4(G) = \frac{1}{2}\sum_{uv\in E(G)}\Big(\frac{deg_G^2(u)+deg_G^2(v)}{deg_G(u)+deg_G(v)}\Big)^2\pi,$$

$$SO_5(G) = \sum_{uv\in E(G)}\frac{2|deg_G^2(u)-deg_G^2(v)|}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\pi, \tag{3}$$

$$SO_6(G) = \sum_{uv\in E(G)}\Big(\frac{deg_G^2(u)-deg_G^2(v)}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\Big)^2\pi, \tag{4}$$

where $deg_G(u)$ and $deg_G(v)$ stand for the degrees of vertex u and v in G, respectively. Recently, studying the properties of Sombor-index-like graph invariants is a research focus. Tang, Li and Deng [11] characterized some extremal trees and molecular trees of Sombor-index-like graph invariants, and they concluded that compared with some popular and commonly used indices, nearly all these six graph invariants have high accuracy in predicting physical and chemical properties. Ali et al. [1] solved most of the open problems proposed in [11]. In addition to the results on Sombor-index-like graph invariants already obtained above, for details on the fashioned Sombor index, one can see the recent papers [3, 4, 10, 13], review papers [6, 9] and the references therein.

In this article, just simple connected graphs are taken into account. For such a graph G, we represent the sets of vertices and edges by $V(G)$ and $E(G)$, respectively. Define $m = |E(G)|$ and $n = |V(G)|$. For $m = n-1$, $m = n$ and $m = n+1$, G is a tree, unicyclic graph and bicycle graph, respectively. A one-degree vertex is called a pendent vertex. Let $G - pq$ and $G + pq$ be the graphs obtained from G by deleting the edge $pq \in E(G)$ and by joining two vertices $p, q \in V(G)$ ($pq \notin E(G)$), respectively. Denoted by n_i the number of vertices of degree i in G. Let $P_s = z_0z_1\cdots z_s$ be the path in G with $deg_G(z_1) = deg_G(z_2) = \cdots = deg_G(z_{s-1}) = 2$ (unless $s = 1$). If $deg_G(z_0) \geq 3$ and $deg_G(z_s) = 1$, then P_s is said to be a pendent path of G. If $deg_G(z_0) \geq 3$ and $deg_G(z_s) \geq 3$, then P_s is said to be an internal path of G.

Recall that a chemical graph is a graph G with $deg_G(x) \leq 4$ for all $x \in V(G)$. Let (n, m, k)-graph be the graph of order n with m edges and k pendent vertices. For an (n, m, k)-graph G, define $E_1 = \{pq \in E(G)|deg_G(q) = 2, deg_G(p) = 1\}$, $E_2 = \{pq \in E(G)|deg_G(q) \geq 3,\ deg_G(p) = 1\}$, $E_3 = \{pq \in E(G)|deg_G(p) = 2, deg_G(q) = 2\}$, $E_4 = \{pq \in E(G)|deg_G(p) = 2, deg_G(q) \geq 3\}$ and $E_5 = \{pq \in E(G)|deg_G(p) \geq 3, deg_G(q) \geq 3\}$. For terminology and notation, not defined here, we refer the readers to relevant standard books[2, 12, 14].

In this work, by analyzing the irregularity of the chemical (n, m, k)-graphs, we get a lower bound of four Sombor-index-like graph invariants (SO_1, SO_2, SO_5 and SO_6) for all chemical (n, m, k)-graphs. Furthermore, we characterize the corresponding extremal graphs.

2. Preliminaries

Lemma 2.1. *If*

$$f_1(x,a) = \frac{x^2-a^2}{x^2+a^2},\ f_2(x,a) = \frac{2(x^2-a^2)}{\sqrt{2}+2\sqrt{x^2+a^2}}\pi,$$
$$f_3(x,a) = \Big(\frac{x^2-a^2}{\sqrt{2}+2\sqrt{x^2+a^2}}\Big)^2\pi,$$

where $x > a \geq 1$, then $f_1(x,a)$, $f_2(x,a)$ and $f_3(x,a)$ are increasing for x, respectively.

Proof. For $x > a \geq 1$, we have

$$\frac{\partial f_1(x,a)}{\partial x} = \frac{4xa^2}{(x^2+a^2)^2} > 0,$$

$$\begin{aligned}\frac{\partial f_2(x,a)}{\partial x} &= 2\pi\frac{2x(\sqrt{2}+2\sqrt{x^2+a^2}) - (x^2-a^2)\frac{2x}{\sqrt{x^2+a^2}})}{(\sqrt{2}+2\sqrt{x^2+a^2})^2}\\ &= 2\pi\frac{2\sqrt{2}x\sqrt{x^2+a^2}+2x^3+6xa^2}{(\sqrt{2}+2\sqrt{x^2+a^2})^2\sqrt{x^2+a^2}} > 0,\end{aligned}$$

$$\begin{aligned}\frac{\partial f_3(x,a)}{\partial x} &= 2\pi\Big(\frac{x^2-a^2}{\sqrt{2}+2\sqrt{x^2+a^2}}\Big)\frac{2x(\sqrt{2}+2\sqrt{x^2+a^2}) - (x^2-a^2)\frac{2x}{\sqrt{x^2+a^2}})}{(\sqrt{2}+2\sqrt{x^2+a^2})^2}\\ &= 2\pi\Big(\frac{x^2-a^2}{\sqrt{2}+2\sqrt{x^2+a^2}}\Big)\frac{2\sqrt{2}x\sqrt{x^2+a^2}+2x^3+6xa^2}{(\sqrt{2}+2\sqrt{x^2+a^2})^2\sqrt{x^2+a^2}} > 0.\end{aligned}$$

Hence the lemma holds. □

Lemma 2.2. *Let*

$$g(c) = \Big(\frac{c^2-1}{\sqrt{2}+2\sqrt{c^2+1}}\Big)^2 - \Big(\frac{c^2-4}{\sqrt{2}+2\sqrt{c^2+4}}\Big)^2 - \Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2.$$

Then $g(c) > 0$ for $c > 2$.

Proof. For $c \geq 2$, we derive

$$\begin{aligned}g'(c) =& 4c\Big[\frac{(c^2-1)[\sqrt{2}\sqrt{c^2+1}+c^2+3]}{(\sqrt{2}+2\sqrt{c^2+1})^3\sqrt{c^2+1}} - \frac{(c^2-4)[\sqrt{2}\sqrt{c^2+4}+c^2+12]}{(\sqrt{2}+2\sqrt{c^2+4})^3\sqrt{c^2+4}}\Big]\\ =&4c\frac{(c^2-1)[\sqrt{2}\sqrt{c^2+1}+c^2+3](\sqrt{2}+2\sqrt{c^2+4})^3\sqrt{c^2+4}}{(\sqrt{2}+2\sqrt{c^2+1})^3\sqrt{c^2+1}(\sqrt{2}+2\sqrt{c^2+4})^3\sqrt{c^2+4}}\\ &-4c\frac{(c^2-4)[\sqrt{2}\sqrt{c^2+4}+c^2+12](\sqrt{2}+2\sqrt{c^2+1})^3\sqrt{c^2+1}}{(\sqrt{2}+2\sqrt{c^2+1})^3\sqrt{c^2+1}(\sqrt{2}+2\sqrt{c^2+4})^3\sqrt{c^2+4}}\\ =&4c\frac{g_1(c)}{(\sqrt{2}+2\sqrt{c^2+1})^3\sqrt{c^2+1}(\sqrt{2}+2\sqrt{c^2+4})^3\sqrt{c^2+4}},\end{aligned}$$

where $g_1(c) = (c^2-1)[\sqrt{2}\sqrt{c^2+1}+c^2+3](\sqrt{2}+2\sqrt{c^2+4})^3\sqrt{c^2+4} - (c^2-4)[\sqrt{2}\sqrt{c^2+4}+c^2+12](\sqrt{2}+2\sqrt{c^2+1})^3\sqrt{c^2+1}$.

Expanding $g_1(c)$, we have that

$$\begin{aligned}g_1(c) =& 496\sqrt{2}\sqrt{c^2+1} - 70\sqrt{2}\sqrt{c^2+4} + 12\sqrt{c^2+1}\sqrt{c^2+4} + 1308c^2 + 444c^4\\ &+ 564\sqrt{2}c^2\sqrt{c^2+1} - 42\sqrt{2}c^4\sqrt{c^2+1} + 156\sqrt{2}c^2\sqrt{c^2+4} - 4\sqrt{2}c^6\sqrt{c^2+1}\\ &+ 78\sqrt{2}c^4\sqrt{c^2+4} + 4\sqrt{2}c^6\sqrt{c^2+4} + 144c^2\sqrt{c^2+1}\sqrt{c^2+4} + 432\\ =& 2\sqrt{2}\sqrt{c^2+4}(2c^6+39c^4+78c^2-35) - 2\sqrt{2}\sqrt{c^2+1}(2c^6+21c^4-282c^2-248)\\ &+ 444c^4 + 1308c^2 + 432 + (144c^2+12)\sqrt{c^2+4}\sqrt{c^2+1}.\end{aligned}$$

Let $t = c^2 \geq 4$. Note that

$$\begin{aligned}&(c^2+4)(2c^6+39c^4+78c^2-35)^2 - (c^2+1)(2c^6+21c^4-282c^2-248)^2\\ =&(t+4)(2t^3+39t^2+78t-35)^2 - (t+1)(2t^3+21t^2-282t-248)^2\\ =&84t^6+3060t^5+26799t^4-29142t^3-201024t^2-221991t-56604.\end{aligned}$$

Let $g_2(t) = 84t^6 + 3060t^5 + 26799t^4 - 29142t^3 - 201024t^2 - 221991t - 56604$, where $t \geq 4$. Hence

$$\begin{aligned} g_2'(t) =& 504t^5 + 15300t^4 + 107196t^3 - 87426t^2 - 402048t - 221991 \\ =& (504t^5 - 221991) + t^2(15300t^2 - 87426) + t(107196t^2 - 402048) \\ \geq& (504 \times 4^5 - 221991) + t^2(15300 \times 4^2 - 87426) + t(107196 \times 4^2 - 402048) \\ =& 294105 + 157374t^2 + 1313088t > 0. \end{aligned}$$

So $g_2'(t) > 0$ for $t \geq 4$ and $g_2(t) \geq g_2(4) = 4312008 > 0$. It implies that $(c^2+4)(2c^6+39c^4+78c^2-35)^2 - (c^2+1)(2c^6+21c^4-282c^2-248)^2 > 0$. Moreover, $444c^4 + 1308c^2 + 432 + (144c^2+12)\sqrt{c^2+4}\sqrt{c^2+1} > 0$ for $c \geq 2$. These yield $g_1(c) > 0$ and $g(c)$ is increasing for $c \geq 2$. Hence for $c > 2$, $g(c) > g(2) = 0$. □

Lemma 2.3. *Let*

$$h(a,b) = \left(\frac{a^2-4}{\sqrt{2}+2\sqrt{a^2+4}}\right)^2 + \left(\frac{b^2-4}{\sqrt{2}+2\sqrt{b^2+4}}\right)^2 - \left(\frac{a^2-b^2}{\sqrt{2}+2\sqrt{a^2+b^2}}\right)^2.$$

Then $h(a,b) > 0$ for $a \geq b \geq 3$, where a, b are integers.

Proof. By calculating the partial derivative of the function $h(a,b)$ with respect to a, we have

$$\begin{aligned} \frac{\partial h(a,b)}{\partial a} =& 4a\frac{(a^2-4)[\sqrt{2}\sqrt{a^2+4}+a^2+12](\sqrt{2}+2\sqrt{a^2+b^2})^3\sqrt{a^2+b^2}}{(\sqrt{2}+2\sqrt{a^2+4})^3\sqrt{a^2+4}(\sqrt{2}+2\sqrt{a^2+b^2})^3\sqrt{a^2+b^2}} \\ &- 4a\frac{(a^2-b^2)[\sqrt{2}\sqrt{a^2+b^2}+a^2+3b^2](\sqrt{2}+2\sqrt{a^2+4})^3\sqrt{a^2+4}}{(\sqrt{2}+2\sqrt{a^2+4})^3\sqrt{a^2+4}(\sqrt{2}+2\sqrt{a^2+b^2})^3\sqrt{a^2+b^2}} \\ =& 4a\frac{h_1(a,b)}{(\sqrt{2}+2\sqrt{a^2+4})^3\sqrt{a^2+4}(\sqrt{2}+2\sqrt{a^2+b^2})^3\sqrt{a^2+b^2}}, \end{aligned}$$

where $h_1(a,b) = (a^2-4)[\sqrt{2}\sqrt{a^2+4}+a^2+12](\sqrt{2}+2\sqrt{a^2+b^2})^3\sqrt{a^2+b^2} - (a^2-b^2)[\sqrt{2}\sqrt{a^2+b^2}+a^2+3b^2](\sqrt{2}+2\sqrt{a^2+4})^3\sqrt{a^2+4}$.

Expanding $h_1(a,b)$, it follows that

$$\begin{aligned} h_1(a,b) =& 144b^4 - 576a^2 - 464a^4 - 576b^2 - 16\sqrt{a^2+4}\sqrt{a^2+b^2} - 1024a^2b^2 \\ &+ 292a^2b^4 - 12a^4b^2 + 32a^4b^4 - 96\sqrt{2}\sqrt{a^2+b^2} - 736\sqrt{2}a^2\sqrt{a^2+b^2} \\ &+ 22\sqrt{2}a^4\sqrt{a^2+b^2} + 4\sqrt{2}a^6\sqrt{a^2+b^2} - 400\sqrt{2}b^2\sqrt{a^2+b^2} \\ &- 192a^2\sqrt{a^2+4}\sqrt{a^2+b^2} + 4b^2\sqrt{a^2+4}\sqrt{a^2+b^2} - 48\sqrt{2}a^2\sqrt{a^2+4} \\ &- 70\sqrt{2}a^4\sqrt{a^2+4} - 4\sqrt{2}a^6\sqrt{a^2+4} - 48\sqrt{2}b^2\sqrt{a^2+4} + 118\sqrt{2}b^4\sqrt{a^2+4} \\ &+ 172\sqrt{2}a^2b^2\sqrt{a^2+b^2} + 20\sqrt{2}a^4b^2\sqrt{a^2+b^2} + 48a^2b^2\sqrt{a^2+4}\sqrt{a^2+b^2} \\ &- 152\sqrt{2}a^2b^2\sqrt{a^2+4} + 44\sqrt{2}a^2b^4\sqrt{a^2+4} - 8\sqrt{2}a^4b^2\sqrt{a^2+4} \\ =& a^4(32b^4 - 12b^2 - 464) + a^2(292b^4 - 1024b^2 - 576) + 114b^4 - 576b^2 \\ &+ (48b^2a^2 - 192a^2 + 4b^2 - 16)\sqrt{a^2+b^2}\sqrt{a^2+4^2} \\ &+ 2\sqrt{2}\sqrt{a^2+b^2}(2a^6 + 10b^2a^4 + 11a^4 + 86b^2a^2 - 368a^2 - 200b^2 - 48) \\ &- 2\sqrt{2}\sqrt{a^2+4^2}(2a^6 + 4b^2a^4 + 35a^4 - 22b^4a^2 + 76b^2a^2 + 24a^2 + 24b^2 - 59b^4) \\ =& l_1(a,b) + l_2(a,b) + 2\sqrt{2}l_3(a,b), \end{aligned}$$

where $l_1(a,b) = a^4(32b^4 - 12b^2 - 464) + a^2(292b^4 - 1024b^2 - 576) + 114b^4 - 576b^2$, $l_2(a,b) = (48b^2a^2 - 192a^2 + 4b^2 - 16)\sqrt{a^2+b^2}\sqrt{a^2+4^2}$ and $l_3(a,b) = \sqrt{a^2+b^2}(2a^6 + 10b^2a^4 + 11a^4 + 86b^2a^2 - 368a^2 - 200b^2 - 48) - \sqrt{a^2+4^2}(2a^6 +$

$4b^2a^4 + 35a^4 - 22b^4a^2 + 76b^2a^2 + 24a^2 + 24b^2 - 59b^4)$. Next, we shall prove that $l_1(a,b) > 0$, $l_2(a,b) > 0$ and $l_3(a,b) > 0$.

Note that for $b^2 \geq 9$, $32b^4 - 12b^2 - 464 = 4[b^2(8b^2-3)-116] \geq 4[b^2(8\cdot 9-3)-116] > 0$, $292b^4 - 1024b^2 - 576 = 4[b^2(73b^2-256)-144] \geq 4[b^2(73\cdot 9-256)-144] > 0$ and $114b^4 - 576b^2 = b^2(114b^2-576) > 0$. These mean that $l_1(a,b) > 0$.

We notice that $48b^2a^2 - 192a^2 + 4b^2 - 16 = 48a^2(b^2-4) + 4(b^2-4) > 0$ for $b^2 \geq 9$. So $l_2(a,b) > 0$.

Let $r = a^2$ and $s = b^2$. If $a = b$, then $r = s \geq 9$. If $a \geq b+1$, then $a^2 \geq (b+1)^2 \geq b^2 + 2b + 1 \geq b^2 + 7$, i.e., $r \geq s + 7$. To prove $l_3(a,b) > 0$, we first calculate the following equation.

$$\begin{aligned}
&(a^2+b^2)(2a^6+10b^2a^4+11a^4+86b^2a^2-368a^2-200b^2-48)^2\\
&\quad-(a^2+4^2)(2a^6+4b^2a^4+35a^4-22b^4a^2+76b^2a^2+24a^2+24b^2-59b^4)^2\\
=&(r+s)(2r^3+10sr^2+11r^2+86sr-368r-200s-48)^2\\
&\quad-(r+4)(2r^3+4sr^2+35r^2-22s^2r+76sr+24r+24s-59s^2)^2\\
=&28\,r^6\,s-112\,r^6+212\,r^5\,s^2-40\,r^5\,s-3232\,r^5+276\,r^4\,s^3+3740\,r^4\,s^2-15563\,r^4\,s\\
&\quad-15252\,r^4-484\,r^3\,s^4+6240\,r^3\,s^3+1018\,r^3\,s^2-104704\,r^3\,s+127072\,r^3-4532\,r^2\,s^4\\
&\quad+28684\,r^2\,s^3-107000\,r^2\,s^2+250848\,r^2\,s+33024\,r^2-13865\,r\,s^4+8528\,r\,s^3\\
&\quad+175104\,r\,s^2+49920\,r\,s+2304\,r-13924\,s^4+51328\,s^3+16896\,s^2+2304\,s\\
=&(28s-112)r^6+(212\,s^2-40\,s-3232)r^5+(276\,s^3+3740\,s^2-15563\,s-15252)r^4\\
&\quad+(-484\,s^4+6240\,s^3+1018\,s^2-104704\,s+127072)r^3\\
&\quad+(-4532\,s^4+28684\,s^3-107000\,s^2+250848\,s+33024\,)r^2\\
&\quad+(-13865\,s^4+8528\,s^3+175104\,s^2+49920\,s+2304)r\\
&\quad+(-13924\,s^4+51328\,s^3+16896\,s^2+2304\,s)\\
=&l_4(r,s).
\end{aligned}$$

If $r = s$ $(a = b)$, for $s \geq 9$, we have

$$\begin{aligned}
l_4(s,s)=&32\,s^7+5296\,s^6-2958\,s^5-232352\,s^4+604352\,s^3+99840\,s^2+4608\,s\\
=&16(2\,s^7+331\,s^6-184.875\,s^5-14522\,s^4+37772\,s^3+6240\,s^2+288\,s)\\
>&16(2\,s^7+331\,s^6-184.875\,s^5-14522\,s^4)\\
=&16[s^5(2s^2+131s-184.875)+s^4(200s^2-14522)]\\
\geq&16[s^5(2\cdot 9^2+131\cdot 9-184.875)+s^4(200\cdot 9^2-14522)]>0.
\end{aligned}$$

If $r \geq s+7$ $(a \geq b+1)$, for $s \geq 9$, we have

$$\begin{aligned}
\frac{\partial l_4(r,s)}{\partial r}=&6(28s-112)r^5+5(212\,s^2-40\,s-3232)r^4\\
&+4(276\,s^3+3740\,s^2-15563\,s-15252)r^3\\
&+3(-484\,s^4+6240\,s^3+1018\,s^2-104704\,s+127072)r^2\\
&+2(-4532\,s^4+28684\,s^3-107000\,s^2+250848\,s+33024\,)r\\
&+(-13865\,s^4+8528\,s^3+175104\,s^2+49920\,s+2304)\\
=&[6(28s-112)r^5-13865\,s^4]+(8528\,s^3+175104\,s^2+49920\,s+2304)\\
&+5(212\,s^2-40\,s-3232)r^4+4\cdot 276\,s^3\,r^3-3\cdot 484\,s^4\,r^2-2\cdot 4532\,s^4\,r\\
&+4(3740\,s^2-15563\,s-15252)r^3+3(6240\,s^3+1018\,s^2-104704\,s+127072)r^2\\
&+2(28684\,s^3-107000\,s^2+250848\,s+33024\,)r.
\end{aligned}$$

Observed that for $s \geq 9$,

$$\begin{aligned}
&6(28s-112)r^5 - 13865\,s^4 \geq 6(28s-112)(s+7)^5 - 13865\,s^4\\
=&168\,s^6 + 5208\,s^5 + 44935\,s^4 + 246960\,s^3 - 288120\,s^2 - 5243784\,s - 11294304\\
=&168\,s^6 + 5208\,s^5 - 11294304 + (44935\,s^3 - 5243784)s + (246960\,s - 288120\,)s^2\\
\geq&168\,\cdot 9^6 + 5208\,\cdot 9^5 - 11294304 + (44935\,\cdot 9^3 - 5243784)s + (246960\,\cdot 9 - 288120\,)s^2\\
=&387286446 + 27513831s + 1934520s^2 > 0;\\
&8528\,s^3 + 175104\,s^2 + 49920\,s + 2304 > 0;
\end{aligned}$$

$$\begin{aligned}
&5(212\,s^2 - 40\,s - 3232)r^4 + 4\cdot 276\,s^3\,r^3 - 3\cdot 484\,s^4\,r^2 - 2\cdot 4532\,s^4\,r\\
=&5(164\,s^2 + s(8s-40) + 8(5s^2-404))r^4 + 4\cdot 276\,s^3\,r^3 - 3\cdot 484\,s^4\,r^2 - 2\cdot 4532\,s^4\,r\\
>&5\cdot 164\,s^2\,r^4 + 4\cdot 276\,s^3\,r^3 - 3\cdot 484\,s^4\,r^2 - 2\cdot 4532\,s^4\,r\\
=&4s^2r(205\,r^3 + 276\,s\,r^2 - 363\,s^2\,r - 2266\,s^2)\\
\geq&4s^2r[205\,(s+7)^3 + 276\,s\,(s+7)^2 - 363\,s^2\,(s+7) - 2266\,s^2]\\
=&4s^2r(118\,s^3 + 3362\,s^2 + 43659\,s + 70315) > 0
\end{aligned}$$

since $\frac{\partial}{\partial r}(205\,r^3 + 276\,s\,r^2 - 363\,s^2\,r - 2266\,s^2) = 615r^2 + 552sr - 363s^2 > 0$;

$$\begin{aligned}
&3740\,s^2 - 15563\,s - 15252 \geq s(3740\cdot 9 - 15563) - 15252 = 18097s - 15252 > 0;\\
&6240\,s^3 + 1018\,s^2 - 104704\,s + 127072 \geq 6240\cdot 9^2\,s - 104704\,s + 1018\,s^2 + 127072 > 0;\\
&28684\,s^3 - 107000\,s^2 + 250848\,s + 33024 \geq 28684\cdot 9\,s^2 - 107000\,s^2 + 250848\,s + 33024 > 0.
\end{aligned}$$

These mean that $\frac{\partial l_4(r,s)}{\partial r} > 0$ and $l_4(r,s) > l_4(s,s) > 0$, which yields $l_3(a,b) > 0$.

So $\frac{\partial h(a,b)}{\partial a} > 0$ and $h(a,b) \geq h(b,b) = 2\Big(\frac{b^2-4}{\sqrt{2}+2\sqrt{b^2+4}}\Big)^2 > 0$ for $b \geq 3$. □

Lemma 2.4. *Let*

$$\begin{aligned}
\varphi_1(a,b) &= \frac{a^2-4}{a^2+4} + \frac{b^2-4}{b^2+4} - \frac{a^2-b^2}{a^2+b^2},\\
\varphi_2(a,b) &= \frac{2(a^2-4)}{\sqrt{2}+2\sqrt{a^2+4}}\pi + \frac{2(b^2-4)}{\sqrt{2}+2\sqrt{b^2+4}}\pi - \frac{2(a^2-b^2)}{\sqrt{2}+2\sqrt{a^2+b^2}}\pi.
\end{aligned}$$

Then $\varphi_1(a,b) > 0$ and $\varphi_2(a,b) > 0$ for $a \geq b \geq 3$.

Proof. It is not difficult to check that for $a \geq b \geq 3$, $\frac{\partial \varphi_1(a,b)}{\partial b}, \frac{\partial \varphi_2(a,b)}{\partial b} > 0$. So for $a \geq b \geq 3$, we have

$$\begin{aligned}
\varphi_1(a,b) =&\frac{a^2-4}{a^2+4} + \frac{b^2-4}{b^2+4} - \frac{a^2-b^2}{a^2+b^2}\\
\geq&\frac{a^2-4}{a^2+4} + \frac{5}{13} - \frac{a^2-9}{a^2+9}\\
=&\frac{10a^2}{(a^2+4)(a^2+9)} + \frac{5}{13} > 0
\end{aligned}$$

and

$$\begin{aligned}\varphi_2(a,b) =&\frac{2(a^2-4)}{\sqrt{2}+2\sqrt{a^2+4}}\pi + \frac{2(b^2-4)}{\sqrt{2}+2\sqrt{b^2+4}}\pi - \frac{2(a^2-b^2)}{\sqrt{2}+2\sqrt{a^2+b^2}}\pi\\ \geq&\frac{2(a^2-4)}{\sqrt{2}+2\sqrt{a^2+4}}\pi + \frac{10}{\sqrt{2}+2\sqrt{13}}\pi - \frac{2(a^2-9)}{\sqrt{2}+2\sqrt{a^2+9}}\pi\\ =&2\frac{5\sqrt{2}+2(a^2-4)\sqrt{a^2+9}-2(a^2-9)\sqrt{a^2+4}}{(\sqrt{2}+2\sqrt{a^2+4})(\sqrt{2}+2\sqrt{a^2+9})}+\frac{10}{\sqrt{2}+2\sqrt{13}} > 0\end{aligned}$$

since $a^2-4 > a^2-9$ and $\sqrt{a^2+9} > \sqrt{a^2+4}$ for $a \geq 3$. □

Lemma 2.5. *Let*

$$\psi(a) = \frac{6}{\sqrt{2}+2\sqrt{5}} + \frac{2(a^2-4)}{\sqrt{2}+2\sqrt{a^2+4}} - \frac{2(a^2-1)}{\sqrt{2}+2\sqrt{a^2+1}}.$$

Then $\psi(a) > 0$ *for* $a \geq 3$.

Proof. Notice that

$$\psi(a) = \frac{6}{\sqrt{2}+2\sqrt{5}} + \sqrt{2}\frac{a^2-4}{1+\sqrt{2a^2+8}} - \sqrt{2}\frac{a^2-1}{1+\sqrt{2a^2+2}}.$$

For $a \geq 3$, we derive

$$\begin{aligned}\psi'(a) =& \sqrt{2}\Big[\frac{2a(1+\sqrt{2a^2+8})-(a^2-4)\frac{2a}{\sqrt{2a^2+8}})}{(1+\sqrt{2a^2+8})^2}-\frac{2a(1+\sqrt{2a^2+2})-(a^2-1)\frac{2a}{\sqrt{2a^2+2}})}{(1+\sqrt{2a^2+2})^2}\Big]\\ =&2\sqrt{2}a\Big[\frac{\sqrt{2a^2+8}+a^2+12}{(1+\sqrt{2a^2+8})^2\sqrt{2a^2+8}}-\frac{\sqrt{2a^2+2}+a^2+3}{(1+\sqrt{2a^2+2})^2\sqrt{2a^2+2}}\Big]\\ =&2\sqrt{2}a\frac{(\sqrt{2a^2+8}+a^2+12)(1+\sqrt{2a^2+2})^2\sqrt{2a^2+2}}{(1+\sqrt{2a^2+8})^2\sqrt{2a^2+8}(1+\sqrt{2a^2+2})^2\sqrt{2a^2+2}}\\ &-2\sqrt{2}a\frac{(\sqrt{2a^2+2}+a^2+3)(1+\sqrt{2a^2+8})^2\sqrt{2a^2+8}}{(1+\sqrt{2a^2+8})^2\sqrt{2a^2+8}(1+\sqrt{2a^2+2})^2\sqrt{2a^2+2}}\\ =&2\sqrt{2}a\frac{\sqrt{2}\sqrt{a^2+1}(2a^4+23a^2+20)+24a^2}{(1+\sqrt{2a^2+8})^2\sqrt{2a^2+8}(1+\sqrt{2a^2+2})^2\sqrt{2a^2+2}}\\ &-2\sqrt{2}a\frac{\sqrt{2}\sqrt{a^2+4}(2a^4+11a^2+23)+12\sqrt{a^2+1}\sqrt{a^2+4}}{(1+\sqrt{2a^2+8})^2\sqrt{2a^2+8}(1+\sqrt{2a^2+2})^2\sqrt{2a^2+2}}\\ =&2\sqrt{2}a\frac{\sqrt{2}\psi_1(a)+12\psi_2(a)}{(1+\sqrt{2a^2+8})^2\sqrt{2a^2+8}(1+\sqrt{2a^2+2})^2\sqrt{2a^2+2}},\end{aligned}$$

where $\psi_1(a) = \sqrt{a^2+1}(2a^4+23a^2+20) - \sqrt{a^2+4}(2a^4+11a^2+23)$ and $\psi_2(a) = 2a^2 - \sqrt{a^2+1}\sqrt{a^2+4}$.

For $a \geq 3$, it follows that

$$\begin{aligned}&(a^2+1)(2a^4+23a^2+20)^2-(a^2+4)(2a^4+11a^2+23)^2\\ =&36a^8+312a^6+171a^4-1233a^2-1716\\ =&3[a^2(12a^6-411)+104a^6+57a^4-572] > 0.\end{aligned}$$

Thus, $\psi_1(a) > 0$. Furthermore, we notice that $\psi_2(a) = 2a^2 - \sqrt{a^2+1}\sqrt{a^2+4} = \frac{3a^4-5a^2-4}{2a^2+\sqrt{a^2+1}\sqrt{a^2+4}} = \frac{a^2(2a^2-5)+a^4-4}{2a^2+\sqrt{a^2+1}\sqrt{a^2+4}} > 0$ for $a \geq 3$. These imply that $\psi'(a) > 0$ and $\psi(a)$ is increasing for $a \geq 3$. Hence for $a \geq 3$, $\psi(a) \geq \psi(3) \approx 0.1112 > 0$. □

3. Main results

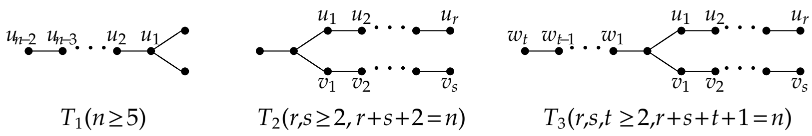

Figure 1. Three types of trees with n vertices and 3 pendent vertices

Note that $m \geq n-1$ and $k \geq 0$ for a chemical (n,m,k)-graph. When $k=0$, by the definition of SO_i $(i=1,2,5,6)$, the chemical $(n,m,0)$-graph with minimum SO_i $(i=1,2,5,6)$ index is an l-regular $(l=2,3,4)$ graph. Furthermore, the chemical $(n,n-1,2)$-graphs are paths, the chemical $(n,n-1,3)$-graphs are T_1, T_2 and T_3 (see Figure 1). We can easily check that $SO_1(T_1)=SO_1(T_2)=SO_1(T_3)$, $SO_2(T_1)<SO_2(T_2)<SO_1(T_3)$, $SO_5(T_1)<SO_5(T_2)<SO_5(T_3)$, $SO_6(T_1)>SO_6(T_2)>SO_6(T_3)$. So in what follows, we shall suppose that $k \geq 4$ for $m=n-1$ and $k \geq 1$ for $m \geq n$ to all chemical (n,m,k)-graphs.

We use $\boldsymbol{G}_{n,m,k}$ (resp. $\boldsymbol{CG}_{n,m,k}$) to denote the set of all (n,m,k)-graphs (resp. chemical (n,m,k)-graphs) with $k \geq 1$ when $m \geq n$ and $k \geq 4$ when $m=n-1$. Next, let us seek the minimal SO_i $(i=1,2,5,6)$ index of $\boldsymbol{G}_{n,m,k}$ satisfying $k \geq 1$ for $m \geq n$ and $k \geq 4$ for $m=n-1$.

Assume that p,q,k are positive integers with $p \geq 6$ and $q=\frac{3p-2k}{2} \geq p-1$. If H is a (p,q,k)-graph in which every non-pendent vertex is degree 3, we call H a $(p,q,k,3)$-semi-regular graph. It is easy to see that $k \geq 4$ for $q=p-1$, $k \geq 3$ for $q=p$, $k \geq 2$ for $q=p+1$ and $k \geq 1$ for $q \geq p+2$ in a $(p,q,k,3)$-semi-regular graph.

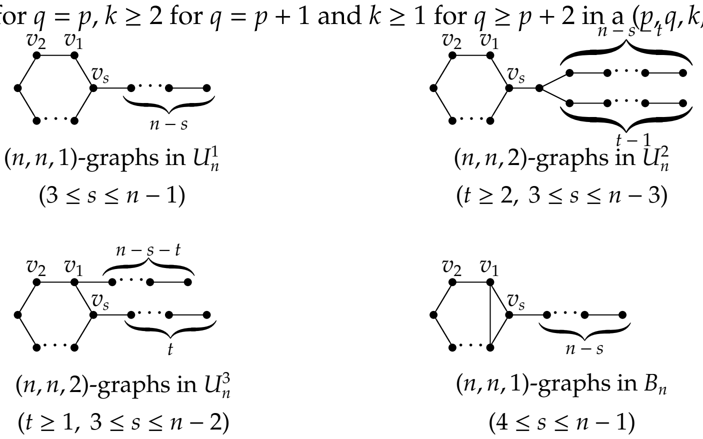

Figure 2. Four types of (n,m,k)-graphs, where $k=1$ or 2

Let $\mathbb{G}^{(1)}_{n,m,k}$ be a collection of $(n,m,k,3)$-semi-regular graphs or (n,m,k)-graphs obtained from $(p,q,k,3)$-semi-regular graphs by inserting several new vertices on some pendent edge. Let $\mathbb{G}^{(2)}_{n,m,k}$ be a collection of $(n,m,k,3)$-semi-regular graphs or (n,m,k)-graphs gotten from $(p,q,k,3)$-semi-regular graphs by inserting several new vertices on one pendent edge. Let $\mathbb{G}^{(3)}_{n,m,k}$ be a collection of (n,m,k)-graphs gotten from $(p,q,k,3)$-semi-regular graphs by inserting several new vertices on each pendent edge. Since $k+n_2+n_3=n$ and $k+2n_2+3n_3=2m$ for $\mathbb{G}^{(i)}_{n,m,k}$ $(i=1,2,3)$, it shows that $n_2=3n-2m-2k$ and the number of newly added vertices is all $3n-2(k+m)$ if there are new vertices added. One can easily see that $\mathbb{G}^{(2)}_{n,m,k}, \mathbb{G}^{(3)}_{n,m,k} \subseteq \mathbb{G}^{(1)}_{n,m,k}$ and $\mathbb{G}^{(1)}_{n,m,k}, \mathbb{G}^{(2)}_{n,m,k}, \mathbb{G}^{(3)}_{n,m,k} \subseteq \boldsymbol{G}_{n,m,k}$ (resp. $\boldsymbol{CG}_{n,m,k}$). The graphs of U_n^1, U_n^2, U_n^3 and B_n used in the following contents are depicted in Figure 2.

3.1. *Minimum SO_1 index of chemical graphs with a given order, number of edges and pendent vertices*

Theorem 3.1. *Consider $G \in \boldsymbol{G}_{n,n,1}$ or $\boldsymbol{G}_{n,n+1,1}$. Then*

$$SO_1(G) \geq 9.$$

Equality occurs if and only if $G \in U_n^1$, $n \geq 4$ or $G \in B_n$, $n \geq 5$ (see Figure 2).

Proof. For $G \in \boldsymbol{G}_{n,n,1}$ or $\boldsymbol{G}_{n,n+1,1}$, we have $E(G) = \bigcup_{i=1}^{5} E_i$ and $|E_1| + |E_2| = 1$. By using (1), one has

$$\begin{aligned} SO_1(G) =& \frac{1}{2} \sum_{uv \in E(G)} |deg_G^2(u) - deg_G^2(v)| \\ =& \frac{1}{2}\Big[3|E_1| + \sum_{uv \in E_2} (deg_G^2(v) - 1) + \sum_{uv \in E_4} (deg_G^2(v) - 4) + \sum_{uv \in E_5} |deg_G^2(u) - deg_G^2(v)|\Big] \\ \geq& \frac{1}{2}\Big[3|E_1| + \sum_{uv \in E_2} (deg_G^2(v) - 1) + \sum_{uv \in E_4} (deg_G^2(v) - 4)\Big] \\ \geq& \frac{1}{2}\Big[3|E_1| + 8|E_2| + 5|E_4|\Big] \\ =& \frac{1}{2}\Big[3 + 5|E_2| + 5|E_4|\Big]. \end{aligned} \tag{5}$$

Case 1. $G \in \boldsymbol{G}_{n,n,1} (n \geq 4)$ is a unicyclic graph.

In this case, $|E_5| = 0$ since $G \in \boldsymbol{G}_{n,n,1}$.

For $|E_1| = 0, |E_2| = 1$, one has $|E_4| = 2$. From (5), we get $SO_1(G) \geq 9$. If $SO_1(G) = 9$, then (I) $|E_1| = 0, |E_2| = 1$; (II) When $uv \in E_4$, $deg_G(u) = 2, deg_G(v) = 3$ and $|E_4| = 2$. These indicate that $G \in U_n^1$ ($n \geq 4$, $s = n - 1$).

For $|E_1| = 1, |E_2| = 0$, one has $|E_4| = 3$. From (5), we get $SO_1(G) \geq \frac{1}{2}(3 + 15) = 9$. If $SO_1(G) = 9$, then (I) $|E_1| = 1, |E_2| = 0$; (II) When $uv \in E_4$, $deg_G(u) = 2, deg_G(v) = 3$ and $|E_4| = 3$. That is $G \in U_n^1$ ($n \geq 5, 3 \leq s \leq n-2$).

Case 2. $G \in \boldsymbol{G}_{n,n+1,1}$ ($n \geq 5$) is a bicyclic graph.

For $|E_1| = 1, |E_2| = 0$, one has $|E_4| \geq 3$. From (5), we derive $SO_1(G) \geq 9$. If $SO_1(G) = 9$, then (I) $|E_1| = 1, |E_2| = 0$; (II) When $uv \in E_4$, $deg_G(u) = 2, deg_G(v) = 3$ and $|E_4| = 3$; (III) For $uv \in E_5$, $deg_G(u) = deg_G(v)$. Moreover, since every edge of E_4 is associated with an edge of E_5 and a 2-degree vertex, respectively, then $deg_G(u) = deg_G(v) = 3$ for $uv \in E_5$. These mean that $G \in B_n$ ($n \geq 6$, $4 \leq s \leq n-2$).

For $|E_1| = 0, |E_2| = 1$, one has $|E_4| \geq 2$. From (5), we derive $SO_1(G) \geq 9$. If $SO_1(G) = 9$, then (I) $|E_1| = 0, |E_2| = 1$; (II) $deg_G(u) = 2, deg_G(v) = 3$ when $uv \in E_3$ and $|E_3| = 3$; (III) When $uv \in E_5$, $deg_G(u) = deg_G(v) = 3$. These imply that $G \in B_n$ ($n \geq 5$, $s = n - 1$). □

Theorem 3.2. *Let $G \in \boldsymbol{G}_{n,n,2}$. Then*

$$SO_1(G) \geq 13,$$

where equality holds only if $G \in U_n^2$, $n \geq 6$ or $G \in U_n^3$, $n \geq 5$ (see Figure 2).

Proof. For $G \in \boldsymbol{G}_{n,n,2}$, $E(G) = \bigcup_{i=1}^{5} E_i$ and $|E_1| + |E_2| = 2$. By using (1), we derive

$$\begin{aligned} SO_1(G) =& \frac{1}{2} \sum_{uv \in E(G)} |deg_G^2(u) - deg_G^2(v)| \\ =& \frac{1}{2}\Big[3|E_1| + \sum_{uv \in E_2} (deg_G^2(v) - 1) + \sum_{uv \in E_4} (deg_G^2(v) - 4) + \sum_{uv \in E_5} |deg_G^2(u) - deg_G^2(v)|\Big] \\ \geq& \frac{1}{2}\Big[3|E_1| + 8|E_2| + 5|E_4|\Big] \\ =& \frac{1}{2}\Big[6 + 5|E_2| + 5|E_4|\Big]. \end{aligned} \tag{6}$$

For $|E_1| = 2, |E_2| = 0$, we have $|E_4| \geq 4$. From (6), one gets $SO_1(G) \geq 13$. If $SO_1(G) = 13$, similar to the proof of Theorem 3.1, it is not difficult to check that $G \in U_n^2$ ($n \geq 8$, $t \geq 3$, $3 \leq s \leq n-5$) or $G \in U_n^3$ ($n \geq 7$, $t \geq 2$, $3 \leq s \leq n-4$).

For $|E_1| = 1, |E_2| = 1$, we have $|E_4| \geq 3$. From (6), one gets $SO_1(G) \geq 13$. If $SO_1(G) = 13$, it is easy to check that $G \in U_n^2$ ($n \geq 7, t = 2, 3 \leq s \leq n-4$) or $G \in U_n^3$ ($n \geq 6, t = 1, 3 \leq s \leq n-3$).

If $|E_1| = 0, |E_2| = 2$, we have $|E_4| \geq 2$. From (6), one gets $SO_1(G) \geq 13$. If $SO_1(G) = 13$, it can be seen that $G \in U_n^2$ ($n \geq 6, t = 2, s = n-3$) or $G \in U_n^3$ ($n \geq 5, t = 1, s = n-2$). □

Lemma 3.1. *Let $H \in \boldsymbol{G}_{n,m,k}$. Assume that $x \in V(H)$ is a 2-degree vertex that is not contained in any pendent path, nor in any cycle of length three. Then there exists a graph $H' \in \boldsymbol{G}_{n,m,k}$ satisfying one of the following properties:*

1) $SO_1(H') < SO_1(H)$;

2) $SO_1(H') = SO_1(H)$ and H' contains more 2-degree vertices in the cycle of length three than H.

Proof. Let $P = x_1x_2\cdots x_l$ ($l \geq 3$) be the internal path containing x in H, where $x = x_i, i \in \{2, \cdots, l-1\}$. Without loss of generality we assume that $deg_H(x_1) = a \geq deg_H(x_r) = b \geq 3$. Let u be a pendent vertex and v be the neighbor of u in H. Clearly, $deg_H(v) = c \geq 2$. Next, we discuss two cases.

Case 1. $l = 3$.

Now, $x = x_2$ and $x_1x_3 \notin E(H)$ since x does not belong to the cycle of length 3. Let $H' = H - x_1x_2 - x_2x_3 - uv + x_1x_3 + vx_2 + x_2u$. Then $H' \in \boldsymbol{G}_{n,m,k}$. Notice that

$$\begin{aligned} SO_1(H) - SO_1(H') =& \frac{1}{2}[(a^2-4)+(b^2-4)+(c^2-1)-(a^2-b^2)-(c^2-4)-(4-1)] \\ =& \frac{1}{2}(2b^2-8) > 0. \end{aligned}$$

Case 2. $l \geq 4$.

If $x_1x_l \notin E(H)$, set $H' = H - x_1x_2 - x_{l-1}x_l - uv + x_1x_l + vx_2 + x_{l-1}u$. Then $H' \in \boldsymbol{G}_{n,m,k}$. Note that

$$\begin{aligned} SO_1(H) - SO_1(H') =& \frac{1}{2}[(a^2-4)+(b^2-4)+(c^2-1)-(a^2-b^2)-(c^2-4)-(4-1)] \\ =& \frac{1}{2}(2b^2-8) > 0. \end{aligned}$$

If $x_1x_l \in E(H)$, set $H' = H - x_2x_3 - x_{l-1}x_l - uv + x_2x_l + vx_3 + x_{l-1}u$. Then $H' \in \boldsymbol{G}_{n,m,k}$. Note that

$$SO_1(H) - SO_1(H') = \frac{1}{2}[(c^2-1)-(c^2-4)-(4-1)] = 0.$$

Clearly, H' has more 2-degree vertices in the cycle of length 3 than H. □

Theorem 3.3. *Suppose $G \in \boldsymbol{G}_{n,m,k}$ with $k \geq 4$ for $m = n-1$, or $k \geq 3$ for $m = n$, or $k \geq 2$ for $m = n+1$, or $k \geq 1$ for $m \geq n+2$, then*

$$SO_1(G) \geq 4k.$$

Moreover, equality holds if and only if $G \in \mathbb{G}_{n,m,k}^{(1)}$.

Proof. Pick $G \in \boldsymbol{G}_{n,m,k}$ such that G has the minimum SO_1. By this hypothesis and Lemma 3.1, without loss of generality, we suppose that all 2-degree vertices lie on the pendent paths except the 2-degree vertices on the cycles whose length is 3 in G. We shall prove the theorem in two cases.

Case 1. G does not contain the 2-degree vertices on the cycles with length 3.

Clearly, $E(G)=\bigcup_{i=1}^{5}E_i$, $|E_1|+|E_2|=k$ and $|E_1|=|E_4|$. By using (1), one has

$$\begin{aligned}SO_1(G)=&\frac{1}{2}\sum_{uv\in E(G)}|deg_G^2(u)-deg_G^2(v)|\\=&\frac{1}{2}\Big[3|E_1|+\sum_{uv\in E_2}(deg_G^2(v)-1)+\sum_{uv\in E_4}(deg_G^2(v)-4)+\sum_{uv\in E_5}|deg_G^2(u)-deg_G^2(v)|\Big]\\\geq&\frac{1}{2}\Big[3|E_1|+8|E_2|+5|E_4|\Big]\\=&\frac{1}{2}\Big[8|E_1|+8|E_2|\Big]\\=&4k.\end{aligned}\tag{7}$$

If the equality in (7) holds, all inequalities in the above argument must be equalities. Note that $|E_1|+|E_2|=k$, we differentiate the following three cases when the equality in (7) occurs.

For $|E_1|=0$ and $|E_2|=k$, one has (I) $|E_4|=0$ cause $|E_3|=0$; (II) $deg_G(u)=1, deg_G(v)=3$ for $uv\in E_2$; (III) $deg_G(v)=deg_G(v)$ for $uv\in E_5$. Moreover, $deg_G(u)=deg_G(v)=3$ for $uv\in E_5$ since an edge of E_2 is incident to a 3-degree vertex of E_5. Thus, G belongs to the $(n,m,k,3)$-semi-regular graphs and $3n=2m+2k$. Clearly, $G\in\mathbb{G}_{n,m,k}^{(1)}$.

For $|E_1|=k$ and $|E_2|=0$, one has (I) $deg_G(v)=3$ and $deg_G(u)=2$ for $uv\in E_4$; (II) $deg_G(u)=deg_G(v)$ for $uv\in E_5$. Moreover, $deg_G(u)=deg_G(v)=3$ for $uv\in E_5$ and $n_2\geq k$ since an edge of E_4 is associated with one edge of E_5 and a 2-degree vertex. Hence, the maximal degree of G is three and $k+n_2+n_3=n$, $k+2n_2+3n_3=2m$ since $G\in\boldsymbol{G}_{n,m,k}$. It follows that $n_2=3n-2m-2k$, $3n\geq 2m+3k$ and $G\in\mathbb{G}_{n,m,k}^{(1)}$.

For $|E_1|,|E_2|\geq 1$, one has (I) $deg_G(v)=3$ and $deg_G(u)=2$ for $uv\in E_4$; (II) $deg_G(u)=1, deg_G(v)=3$ for $uv\in E_2$; (III) $deg_G(u)=deg_G(v)=3$ for $uv\in E_5$ since an edge of E_4 is incident to an edge of E_5 as well as a 2-degree vertex, and one edge of E_2 is incident to a 3-degree vertex of E_5, respectively. So the maximal degree of G is three and $G\in\mathbb{G}_{n,m,k}^{(1)}$.

Case 2. G contains at least a 2-degree vertex on the cycle of length 3.

We use r to represent the number of 3-length cycles having the 2-degree vertices in G. Now, $E(G)=\bigcup_{i=1}^{5}E_i$, $|E_1|+|E_2|=k$ and $|E_4|=|E_1|+2r$, where $r>0$. By using (1), we have

$$\begin{aligned}SO_1(G)=&\frac{1}{2}\sum_{uv\in E(G)}|deg_G^2(u)-deg_G^2(v)|\\=&\frac{1}{2}\Big[3|E_1|+\sum_{uv\in E_2}(deg_G^2(v)-1)+\sum_{uv\in E_4}(deg_G^2(v)-4)+\sum_{uv\in E_5}|deg_G^2(u)-deg_G^2(v)|\Big]\\\geq&\frac{1}{2}\Big[3|E_1|+8|E_2|+5|E_4|\Big]\\=&\frac{1}{2}\Big[8|E_1|+8|E_2|+10r\Big]\\=&4k+5r\\>&4k.\end{aligned}$$

The proof is completed. □

3.2. *Minimum SO_2 and SO_5 indices of chemical graphs with a given order, number of edges and pendent vertices*

Theorem 3.4. *Let $G\in\boldsymbol{G}_{n,n,1}$ or $\boldsymbol{G}_{n,n+1,1}$. Then*

$$SO_2(G)\geq\frac{102}{65}$$

and

$$SO_5(G) \geq \frac{16}{\sqrt{2}+\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi.$$

Equalities hold only when $G \in U_n^1$, $n \geq 4, s = n-1$, or $G \in B_n$, $n \geq 5, s = n-1$ (see Figure 2).

Proof. For $G \in \boldsymbol{G}_{n,n,1}$ or $\boldsymbol{G}_{n,n+1,1}$, one has $E(G) = \bigcup_{i=1}^{5} E_i$ and $|E_1| + |E_2| = 1$. By using (2), (3) and Lemma 2.1, we deduce that

$$\begin{aligned} SO_2(G) &= \sum_{uv\in E(G)} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)} \\ &= \frac{3}{5}|E_1| + \sum_{uv\in E_2} \frac{deg_G^2(v) - 1}{deg_G^2(v) + 1} + \sum_{uv\in E_4} \frac{deg_G^2(v) - 4}{deg_G^2(v) + 4} + \sum_{uv\in E_5} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)} \\ &\geq \frac{3}{5}|E_1| + \frac{4}{5}|E_2| + \frac{5}{13}|E_4| \end{aligned} \tag{8}$$

and

$$\begin{aligned} SO_5(G) &= \sum_{uv\in E(G)} \frac{2|deg_G^2(u) - deg_G^2(v)|}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\pi \\ &= \frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1| + \sum_{uv\in E_2} \frac{2(deg_G^2(v) - 1)}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 1}}\pi \\ &\quad + \sum_{uv\in E_4} \frac{2(deg_G^2(v) - 4)}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 4}}\pi \\ &\quad + \sum_{uv\in E_5} \frac{2|deg_G^2(u) - deg_G^2(v)|}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\pi \\ &\geq \frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1| + \frac{16}{\sqrt{2}+2\sqrt{10}}\pi|E_2| + \frac{10}{\sqrt{2}+2\sqrt{13}}\pi|E_4|. \end{aligned} \tag{9}$$

Case 1. $G \in \boldsymbol{G}_{n,n,1} (n \geq 4)$.

For $|E_1| = 1, |E_2| = 0$, one has $|E_4| = 3$. From (8) and (9), we get $SO_2(G) \geq \frac{3}{5} + 3 \times \frac{5}{13} = \frac{114}{65} > \frac{102}{65}$ and $SO_5(G) \geq \frac{6}{\sqrt{2}+2\sqrt{5}}\pi + 3\frac{10}{\sqrt{2}+2\sqrt{13}}\pi > \frac{16}{\sqrt{2}+\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$, respectively.

For $|E_1| = 0, |E_2| = 1$, one has $|E_4| = 2$. From (8) and (9), we get $SO_2(G) \geq \frac{4}{5} + 2 \times \frac{5}{13} = \frac{102}{65}$ and $SO_5(G) \geq \frac{16}{\sqrt{2}+\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$. If $SO_2(G) = \frac{102}{65}$ or $SO_5(G) = \frac{16}{\sqrt{2}+\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$, then (I) $|E_1| = 0, |E_2| = 1$; (II) $deg_G(u) = 2, deg_G(v) = 3$ for $uv \in E_4$ and $|E_4| = 2$. Furthermore, $|E_5| = 0$. These mean that $G \in U_n^1$ $(s = n-1)$.

Case 2. $G \in \boldsymbol{G}_{n,n+1,1} (n \geq 5)$.

For $|E_1| = 1, |E_2| = 0$, one has $|E_4| \geq 3$. From (8) and (9), we derive $SO_2(G) \geq \frac{114}{65} > \frac{102}{65}$ and $SO_5(G) \geq \frac{6}{\sqrt{2}+2\sqrt{5}}\pi + 3\frac{10}{\sqrt{2}+2\sqrt{13}}\pi > \frac{16}{\sqrt{2}+\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$, respectively.

For $|E_1| = 0, |E_2| = 1$, one has $|E_4| \geq 2$. From (8) and (9), we derive $SO_2(G) \geq \frac{102}{65}$ and $SO_5(G) \geq \frac{16}{\sqrt{2}+\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$. If $SO_2(G) = \frac{102}{65}$ or $SO_5(G) = \frac{16}{\sqrt{2}+\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$, then (I) $|E_1| = 0, |E_2| = 1$; (II) $deg_G(u) = 2, deg_G(v) = 3$ for $uv \in E_4$, and $|E_4| = 2$; (III) $deg_G(u) = deg_G(v) = 3$ for $uv \in E_5$. These indicate that $G \in B_n$ $(s = n-1)$. □

Theorem 3.5. *Let $G \in \boldsymbol{G}_{n,n,2}$. Then*

$$SO_2(G) \geq \frac{154}{65}$$

and

$$SO_5(G) \geq \frac{32}{\sqrt{2}+2\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi.$$

Equalities hold only if $G \in U_n^2$, $n \geq 6$, $t = 2$, $s = n-3$ or $G \in U_n^3$, $n \geq 5$, $t = 1$, $s = n-2$ (see Figure 2).

Proof. For $G \in \boldsymbol{G}_{n,n,2}$, $E(G) = \bigcup_{i=1}^{5} E_i$ and $|E_1| + |E_2| = 2$. By using (2), (3) and Lemma 2.1, we derive

$$\begin{aligned} SO_2(G) &= \sum_{uv\in E(G)} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)} \\ &= \frac{3}{5}|E_1| + \sum_{uv\in E_2} \frac{deg_G^2(v) - 1}{deg_G^2(v) + 1} + \sum_{uv\in E_4} \frac{deg_G^2(v) - 4}{deg_G^2(v) + 4} + \sum_{uv\in E_5} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)} \\ &\geq \frac{3}{5}|E_1| + \frac{4}{5}|E_2| + \frac{5}{13}|E_4| \end{aligned} \tag{10}$$

and

$$\begin{aligned} SO_5(G) &= \sum_{uv\in E(G)} \frac{2|deg_G^2(u) - deg_G^2(v)|}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\pi \\ &= \frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1| + \sum_{uv\in E_2} \frac{2(deg_G^2(v) - 1)}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 1}}\pi \\ &\quad + \sum_{uv\in E_4} \frac{2(deg_G^2(v) - 4)}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 4}}\pi \\ &\quad + \sum_{uv\in E_5} \frac{2|deg_G^2(u) - deg_G^2(v)|}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\pi \\ &\geq \frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1| + \frac{16}{\sqrt{2}+2\sqrt{10}}\pi|E_2| + \frac{10}{\sqrt{2}+2\sqrt{13}}\pi|E_4|. \end{aligned} \tag{11}$$

If $|E_1| = 2, |E_2| = 0$, then $|E_4| \geq 4$. From (10) and (11), one has $SO_2(G) \geq 2 \times \frac{3}{5} + 4 \times \frac{5}{13} = \frac{178}{65} > \frac{154}{65}$ and $SO_5(G) \geq 2\frac{6}{\sqrt{2}+2\sqrt{5}}\pi + 4\frac{10}{\sqrt{2}+2\sqrt{13}}\pi > \frac{32}{\sqrt{2}+2\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$, respectively.

If $|E_1| = 1, |E_2| = 1$, then $|E_4| \geq 3$. From (10) and (11), one has $SO_2(G) \geq \frac{3}{5} + \frac{4}{5} + 3 \times \frac{5}{13} = \frac{166}{65} > \frac{154}{65}$ and $SO_5(G) \geq \frac{6}{\sqrt{2}+2\sqrt{5}}\pi + \frac{16}{\sqrt{2}+2\sqrt{10}}\pi + 3\frac{10}{\sqrt{2}+2\sqrt{13}}\pi > \frac{32}{\sqrt{2}+2\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$, respectively.

If $|E_1| = 0, |E_2| = 2$, then $|E_4| \geq 2$. From (10) and (11), one has $SO_2(G) \geq 2 \times \frac{4}{5} + 2 \times \frac{5}{13} = \frac{154}{65}$ and $SO_5(G) \geq 2\frac{16}{\sqrt{2}+2\sqrt{10}}\pi + 2\frac{10}{\sqrt{2}+2\sqrt{13}}\pi$, respectively. If $SO_2(G) = \frac{154}{65}$ or $SO_5(G) = \frac{32}{\sqrt{2}+2\sqrt{10}}\pi + \frac{20}{\sqrt{2}+2\sqrt{13}}\pi$, it is not difficult to check that $G \in U_n^2$ ($t = 2$, $s = n-3$) or $G \in U_n^3$ ($t = 1$, $s = n-2$). □

Lemma 3.2. *Suppose $H \in \boldsymbol{G}_{n,m,k}$ and H contains at least one 2-degree vertex in a pendent path. Let $x \in V(H)$ be a 2-degree vertex that is not contained in any 3-length cycle and any pendent path. Then there exists a graph $H' \in \boldsymbol{G}_{n,m,k}$ satisfying one of the following properties:*

1) *$SO_2(H') < SO_2(H)$ and $SO_5(H') < SO_5(H)$;*

2) *$SO_2(H') = SO_2(H)$, $SO_5(H') = SO_5(H)$ and H' contains more 2-degree vertices in the 3-length cycle than H.*

Proof. Let $P = x_1x_2\cdots x_l$ ($l \geq 3$) be the internal path containing x in H, where $x = x_i$, $i \in \{2, \cdots, l-1\}$. Without loss of generality we assume that $deg_H(x_1) = a \geq deg_H(x_l) = b \geq 3$. Let u be a pendent vertex in the pendent path containing the 2-degree vertices and v be the neighbor of u in H. Then $deg_H(v) = 2$. Next, we discuss in two cases.

Case 1. $l = 3$.

Now, $x = x_2$ and $x_1x_3 \notin E(H)$ since x does not belong to the cycle of length 3. Let $H' = H - x_1x_2 - x_2x_3 - uv + x_1x_3 + vx_2 + x_2u$. Then $H' \in \mathbf{G}_{n,m,k}$. By Lemma 2.4, we derive

$$SO_2(H) - SO_2(H') = \frac{a^2-4}{a^2+4} + \frac{b^2-4}{b^2+4} - \frac{a^2-b^2}{a^2+b^2} > 0$$

and

$$SO_5(H) - SO_5(H') = \frac{2(a^2-4)}{\sqrt{2}+2\sqrt{a^2+4}}\pi + \frac{2(b^2-4)}{\sqrt{2}+2\sqrt{b^2+4}}\pi - \frac{2(a^2-b^2)}{\sqrt{2}+2\sqrt{a^2+b^2}}\pi > 0.$$

Case 2. $l \geq 4$.

If $x_1x_l \notin E(H)$, set $H' = H - x_1x_2 - x_{l-1}x_l - uv + x_1x_l + vx_2 + x_{l-1}u$. Then $H' \in \mathbf{G}_{n,m,k}$. Note that

$$SO_2(H) - SO_2(H') = \frac{a^2-4}{a^2+4} + \frac{b^2-4}{b^2+4} - \frac{a^2-b^2}{a^2+b^2} > 0$$

and

$$SO_5(H) - SO_5(H') = \frac{2(a^2-4)}{\sqrt{2}+2\sqrt{a^2+4}}\pi + \frac{2(b^2-4)}{\sqrt{2}+2\sqrt{b^2+4}}\pi - \frac{2(a^2-b^2)}{\sqrt{2}+2\sqrt{a^2+b^2}}\pi > 0.$$

If $x_1x_l \in E(H)$, set $H' = H - x_2x_3 - x_{l-1}x_l - uv + x_2x_l + vx_3 + x_{l-1}u$. Then $H' \in \mathbf{G}_{n,m,k}$. Note that

$$SO_2(H) - SO_2(H') = \frac{3}{5} - \frac{3}{5} = 0$$

and

$$SO_5(H) - SO_5(H') = \frac{6}{\sqrt{2}+2\sqrt{5}}\pi - \frac{6}{\sqrt{2}+2\sqrt{5}}\pi = 0.$$

Obviously, H' contains more 2-degree vertices in the cycle of length 3 than H. □

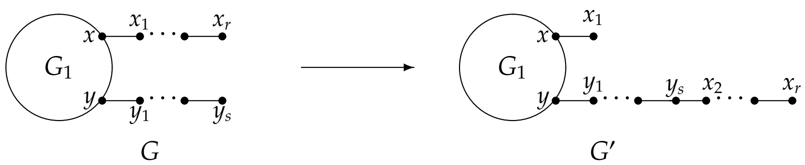

Figure 3. The graphs G and G' in Lemma 3.3

Lemma 3.3. *Let G be a graph as shown in Figure 3, where $x, y \in V(G_1)$ (possibly, $x = y$) and $d_G(x) = a \geq 3, d_G(y) = b \geq 3$. $xx_1x_2\cdots x_r$ and $yy_1y_2\cdots y_s$ are two paths attached to x and y of G_1, respectively, where $r, s \geq 2$. Set $G' = G - x_1x_2 + y_sx_2$, as shown in Figure 3. Then $SO_2(G) > SO_2(G')$ and $SO_5(G) > SO_5(G')$.*

Proof. For $a \geq 3$, we derive

$$SO_2(G) - SO_2(G') = \frac{a^2-4}{a^2+4} + \frac{3}{5} - \frac{a^2-1}{a^2+1} = \frac{3(a^2-1)(a^2-4)}{5(a^2+1)(a^2+4)} > 0$$

and

$$SO_5(G) - SO_5(G') = \frac{6}{\sqrt{2}+2\sqrt{5}}\pi + \frac{2(a^2-4)}{\sqrt{2}+2\sqrt{a^2+4}}\pi - \frac{2(a^2-1)}{\sqrt{2}+2\sqrt{a^2+1}}\pi > 0$$

from Lemma 2.5. □

Theorem 3.6. *Let $G \in \boldsymbol{G}_{n,m,k}$, where $k \geq 4$ for $m = n-1$, or $k \geq 3$ for $m = n$, or $k \geq 2$ for $m = n+1$, or $k \geq 1$ for $m \geq n+2$. Then*

$$SO_2(G) \geq \begin{cases} \frac{4}{5}k & \text{if } |E_1| = 0, \\ \frac{4}{5}k + \frac{12}{65} & \text{if } |E_1| > 0 \end{cases}$$

and

$$SO_5(G) \geq \begin{cases} \pi \frac{16}{\sqrt{2}+2\sqrt{10}} k & \text{if } |E_1| = 0, \\ \pi \frac{16}{\sqrt{2}+2\sqrt{10}} k + \frac{6}{\sqrt{2}+2\sqrt{5}}\pi + \frac{10}{\sqrt{2}+2\sqrt{13}}\pi - \frac{16}{\sqrt{2}+2\sqrt{10}}\pi & \text{if } |E_1| > 0. \end{cases}$$

Moreover, equalities hold only if $G \in \mathbb{G}^{(2)}_{n,m,k}$ with $3n = 2m + 2k$ when $|E_1| = 0$ and with $3n \geq 2m + 2k + 1$ when $|E_1| > 0$, respectively.

Proof. Choose $G \in \boldsymbol{G}_{n,m,k}$ such that G has the minimum SO_2 or SO_5. Clearly, $E(G) = \bigcup_{i=1}^{5} E_i$, $|E_1| + |E_2| = k$. We discuss in two cases.

Case 1. G contains no 2-degree vertex in any pendent path, that is $|E_1| = 0$, $|E_2| = k$.

Now, by using (2), (3) and Lemma 2.1, we derive

$$\begin{aligned} SO_2(G) &= \sum_{uv \in E(G)} \frac{|deg^2_G(u) - deg^2_G(v)|}{deg^2_G(u) + deg^2_G(v)} \\ &= \sum_{uv \in E_2} \frac{deg^2_G(v) - 1}{deg^2_G(v) + 1} + \sum_{uv \in E_4} \frac{deg^2_G(v) - 4}{deg^2_G(v) + 4} + \sum_{uv \in E_5} \frac{|deg^2_G(u) - deg^2_G(v)|}{deg^2_G(u) + deg^2_G(v)} \\ &\geq \frac{4}{5}|E_2| + \frac{5}{13}|E_4| \\ &\geq \frac{4}{5}k \end{aligned} \tag{12}$$

and

$$\begin{aligned} SO_5(G) &= \sum_{uv \in E(G)} \frac{2|deg^2_G(u) - deg^2_G(v)|}{\sqrt{2} + 2\sqrt{deg^2_G(u) + deg^2_G(v)}}\pi \\ &= \sum_{uv \in E_2} \frac{2(deg^2_G(v) - 1)}{\sqrt{2} + 2\sqrt{deg^2_G(v) + 1}}\pi + \sum_{uv \in E_4} \frac{2(deg^2_G(v) - 4)}{\sqrt{2} + 2\sqrt{deg^2_G(v) + 4}}\pi \\ &\quad + \sum_{uv \in E_5} \frac{2|deg^2_G(u) - deg^2_G(v)|}{\sqrt{2} + 2\sqrt{deg^2_G(u) + deg^2_G(v)}}\pi \\ &\geq \frac{16}{\sqrt{2} + 2\sqrt{10}}\pi|E_2| + \frac{10}{\sqrt{2} + 2\sqrt{13}}\pi|E_4| \\ &\geq \pi \frac{16}{\sqrt{2} + 2\sqrt{10}} k. \end{aligned} \tag{13}$$

If the equalities in (12) and (13) follow, all inequalities above-mentioned have to be equalities. So we obtain (I) $|E_1| = 0$, $|E_2| = k$ and $|E_4| = 0$; (II) $deg_G(u) = 1, deg_G(v) = 3$ for $uv \in E_2$; (III) $deg_G(u) = deg_G(v) = 3$ for $uv \in E_5$. Hence the maximal degree of G is three and $k + n_3 = n$ and $k + 3n_3 = 2m$ for $G \in \boldsymbol{G}_{n,m,k}$. It follows that $3n = 2m + 2k$, G belongs to the $(n, m, k, 3)$-semi-regular graphs and $G \in \mathbb{G}^{(2)}_{n,m,k}$.

Case 2. $|E_1| > 0$ and G does not contain the 2-degree vertices on the 3-length cycle in G.

In this case, by Lemmas 3.2 and 3.3, we suppose that all 2-degree vertices lie on a pendent path of G. Now, $|E_1| = 1$, $|E_2| = k - 1$ and $|E_4| = |E_1| = 1$. By using (2), (3) and Lemma 2.1, we deduce that

$$\begin{aligned} SO_2(G) =& \sum_{uv\in E(G)} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)} \\ =& \frac{3}{5}|E_1| + \sum_{uv\in E_2} \frac{deg_G^2(v) - 1}{deg_G^2(v) + 1} + \sum_{uv\in E_4} \frac{deg_G^2(v) - 4}{deg_G^2(v) + 4} + \sum_{uv\in E_5} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)} \\ \geq& \frac{3}{5}|E_1| + \frac{4}{5}|E_2| + \frac{5}{13}|E_4| \\ =& \frac{3}{5} + \frac{4}{5}(k-1) + \frac{5}{13} \\ =& \frac{4}{5}k + \frac{12}{65} \end{aligned} \tag{14}$$

and

$$\begin{aligned} SO_5(G) =& \sum_{uv\in E(G)} \frac{2|deg_G^2(u) - deg_G^2(v)|}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\pi \\ =& \frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1| + \sum_{uv\in E_2} \frac{2(deg_G^2(v) - 1)}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 1}}\pi \\ &+ \sum_{uv\in E_4} \frac{2(deg_G^2(v) - 4)}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 4}}\pi \\ &+ \sum_{uv\in E_5} \frac{2|deg_G^2(u) - deg_G^2(v)|}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\pi \\ \geq& \frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1| + \frac{16}{\sqrt{2}+2\sqrt{10}}\pi|E_2| + \frac{10}{\sqrt{2}+2\sqrt{13}}\pi|E_4| \\ =& \pi\frac{16}{\sqrt{2}+2\sqrt{10}}k + \frac{6}{\sqrt{2}+2\sqrt{5}}\pi + \frac{10}{\sqrt{2}+2\sqrt{13}}\pi - \frac{16}{\sqrt{2}+2\sqrt{10}}\pi. \end{aligned} \tag{15}$$

If the equalities in (14) and (15) follow, all inequalities above-mentioned have to be equalities. Therefore one get (I) $|E_1| = |E_4| = 1$ and $|E_2| = k-1$; (II) $deg_G(v) = 3$ and $deg_G(u) = 2$ for $uv \in E_4$; (III) $deg_G(u) = deg_G(v) = 3$ for $uv \in E_5$ and $n_2 \geq 1$. So the maximum degree of G is 3. We have $k + n_2 + n_3 = n$ and $k + 2n_2 + 3n_3 = 2m$ for $G \in \boldsymbol{G}_{n,m,k}$. It follows that $n_2 = 3n - 2m - 2k$, and $3n \geq 2m + 2k + 1$, $G \in \mathbb{G}_{n,m,k}^{(2)}$.

Case 3. $|E_1| > 0$ and G contains at least one 2-degree vertex on the 3-length cycles.

We use r to represent the number of the 3-length cycles having the 2-degree vertices in G. So $|E_4| = |E_1| + 2r$, where $r > 0$. By Lemmas 3.2 and 3.3, we assume that all 2-degree vertices are on the 3-length cycles or a pendent path in G. Now, $|E_1| = 1$, $|E_2| = k - 1$ and $|E_4| = |E_1| + 2r = 1 + 2r$. By using (2), (3) and Lemma 2.1, one has

$$\begin{aligned} SO_2(G) =& \sum_{uv\in E(G)} \frac{|deg_G^2(u) - deg_G^2(v)|}{deg_G^2(u) + deg_G^2(v)} \\ =& \frac{3}{5}|E_1| + \sum_{uv\in E_2} \frac{deg_G^2(v) - 1}{deg_G^2(v) + 1} + \sum_{uv\in E_4} \frac{deg_G^2(v) - 4}{deg_G^2(v) + 4} \end{aligned}$$

$$
\begin{aligned}
&+\sum_{uv\in E_5}\frac{|deg_G^2(u)-deg_G^2(v)|}{deg_G^2(u)+deg_G^2(v)}\\
\geq&\frac{3}{5}|E_1|+\frac{4}{5}|E_2|+\frac{5}{13}|E_4|\\
=&\frac{3}{5}+\frac{4}{5}(k-1)+\frac{5}{13}(1+2r)\\
>&\frac{4}{5}k+\frac{12}{65}
\end{aligned}
$$

and

$$
\begin{aligned}
SO_5(G)=&\sum_{uv\in E(G)}\frac{2|deg_G^2(u)-deg_G^2(v)|}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\pi\\
=&\frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1|+\sum_{uv\in E_2}\frac{2(deg_G^2(v)-1)}{\sqrt{2}+2\sqrt{deg_G^2(v)+1}}\pi\\
&+\sum_{uv\in E_4}\frac{2(deg_G^2(v)-4)}{\sqrt{2}+2\sqrt{deg_G^2(v)+4}}\pi\\
&+\sum_{uv\in E_5}\frac{2|deg_G^2(u)-deg_G^2(v)|}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\pi\\
\geq&\frac{6}{\sqrt{2}+2\sqrt{5}}\pi|E_1|+\frac{16}{\sqrt{2}+2\sqrt{10}}\pi|E_2|+\frac{10}{\sqrt{2}+2\sqrt{13}}\pi|E_4|\\
=&\frac{6}{\sqrt{2}+2\sqrt{5}}\pi+\frac{16}{\sqrt{2}+2\sqrt{10}}\pi(k-1)+\frac{10}{\sqrt{2}+2\sqrt{13}}\pi(1+2r)\\
>&\pi\frac{16}{\sqrt{2}+2\sqrt{10}}k+\frac{6}{\sqrt{2}+2\sqrt{5}}\pi+\frac{10}{\sqrt{2}+2\sqrt{13}}\pi-\frac{16}{\sqrt{2}+2\sqrt{10}}\pi.
\end{aligned}
$$

The proof is completed. □

3.3. Minimum SO_6 index of chemical graphs with a given order, number of edges and pendent vertices

Theorem 3.7. *Let $G\in \boldsymbol{G}_{n,n,1}$ or $\boldsymbol{G}_{n,n+1,1}$. Then*

$$
SO_6(G)\geq\left(\frac{3}{\sqrt{2}+2\sqrt{5}}\right)^2\pi+3\left(\frac{5}{\sqrt{2}+2\sqrt{13}}\right)^2\pi.
$$

Equality holds if and only if $G\in U_n^1$, $n\geq 5, 3\leq s\leq n-2$, or $G\in B_n$, $n\geq 6, 4\leq s\leq n-2$ (see Figure 2).

Proof. For $G\in \boldsymbol{G}_{n,n,1}$ or $\boldsymbol{G}_{n,n+1,1}$, one gets $E(G)=\bigcup_{i=1}^{5}E_i$ and $|E_1|+|E_2|=1$. By using (4) and Lemma 2.1, it follows that

$$
\begin{aligned}
SO_6(G) &= \sum_{uv\in E(G)} \Big(\frac{deg_G^2(u) - deg_G^2(v)}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\Big)^2 \pi \\
&= \Big(\frac{3}{\sqrt{2} + 2\sqrt{5}}\Big)^2 \pi |E_1| + \sum_{uv\in E_2} \Big(\frac{deg_G^2(v) - 1}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 1}}\Big)^2 \pi \\
&\quad + \sum_{uv\in E_4} \Big(\frac{deg_G^2(v) - 4}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 4}}\Big)^2 \pi \\
&\quad + \sum_{uv\in E_5} \Big(\frac{deg_G^2(u) - deg_G^2(v)}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\Big)^2 \pi \\
&\geq \Big(\frac{3}{\sqrt{2} + 2\sqrt{5}}\Big)^2 \pi |E_1| + \Big(\frac{8}{\sqrt{2} + 2\sqrt{10}}\Big)^2 \pi |E_2| \\
&\quad + \Big(\frac{5}{\sqrt{2} + 2\sqrt{13}}\Big)^2 \pi |E_4|. \qquad (16)
\end{aligned}
$$

Case 1. $G \in \boldsymbol{G}_{n,n,1} (n \geq 5)$.

Now, $|E_5| = 0$. For $|E_1| = 1, |E_2| = 0$, one has $|E_4| = 3$. From (16), we get $SO_6(G) \geq \big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2\pi + 3\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi$. If $SO_6(G) = \big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2\pi + 3\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi$, then (I) $|E_1| = 1, |E_2| = 0$; (II) $deg_G(u) = 2, deg_G(v) = 3$ for $uv \in E_4$ and $|E_4| = 3$. That is $G \in U_n^1$ $(3 \leq s \leq n-2)$.

For $|E_1| = 0, |E_2| = 1$, one has $|E_4| = 2$. From (16), we get $SO_6(G) \geq \big(\frac{8}{\sqrt{2}+2\sqrt{10}}\big)^2\pi + 2\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi > \big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2\pi + 3\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi$.

Case 2. $G \in \boldsymbol{G}_{n,n+1,1} (n \geq 6)$.

For $|E_1| = 1, |E_2| = 0$, one has $|E_4| \geq 3$. From (16), we derive $SO_6(G) \geq \big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2\pi + 3\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi$. If $SO_6(G) = \big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2\pi + 3\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi$, then (I) $|E_1| = 1, |E_2| = 0$; (II) $deg_G(u) = 2, deg_G(v) = 3$ for $uv \in E_4$ and $|E_4| = 3$; (III) $deg_G(u) = deg_G(v) = 3$ for $uv \in E_5$. This means that $G \in B_n$ $(4 \leq s \leq n-2)$.

For $|E_1| = 0, |E_2| = 1$, one has $|E_4| \geq 2$. From (16), we derive $SO_6(G) \geq \big(\frac{8}{\sqrt{2}+2\sqrt{10}}\big)^2\pi + 2\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi > \big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2\pi + 3\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2\pi$. □

Theorem 3.8. *Let $G \in \boldsymbol{G}_{n,n,2}$. Then*

$$SO_6(G) \geq 2\Big(\frac{3}{\sqrt{2} + 2\sqrt{5}}\Big)^2 \pi + 4\Big(\frac{5}{\sqrt{2} + 2\sqrt{13}}\Big)^2 \pi,$$

where equality holds only if $G \in U_n^2$, $n \geq 8$, $t \geq 3$, $3 \leq s \leq n-5$ or $G \in U_n^3$, $n \geq 7$, $t \geq 2$, $3 \leq s \leq n-4$ (see Figure 2).

Proof. For $G \in \boldsymbol{G}_{n,n,2}$, $E(G) = \bigcup_{i=1}^{5} E_i$ and $|E_1| + |E_2| = 2$. By using (4) and Lemma 2.1, we derive

$$\begin{aligned} SO_6(G) =& \sum_{uv\in E(G)} \Big(\frac{deg_G^2(u) - deg_G^2(v)}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\Big)^2 \pi \\ =& \Big(\frac{3}{\sqrt{2} + 2\sqrt{5}}\Big)^2 \pi |E_1| + \sum_{uv\in E_2} \Big(\frac{deg_G^2(v) - 1}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 1}}\Big)^2 \pi \\ &+ \sum_{uv\in E_4} \Big(\frac{deg_G^2(v) - 4}{\sqrt{2} + 2\sqrt{deg_G^2(v) + 4}}\Big)^2 \pi \\ &+ \sum_{uv\in E_5} \Big(\frac{deg_G^2(u) - deg_G^2(v)}{\sqrt{2} + 2\sqrt{deg_G^2(u) + deg_G^2(v)}}\Big)^2 \pi \\ \geq& \Big(\frac{3}{\sqrt{2} + 2\sqrt{5}}\Big)^2 \pi |E_1| + \Big(\frac{8}{\sqrt{2} + 2\sqrt{10}}\Big)^2 \pi |E_2| \\ &+ \Big(\frac{5}{\sqrt{2} + 2\sqrt{13}}\Big)^2 \pi |E_4| \\ =& 2\Big(\frac{3}{\sqrt{2} + 2\sqrt{5}}\Big)^2 \pi + \Big[\Big(\frac{8}{\sqrt{2} + 2\sqrt{10}}\Big)^2 - \Big(\frac{3}{\sqrt{2} + 2\sqrt{5}}\Big)^2\Big] \pi |E_2| \\ &+ \Big(\frac{5}{\sqrt{2} + 2\sqrt{13}}\Big)^2 \pi |E_4|. \end{aligned} \quad (17)$$

If $|E_1| = 2, |E_2| = 0$, then $|E_4| \geq 4$. From (17), one has $SO_6(G) \geq 2\big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2 \pi + 4\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2 \pi$. If $SO_6(G) = 2\big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2 \pi + 4\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2 \pi$, similar to the proof of Theorem 3.7, it is not difficult to check that $G \in U_n^2$ ($t \geq 3$, $3 \leq s \leq n-5$) or $G \in U_n^3$ ($t \geq 2$, $3 \leq s \leq n-4$).

If $|E_1| = 1, |E_2| = 1$, then $|E_4| \geq 3$. From (17), one has $SO_6(G) \geq \big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2 \pi + \big(\frac{8}{\sqrt{2}+2\sqrt{10}}\big)^2 \pi + 3\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2 \pi > 2\big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2 \pi + 4\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2 \pi$.

If $|E_1| = 0, |E_2| = 2$, then $|E_4| \geq 2$. From (17), one has $SO_6(G) \geq 2\big(\frac{8}{\sqrt{2}+2\sqrt{10}}\big)^2 \pi + 2\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2 \pi > 2\big(\frac{3}{\sqrt{2}+2\sqrt{5}}\big)^2 \pi + 4\big(\frac{5}{\sqrt{2}+2\sqrt{13}}\big)^2 \pi$. □

Lemma 3.4. *Let $H \in \boldsymbol{G}_{n,m,k}$. Assume that $x \in V(H)$ is a 2-degree vertex that is not contained in any 3-length cycle and any pendent path. Then there is a graph $H' \in \boldsymbol{G}_{n,m,k}$ satisfying one of the following properties:*

1) *$SO_6(H') < SO_6(H)$;*

2) *$SO_6(H') = SO_6(H)$ and H' contains more 2-degree vertices in pendent paths than H.*

Proof. Assume that the neighbors of x are y and z with $deg_H(y) = a \geq deg_H(z) = b \geq 2$. Let u be a pendent vertex of H and v be the neighbor of u with $deg_H(v) = c \geq 2$. Let $H' = H - xy - xz - uv + yz + ux + vx$. Then

$H' \in \boldsymbol{G}_{n,m,k}$. Note that

$$\begin{aligned}
&SO_6(H) - SO_6(H') \\
=&\Big(\frac{a^2-4}{\sqrt{2}+2\sqrt{a^2+4}}\Big)^2\pi + \Big(\frac{b^2-4}{\sqrt{2}+2\sqrt{b^2+4}}\Big)^2\pi + \Big(\frac{c^2-1}{\sqrt{2}+2\sqrt{c^2+1}}\Big)^2\pi \\
&-\Big(\frac{c^2-4}{\sqrt{2}+2\sqrt{c^2+4}}\Big)^2\pi - \Big(\frac{a^2-b^2}{\sqrt{2}+2\sqrt{a^2+b^2}}\Big)^2\pi - \Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2\pi \\
=&\pi\Big[\Big(\frac{c^2-1}{\sqrt{2}+2\sqrt{c^2+1}}\Big)^2 - \Big(\frac{c^2-4}{\sqrt{2}+2\sqrt{c^2+4}}\Big)^2\pi - \Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2\Big] \\
&+\pi\Big[\Big(\frac{a^2-4}{\sqrt{2}+2\sqrt{a^2+4}}\Big)^2 + \Big(\frac{b^2-4}{\sqrt{2}+2\sqrt{b^2+4}}\Big)^2 - \Big(\frac{a^2-b^2}{\sqrt{2}+2\sqrt{a^2+b^2}}\Big)^2\Big].
\end{aligned}$$

For $a \geq b > 2$ or $c > 2$, in view of Lemmas 2.2 and 2.3, one gets $SO_6(H) > SO_6(H')$. On the other hand, only when $b = 2$ and $c = 2$, $SO_6(H) = SO_6(H')$. Now, obviously H' contains more 2-degree vertices in pendent paths than H. □

Theorem 3.9. *Suppose $G \in \boldsymbol{G}_{n,m,k}$, where $k \geq 4$ for $m = n-1$, or $k \geq 3$ for $m = n$, or $k \geq 2$ for $m = n+1$, or $k \geq 1$ for $m \geq n+2$, then*

$$SO_6(G) \geq \pi\Big[\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2 + \Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\Big]k.$$

Equality holds if and only if $G \in \mathbb{G}^{(3)}_{n,m,k}$ and $3n \geq 3k + 2m$.

Proof. Pick $G \in \boldsymbol{G}_{n,m,k}$ such that G has the minimum SO_6. By this supposition and Lemma 3.4, without loss of generality, we suppose that all 2-degree vertices lie on the pendent paths except the 2-degree vertices on the 3-length cycles in G. In what follows, we prove the theorem in two cases.

Case 1. G does not contain the 2-degree vertices on the 3-length cycle.

Clearly, $E(G) = \bigcup_{i=1}^{5} E_i$, $|E_1| + |E_2| = k$ and $|E_1| = |E_4|$. By using (4) and Lemma 2.1, one has

$$\begin{aligned}
SO_6(G) =& \sum_{uv\in E(G)}\Big(\frac{deg_G^2(u) - deg_G^2(v)}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\Big)^2\pi \\
=&\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2\pi|E_1| + \sum_{uv\in E_2}\Big(\frac{deg_G^2(v)-1}{\sqrt{2}+2\sqrt{deg_G^2(v)+1}}\Big)^2\pi \\
&+\sum_{uv\in E_4}\Big(\frac{deg_G^2(v)-4}{\sqrt{2}+2\sqrt{deg_G^2(v)+4}}\Big)^2\pi \\
&+\sum_{uv\in E_5}\Big(\frac{deg_G^2(u)-deg_G^2(v)}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\Big)^2\pi \\
\geq&\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2\pi|E_1| + \Big(\frac{8}{\sqrt{2}+2\sqrt{10}}\Big)^2\pi|E_2| \\
&+\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\pi|E_4| \\
=&\pi\Big[\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2 + \Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\Big]k
\end{aligned}$$

$$+\pi\Big[\Big(\frac{8}{\sqrt{2}+2\sqrt{10}}\Big)^2-\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2-\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\Big]|E_2|$$
$$\geq\pi\Big[\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2+\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\Big]k. \tag{18}$$

If the equality in (18) holds, all inequalities in the above argument must be equalities. Thus we have (I) $deg_G(u)=2, deg_G(v)=3$ for $uv\in E_4$; (II) $|E_2|=0$; (III) $deg_G(u)=deg_G(v)=3$ for $uv\in E_5$ and $n_2\geq k$ since an edge of E_4 is associated with one edge of E_5 and a 2-degree vertex. Hence, the maximal degree of G is 3 and $k+n_2+n_3=n$, $k+2n_2+3n_3=2m$ for $G\in \boldsymbol{G}_{n,m,k}$. It follows that $n_2=3n-2m-2k$, and thus $3n\geq 2m+3k$, $G\in\mathbb{G}^{(3)}_{n,m,k}$.

Case 2. G contains at least a 2-degree vertex on the 3-length cycles.

We use r to denote the number of the 3-length cycles having 2-degree vertices in G. In this case, $E(G)=\bigcup_{i=1}^{5}E_i$, $|E_1|+|E_2|=k$ and $|E_4|=|E_1|+2r$, where $r>0$. By using (4) and Lemma 2.1, we have

$$SO_6(G)=\sum_{uv\in E(G)}\Big(\frac{deg_G^2(u)-deg_G^2(v)}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\Big)^2\pi$$
$$=\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2\pi|E_1|+\sum_{uv\in E_2}\Big(\frac{deg_G^2(v)-1}{\sqrt{2}+2\sqrt{deg_G^2(v)+1}}\Big)^2\pi$$
$$+\sum_{uv\in E_4}\Big(\frac{deg_G^2(v)-4}{\sqrt{2}+2\sqrt{deg_G^2(v)+4}}\Big)^2\pi$$
$$+\sum_{uv\in E_5}\Big(\frac{deg_G^2(u)-deg_G^2(v)}{\sqrt{2}+2\sqrt{deg_G^2(u)+deg_G^2(v)}}\Big)^2\pi$$
$$\geq\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2\pi|E_1|+\Big(\frac{8}{\sqrt{2}+2\sqrt{10}}\Big)^2\pi|E_2|$$
$$+\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\pi|E_4|$$
$$=\pi\Big[\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2+\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\Big]k+2\pi r\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2$$
$$+\pi\Big[\Big(\frac{8}{\sqrt{2}+2\sqrt{10}}\Big)^2-\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2-\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\Big]|E_2|$$
$$>\pi\Big[\Big(\frac{3}{\sqrt{2}+2\sqrt{5}}\Big)^2+\Big(\frac{5}{\sqrt{2}+2\sqrt{13}}\Big)^2\Big]k.$$

The proof is completed. □

4. Conclusions and discussions

Remark 4.1. *For any graphs in U_n^1, U_n^2, U_n^3, B_n, $\mathbb{G}^{(1)}_{n,m,k}$, $\mathbb{G}^{(2)}_{n,m,k}$ and $\mathbb{G}^{(3)}_{n,m,k}$, the maximum degree of these graphs is less than 4, so Theorems 3.1-3.9 hold for $G\in \boldsymbol{CG}_{n,m,k}$.*

In this paper, we get the minimum value of SO_1, SO_2, SO_5 and SO_6 indices for all (n,m,k)-graphs (resp. chemical (n,m,k)-graphs). One can investigate the chemical (n,m,k)-graphs with the minimum value of SO_3, SO_4 indices and the maximum value of SO_1, SO_2, SO_3, SO_4, SO_5, SO_6 indices as a future work.

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