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# On Diameter, Cyclomatic Number and Inverse Degree of Chemical Graphs

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Abstract. Let $G$ be a chemical graph with vertex set $\{v_1, v_1, \ldots, v_n\}$ and degree sequence $d(G) = (\deg_G(v_1), \deg_G(v_2), \ldots, \deg_G(v_n))$. The inverse degree, $R(G)$ of $G$ is defined as $R(G) = \sum_{i=1}^{n} \frac{1}{\deg_G(v_i)}$. The cyclomatic number of $G$ is defined as $\gamma = m - n + k$, where $m$, $n$ and $k$ are the number of edges, vertices and components of $G$, respectively. In this paper, some upper bounds on the diameter of a chemical graph in terms of its inverse degree are given. We also obtain an ordering of connected chemical graphs with respect to the inverse degree.

## 1. Introduction

Throughout this paper, all graphs are assumed to be undirected, simple and connected. Let $G$ be such a graph. We denote its vertex set and edge set by $V(G)$ and $E(G)$, respectively. The degree of a vertex $v$, $\deg_G(v)$, is defined as the size of $\{w \in V(G) \mid vw \in E(G)\}$. A vertex of degree one is called a pendant vertex.

The number of vertices of degree $i$ in $G$ is denoted by $n_i = n_i(G)$. Obviously $\sum_{i\geq 1} n_i = |V(G)|$. A chemical graph is a graph with a maximum degree of less than or equal to 4. This reflects the fact that chemical graphs represent the structure of organic molecules– carbon atoms being 4-valent and double bonds being counted as single edges.

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The distance $d_G(u,v)$ between two vertices $u$ and $v$ of $G$ is the length of a shortest $u-v$ path in $G$, and the diameter is defined as $\mathrm{diam}(G) = \max\{d_G(u,v) \mid u,v \in V(G)\}$.

The cyclomatic number of a connected graph $G$ is the minimum number of edges that must be removed from the graph to break all its cycles, making it into a tree or forest. The cyclomatic number $\gamma(G)$ can be expressed as $\gamma(G) = m - n + k$, where $n$, $m$ and $k$ denote the number of vertices, edges and components of $G$, respectively.

A graph with cyclomatic number $0, 1, 2, 3, 4$ or $5$ is said to be a tree, unicyclic, bicyclic, tricyclic, tetracyclic or pentacyclic, respectively. Suppose $E'$ is a subset of $E(G)$. The subgraph $G - E'$ of $G$ is obtained by deleting the edges of $E'$. If $uv \notin E(G)$, then the graph $G + uv$ obtained from $G$ by attaching vertices $u$, $v$.

Suppose $r = (r_1, r_2, \dots, r_n)$ and $s = (s_1, s_2, \dots, s_n)$ are two non-increasing vectors in $\mathbb{R}^n$. If $\sum_{i=1}^{k} r_i \leq \sum_{i=1}^{k} s_i$, $1 \leq k \leq n-1$, and $\sum_{i=1}^{n} r_i = \sum_{i=1}^{n} s_i$, then we say that $r$ is majorized by $s$, and we write $r \preceq s$. Moreover, $r \prec s$ means that $r \preceq s$ and $r \neq s$, see [10] for details. The non-increasing sequence $d = (d_1, d_2, \dots, d_n)$ of nonnegative integers is called a graphic sequence if we can find a simple graph $G$ with the vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ such that $d_i = \deg_G(v_i)$, $1 \leq i \leq n$. The *inverse degree*, $R(G)$ of $G$ was defined as $R(G) = \sum_{i=1}^{n} \frac{1}{\deg_G(v_i)}$, under the name *zeroth-order Randić* index by Kier and Hall in [9]. The inverse degree attracted attention through conjectures of the computer program Graffiti [6]. Since then its relationship with other graph invariants, such as diameter, edge-connectivity, matching number, chromatic number, clique number, Wiener index, $GA_1$-index, $ABC$-index and $Kf$-index has been studied by several authors (see, for example, [1, 2, 4, 5, 12]). Some extremal graphs with respect to the inverse degree are given (see, for example, [11]).

In this paper, some upper bounds on the diameter of a chemical graph in terms of its inverse degree are given. We also obtain an ordering of connected chemical graphs with respect to inverse degree.

## 2. Bounds on the Inverse Degree

In this section, some new bounds for inverse degree are presented. We start this section with the following lemma:

**Lemma 2.1.**([8]) *If $G$ is a connected graph with $n$ vertices and cyclomatic number $\gamma$, then $n_1(G) = 2 - 2\gamma + \sum_{i=3}^{\Delta(G)} (i-2) n_i$ and $n_2(G) = 2\gamma + n - 2 - \sum_{i=3}^{\Delta(G)} (i-1) n_i$.*

**Proposition 2.2.** *Let $G$ be a connected graph with $m$ edges.*

(1) *If $G \cong P_n$, then $\gamma(G) = m - \mathrm{diam}(G) - n_1 + 2$.*

(2) *If $G \ncong P_n$, then $\gamma(G) \leq m - \mathrm{diam}(G) - n_1 + 1$.*

*Proof.* It is clear that $\gamma(P_n) = m - \mathrm{diam}(G) - n_1 + 2$. Let $G$ be a graph such that $G \ncong P_n$. Suppose $u, v \in V(G)$, $d_G(u,v) = \mathrm{diam}(G)$ and $u w_1 w_2 \dots w_{\mathrm{diam}(G)-1} v$ is a shortest $u - v$ path in $G$. Let $A = \{u w_1, w_1 w_2, \dots, w_{\mathrm{diam}(G)-2} w_{\mathrm{diam}(G)-1}, w_{\mathrm{diam}(G)-1} v\}$

and $B = \{uv \mid uv \in E(G)$ and $uv$ is a pendant edge in $G\}$. Then observe that $|A \cap B| \leq 2$ and the subgraph $G - \big(E \setminus (A \cup B \cup \{e\})\big)$ is an acyclic graph, where $e \in E \setminus (A \cup B)$. Therefore, $\gamma(G) \leq m - \mathrm{diam}(G) - n_1 + 1$. □

**Corollary 2.3.** *Let $G$ be a connected graph with $n$ vertices and $m$ edges except $P_n$. Then* $\mathrm{diam}(G) \leq n - n_1 + 1$. *Furthermore, if $G$ is a chemical graph, then* $\mathrm{diam}(G) \leq 2n - \gamma(G) - \frac{5}{2}n_1 + 1$.

*Proof.* By Proposition 2.2, we have $\mathrm{diam}(G) \leq n - n_1 + 1$ since $\gamma(G) = m - n + 1$. It is well-known that for a chemical graph $G$, $m \leq 2n - \frac{3}{2}n_1$. Therefore, by Proposition 2.2, $\mathrm{diam}(G) \leq 2n - \gamma(G) - \frac{5}{2}n_1 + 1$. □

**Theorem 2.4.** *Let $G$ be a connected chemical graph with $n$ vertices, $m$ edges and cyclomatic number $\gamma$.*

(1) *If $G \cong P_n$, then* $\mathrm{diam}(G) = 2R(G) - n_1 - 1$.

(2) *If $G \ncong P_n$, then* $\mathrm{diam}(G) \leq 4R(G) - n_1$.

*Proof.* It is easy to see that $\mathrm{diam}(P_n) = 2R(G) - n_1 - 1$. For $G \ncong P_n$, by definition of $R(G)$ and Lemma 2.1,

$$R(G) \quad = \quad 2 - 2\gamma + \frac{1}{2}n_2 + \frac{4}{3}n_3 + \frac{9}{4}n_4.$$

By Proposition 2.2, and the fact that $m = \frac{1}{2}(n_1 + 2n_2 + 3n_2 + 4n_4)$, we have

$$\begin{aligned} R(G) &\geq n_1 - \frac{3}{2}n_2 - \frac{5}{3}n_3 - \frac{7}{4}n_4 + 2\,\mathrm{diam}(G) \\ &= 2n_1 - (n_1 + \frac{3}{2}n_2 + \frac{5}{3}n_3 + \frac{7}{4}n_4) + 2\,\mathrm{diam}(G) \\ &\geq 2n_1 - 7(n_1 + \frac{1}{2}n_2 + \frac{1}{3}n_3 + \frac{1}{4}n_4) + 2\,\mathrm{diam}(G). \end{aligned} \tag{2.1}$$

Thus $\mathrm{diam}(G) \leq 4R(G) - n_1$. □

**Corollary 2.5.** *Let $G$ be a connected chemical graph with $n$ vertices and $m$ edges. Then $R(G) = \frac{3}{2}n - m + \frac{1}{3}n_3 + \frac{3}{4}n_4$. Besides, if $n_4 = 0$,* $\mathrm{diam}(G) \leq 3R(G) - n_1$.

*Proof.* By definition,

$$\begin{aligned} R(G) = \sum_{v \in V(G)} \frac{1}{\deg_G(v)} &= n_1 + \frac{n_2}{2} + \frac{n_3}{3} + \frac{n_4}{4} \\ &= \frac{1}{12}(12n_1 + 6n_2 + 4n_3 + 3n_4). \end{aligned}$$

Now, by Lemma 2.1. and $\gamma(G) = m - n + 1$, we have $R(G) = \frac{3}{2}n - m + \frac{1}{3}n_3 + \frac{3}{4}n_4$. If $n_4 = 0$, then by Eq. (2.1), $R(G) \geq 2n_1 - (n_1 + \frac{3}{2}n_2 + \frac{5}{3}n_3) + 2\,\mathrm{diam}(G)$. Therefore, $\mathrm{diam}(G) \leq 3R(G) - n_1$. □

**Corollary 2.6.** *Let $G$ be a connected chemical graph with $n$ vertices and $m$ edges. Then $R(G) \geq \frac{3}{2}n - m$, with equality if and only if $G \cong P_n$ or $C_n$.*

**Corollary 2.7.** *Let $G$ be a connected chemical graph with $n$ vertices. Then the following hold:*

(1) *If $G$ is a tree, then $R(G) \geq \frac{1}{2}n + 1$, with equality if and only if $G \cong P_n$.*

(2) *If $G$ is unicyclic, then $R(G) \geq \frac{1}{2}n$, with equality if and only if $G \cong C_n$.*

For $n \geq 5$ we set

$$\Gamma_1 = \{B \mid B \text{ is a bicyclic graph, } n_3(B) = 2 \text{ and } n_2(B) = n-2\},$$
$$\Gamma_2 = \{B \mid B \text{ is a bicyclic graph, } n_4(B) = 1 \text{ and } n_2(B) = n-1\}.$$

**Corollary 2.8.** *Let $G$ be a chemical bicyclic graph with $n \geq 5$ vertices. If $B_1 \in \Gamma_1$, $B_2 \in \Gamma_2$ and $G \notin \Gamma_1 \cup \Gamma_2$, then $R(B_1) < R(B_2) = \frac{1}{2}n - \frac{1}{4} < R(G)$.*

*Proof.* By Corollary 2.5, if $n_4(G) \geq 1$, then $R(G) \geq \frac{1}{2}n - \frac{1}{4}$, with equality if and only if $G \in \Gamma_2$. If $n_4(G) = 0$ and $n_3(G) = 0$ or $n_4(G) = 0$ and $n_3(G) = 1$, then $G$ is not a chemical bicyclic graph. If $n_4(G) = 0$ and $n_3(G) = 2$, then $R(G) = \frac{1}{2}n - \frac{1}{3}$; and if $n_4(G) = 0$ and $n_3(G) \geq 3$, then $R(G) \geq \frac{1}{2}n$, proving the corollary. □

For $n \geq 5$ we set

$$\Lambda_1 = \big\{G \mid G \text{ is a tricyclic graph, } n_3(G) = 4 \text{ and } n_2(G) = n-4\big\},$$
$$\Lambda_2 = \big\{G \mid G \text{ is a tricyclic graph, } n_4(G) = 1,\ n_3(G) = 2 \text{ and } n_2(G) = n-3\big\}.$$

**Corollary 2.9.** *Let $G$ be a chemical tricyclic graph with $n \geq 5$ vertices. If $G_1 \in \Lambda_1$, $G_2 \in \Lambda_2$ and $G \notin \Lambda_1 \cup \Lambda_2$, then $R(G_1) < R(G_2) = \frac{1}{2}n + \frac{5}{12} < R(G)$.*

*Proof.* By Corollary 2.5, if $n_4(G) \geq 2$, $R(G) \geq \frac{1}{2}n + \frac{1}{2}$. If $n_4(G) = 1$ and $n_3(G) \leq 1$, or $n_4(G) = 0$ and $n_3(G) \leq 3$, then $G$ is not a chemical tricyclic graph. If $n_4(G) = 0$ and $n_3(G) = 4$, then $R(G) = \frac{1}{2}n + \frac{1}{3}$. If $n_4(G) = 1$ and $n_3(G) = 2$, then $R(G) = \frac{1}{2}n + \frac{5}{12}$. If $n_4(G) = 0$ and $n_3(G) \geq 5$, then $R(G) \geq \frac{1}{2}n + \frac{2}{3}$. If $n_4(G) = 1$ and $n_3(G) \geq 3$, then $R(G) \geq \frac{1}{2}n + \frac{3}{4}$, proving the result. □

The proofs of the following two corollaries are similar to that of Corollary 2.8 and Corollary 2.9. So we omit them.

Next we define the following two sets, when $n \geq 6$,

$$\Theta_1 = \{G \mid G \text{ is a tetracyclic graph, } n_3(G) = 6 \text{ and } n_2(G) = n-6\},$$
$$\Theta_2 = \{G \mid G \text{ is a tetracyclic graph, } n_4(G) = 1,\ n_3(G) = 4 \text{ and } n_2(G) = n-5\}.$$

**Corollary 2.10.** *Let $G$ be a chemical tetracyclic graph with $n \geq 6$ vertices. If $G_1 \in \Theta_1$ and $G_2 \in \Theta_2$ and $G \notin \Theta_1 \cup \Theta_2$, then $R(G_1) < R(G_2) = \frac{1}{2}n + \frac{13}{12} < R(G)$.*

For $n \geq 8$ we define

$$\Upsilon_1 = \{G \mid G \text{ is a pentacyclic graph, } n_3(G) = 8 \text{ and } n_2(G) = n - 8\},$$
$$\Upsilon_2 = \{G \mid G \text{ is a pentacyclic graph, } n_4(G) = 1,\ n_3(G) = 6 \text{ and } n_2(G) = n - 7\}.$$

**Corollary 2.11.** *Let $G$ be a chemical pentacyclic graph with $n \geq 6$ vertices. If $G_1 \in \Upsilon_1$, $G_2 \in \Upsilon_2$ and $G \notin \Upsilon_1 \cup \Upsilon_2$, then $R(G_1) < R(G_2) = \frac{1}{2}n + \frac{7}{4} < R(G)$.*

## 3. Ordering Chemical Trees and Unicyclic Graphs with Respect to the Inverse Degree Index

Recall that if $I \subset \mathbb{R}$ is an interval and $f : I \longrightarrow \mathbb{R}$ is a real-valued function such that $f''(x) \geq 0$ on $I$, then $f$ is convex on $I$. If $f''(x) > 0$, then $f$ is strictly convex on $I$. A real-valued function $\varphi$ defined on a set $\Lambda \subset \mathbb{R}^n$ is said to be Schur-convex on $\Lambda$ if for all $x = (x_1, \ldots, x_n)$ and $y = (y_1 \ldots, y_n) \in \Lambda$, if $x \preceq y$, then $\varphi(x) \leq \varphi(y)$. In addition, $\varphi$ is said to be strictly Schur-convex on $\Lambda$ if $x \prec y$ implies that $\varphi(x) < \varphi(y)$.

**Lemma 3.1.**([10]) *Let $I \subset \mathbb{R}$ be an interval and let $\varphi(x_1, \ldots, x_n) = \sum_{i=1}^{n} g(x_i)$, where $g : I \longrightarrow \mathbb{R}$. If $g$ is strictly convex on $I$, then $\varphi$ is strictly Schur-convex on $I^n$.*

**Theorem 3.2.** *Let $G$ and $G'$ be two connected graphs with the degree sequences $d(G) = (d_1, \ldots, d_n)$ and $d(G') = (d'_1, \ldots, d'_n)$, respectively. If $d(G) \preceq d(G')$, then $R(G) \leq R(G')$, with equality if and only if $d(G) = d(G')$.*

*Proof.* Let $\alpha : (0, \infty) \longrightarrow \mathbb{R}$ be a real-valued function such that $\alpha(x) = \frac{1}{x}$ for all $x \in (0, \infty)$. Then observe that for $x > 0$, $\alpha''(x) = \frac{2}{x^3} > 0$. Therefore, $\alpha$ is strictly convex on $(0, \infty)$. So by Lemma 3.1, inverse degree, $R$, is strictly Schur-convex. Thus $R(G) \leq R(G')$, with equality if and only if $d(G) = d(G')$. □

**Lemma 3.3.** (See [7]) *Suppose that $G_1$ is a graph with given vertices $v_1$ and $v_2$, such that $\deg_{G_1}(v_1) \geq 2$ and $\deg_{G_1}(v_2) = 1$. In addition, assume that $G_2$ is another graph and $w$ is a vertex in $G_2$. Let $G$ be the graph obtained from $G_1$ and $G_2$ by attaching vertices $w$ and $v_1$. If $G' = G - wv_1 + wv_2$, then $d(G') \prec d(G)$.*

**Theorem 3.4.** *Among all graphs with $n$ vertices and cyclomtatic number $\gamma$ ($1 \leq \gamma \leq n - 2$), a graph $G^1_\gamma$ with the degree sequence*

$$d(G^1_\gamma) = (n-1, \gamma+1, \underbrace{2, \ldots, 2}_{\gamma}, \underbrace{1, \ldots, 1}_{n-\gamma-2})$$

*has the maximal inverse degree and a graph $G^2_\gamma$ with the degree sequence*

$$d(G^2_\gamma) = (\underbrace{x+1, \ldots, x+1}_{y}, \underbrace{x, \ldots, x}_{n-y}),$$

*where* $x = \lfloor \frac{2n+2\gamma-2}{n} \rfloor$ *and* $y \equiv 2n+2\gamma-2 \pmod{n}$*, has the minimal inverse degree.*

*Proof.* Let $G$ be an arbitrary simple connected graph with $n$ vertices and with cyclomtatic number $\gamma$ $(1 \leq \gamma \leq n-2)$ which is different from $G^1_\gamma$ and $G^2_\gamma$. Dimitrov and Ali in [3] showed that $d(G^2_\gamma) \prec d(G) \prec d(G^1_\gamma)$. Now, the result follows from Theorem 3.2. □

**Theorem 3.5.** *Let* $T_i \in A_i$*, for* $1 \leq i \leq 31$ *(See Table* 1 *). If* $n \geq 22$ *and* $T$ *is a tree such that* $T \notin \bigcup_{i=1}^{31} A_i$*, then* $R(T_i) < R(T_{i+1})$ *for* $i \in \{1, 2, \ldots, 29\} \setminus \{25\}$*,* $R(T_{25}) = R(T_{26})$*,* $R(T_{30}) = R(T_{31})$ *and* $R(T_{31}) < R(T)$*.*

*Proof.* By data given in the Table 1, and simple calculations one can see that, $R(T_i) < R(T_{i+1})$ for $i \in \{1, 2, \ldots, 29\} \setminus \{25\}$, $R(T_{25}) = R(T_{26})$, $R(T_{30}) = R(T_{31})$ and $R(T_{31}) < R(T)$ for $T \in \cup_{i=32}^{36} A_i$. If $n_1(T) > 12$, then by the repeated application of Lemma 3.3 on the vertices of degree 1, we arrive at a tree $T_l$, in which $R(T_l) < R(T)$ and $n_1(T_l) = 12$. Now, by Lemma 2.1 and simple calculations one can see that, $T$ is a chemical tree of order $n$ with $2 \leq n_1(T) \leq 12$ if and only if $T$ is given in Table 1. Therefore, by Table 1, $R(T_{31}) \leq R(T_l) < R(T)$ and this completes the proof. □

**Theorem 3.6.** *Let* $U_i \in B_i$*, for* $1 \leq i \leq 41$ *and* $U_{42} \in B_{43}$ *(See Table 2). If* $n \geq 24$ *and* $U$ *is a chemical unicyclic graph such that* $U \notin \bigcup_{i=1}^{41} B_i \bigcup B_{43}$*, then for* $i \in \{1, 2, \ldots, 40\} \setminus \{25, 30, 36\}$*,* $R(U_i) < R(U_{i+1})$

$$R(U_{25}) = R(U_{26}), R(U_{30}) = R(U_{31}), R(U_{35}) = R(U_{37}),$$

$$R(U_{36}) = R(U_{38}), R(U_{41}) = R(U_{42}),$$

*and* $R(U_{42}) < R(U)$*.*

*Proof.* By Table 2, we can see that, for $i \in \{1, 2, \ldots, 40\} \setminus \{25, 30, 36\}$, $R(U_i) < R(U_{i+1})$ and

$$R(U_{25}) = R(U_{26}),\ R(U_{30}) = R(U_{31}),\ R(U_{35}) = R(U_{37}),$$
$$R(U_{36}) = R(U_{38}),\ R(U_{41}) = R(U_{42})$$

and $R(U_{42}) < R(U)$ for $U \in \bigcup_{i=43}^{49} B_i$.

If $n_1(U) > 12$, then by the repeated application of Lemma 3.3 on the vertices of degree 1 we arrive at a unicyclic graph $U_l$, in which $R(U_l) < R(U)$ and $n_1(U_l) = 12$. Now, by Lemma 2.1 and simple calculations one can see that, $U$ is a chemical unicyclic graph of order $n$ with $2 \leq n_1(U) \leq 12$ if and only if $U$ is given in Table 2. Therefore, by Table 2, $R(U_{42}) \leq R(U_l) < R(U)$ and this completes the proof. □

Table 1: Degree distributions of the chemical trees with $n_1 \leq 12$.

| E.C. | $n_4$ | $n_3$ | $n_2$ | $n_1$ | $R$ | E.C. | $n_4$ | $n_3$ | $n_2$ | $n_1$ | $R$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $A_1$ | 0 | 0 | $n-2$ | 2 | $\frac{1}{2}n+1$ | $A_{19}$ | 2 | 3 | $n-14$ | 9 | $\frac{1}{2}n+\frac{7}{2}$ |
| $A_2$ | 0 | 1 | $n-4$ | 3 | $\frac{1}{2}n+\frac{4}{3}$ | $A_{20}$ | 3 | 1 | $n-13$ | 9 | $\frac{1}{2}n+\frac{43}{12}$ |
| $A_3$ | 0 | 2 | $n-6$ | 4 | $\frac{1}{2}n+\frac{5}{3}$ | $A_{21}$ | 0 | 8 | $n-18$ | 10 | $\frac{1}{2}n+\frac{11}{3}$ |
| $A_4$ | 1 | 0 | $n-5$ | 4 | $\frac{1}{2}n+\frac{7}{4}$ | $A_{22}$ | 1 | 6 | $n-17$ | 10 | $\frac{1}{2}n+\frac{15}{4}$ |
| $A_5$ | 0 | 3 | $n-8$ | 5 | $\frac{1}{2}n+2$ | $A_{23}$ | 2 | 4 | $n-16$ | 10 | $\frac{1}{2}n+\frac{23}{6}$ |
| $A_6$ | 1 | 1 | $n-7$ | 5 | $\frac{1}{2}n+\frac{25}{12}$ | $A_{24}$ | 3 | 2 | $n-15$ | 10 | $\frac{1}{2}n+\frac{47}{12}$ |
| $A_7$ | 0 | 4 | $n-10$ | 6 | $\frac{1}{2}n+\frac{7}{3}$ | $A_{25}$ | 4 | 0 | $n-14$ | 10 | $\frac{1}{2}n+4$ |
| $A_8$ | 1 | 2 | $n-9$ | 6 | $\frac{1}{2}n+\frac{29}{12}$ | $A_{26}$ | 0 | 9 | $n-20$ | 11 | $\frac{1}{2}n+4$ |
| $A_9$ | 2 | 0 | $n-8$ | 6 | $\frac{1}{2}n+\frac{5}{2}$ | $A_{27}$ | 1 | 7 | $n-19$ | 11 | $\frac{1}{2}n+\frac{49}{12}$ |
| $A_{10}$ | 0 | 5 | $n-12$ | 7 | $\frac{1}{2}n+\frac{8}{3}$ | $A_{28}$ | 2 | 5 | $n-18$ | 11 | $\frac{1}{2}n+\frac{25}{6}$ |
| $A_{11}$ | 1 | 3 | $n-11$ | 7 | $\frac{1}{2}n+\frac{11}{4}$ | $A_{29}$ | 3 | 3 | $n-17$ | 11 | $\frac{1}{2}n+\frac{17}{4}$ |
| $A_{12}$ | 2 | 1 | $n-10$ | 7 | $\frac{1}{2}n+\frac{17}{6}$ | $A_{30}$ | 4 | 1 | $n-16$ | 11 | $\frac{1}{2}n+\frac{13}{3}$ |
| $A_{13}$ | 0 | 6 | $n-14$ | 8 | $\frac{1}{2}n+3$ | $A_{31}$ | 0 | 10 | $n-22$ | 12 | $\frac{1}{2}n+\frac{13}{3}$ |
| $A_{14}$ | 1 | 4 | $n-13$ | 8 | $\frac{1}{2}n+\frac{37}{12}$ | $A_{32}$ | 1 | 8 | $n-21$ | 12 | $\frac{1}{2}n+\frac{53}{12}$ |
| $A_{15}$ | 2 | 2 | $n-12$ | 8 | $\frac{1}{2}n+\frac{19}{6}$ | $A_{33}$ | 2 | 6 | $n-20$ | 12 | $\frac{1}{2}n+\frac{9}{2}$ |
| $A_{16}$ | 3 | 0 | $n-11$ | 8 | $\frac{1}{2}n+\frac{13}{4}$ | $A_{34}$ | 3 | 4 | $n-19$ | 12 | $\frac{1}{2}n+\frac{55}{12}$ |
| $A_{17}$ | 0 | 7 | $n-16$ | 9 | $\frac{1}{2}n+\frac{10}{3}$ | $A_{35}$ | 4 | 2 | $n-18$ | 12 | $\frac{1}{2}n+\frac{14}{3}$ |
| $A_{18}$ | 1 | 5 | $n-15$ | 9 | $\frac{1}{2}n+\frac{41}{12}$ | $A_{36}$ | 5 | 0 | $n-17$ | 12 | $\frac{1}{2}n+\frac{19}{4}$ |

Abbreviation: E.C. = Equivalence Classes.

Table 2: Degree distributions of the connected chemical unicyclic graphs with $0 \leq n_1 \leq 12$.

| E.C. | $n_4$ | $n_3$ | $n_2$ | $n_1$ | $R$ | E.C. | $n_4$ | $n_3$ | $n_2$ | $n_1$ | $R$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $B_1$ | 0 | 0 | $n$ | 0 | $\frac{1}{2}n$ | $B_{26}$ | 0 | 9 | $n-18$ | 9 | $\frac{1}{2}n+3$ |
| $B_2$ | 0 | 1 | $n-2$ | 1 | $\frac{1}{2}n+\frac{1}{3}$ | $B_{27}$ | 1 | 7 | $n-17$ | 9 | $\frac{1}{2}n+\frac{37}{12}$ |
| $B_3$ | 0 | 2 | $n-4$ | 2 | $\frac{1}{2}n+\frac{2}{3}$ | $B_{28}$ | 2 | 5 | $n-16$ | 9 | $\frac{1}{2}n+\frac{19}{6}$ |
| $B_4$ | 1 | 0 | $n-3$ | 2 | $\frac{1}{2}n+\frac{3}{4}$ | $B_{29}$ | 3 | 3 | $n-15$ | 9 | $\frac{1}{2}n+\frac{13}{4}$ |
| $B_5$ | 0 | 3 | $n-6$ | 3 | $\frac{1}{2}n+1$ | $B_{30}$ | 4 | 1 | $n-14$ | 9 | $\frac{1}{2}n+\frac{10}{3}$ |
| $B_6$ | 1 | 1 | $n-5$ | 3 | $\frac{1}{2}n+\frac{13}{12}$ | $B_{31}$ | 0 | 10 | $n-20$ | 10 | $\frac{1}{2}n+\frac{10}{3}$ |
| $B_7$ | 0 | 4 | $n-8$ | 4 | $\frac{1}{2}n+\frac{4}{3}$ | $B_{32}$ | 1 | 8 | $n-19$ | 10 | $\frac{1}{2}n+\frac{41}{12}$ |
| $B_8$ | 1 | 2 | $n-7$ | 4 | $\frac{1}{2}n+\frac{17}{12}$ | $B_{33}$ | 2 | 6 | $n-18$ | 10 | $\frac{1}{2}n+\frac{7}{2}$ |
| $B_9$ | 2 | 0 | $n-6$ | 4 | $\frac{1}{2}n+\frac{3}{2}$ | $B_{34}$ | 3 | 4 | $n-17$ | 10 | $\frac{1}{2}n+\frac{43}{12}$ |
| $B_{10}$ | 0 | 5 | $n-10$ | 5 | $\frac{1}{2}n+\frac{5}{3}$ | $B_{35}$ | 4 | 2 | $n-16$ | 10 | $\frac{1}{2}n+\frac{11}{3}$ |
| $B_{11}$ | 1 | 3 | $n-9$ | 5 | $\frac{1}{2}n+\frac{7}{4}$ | $B_{36}$ | 5 | 0 | $n-15$ | 10 | $\frac{1}{2}n+\frac{15}{4}$ |
| $B_{12}$ | 2 | 1 | $n-8$ | 5 | $\frac{1}{2}n+\frac{11}{6}$ | $B_{37}$ | 0 | 11 | $n-22$ | 11 | $\frac{1}{2}n+\frac{11}{3}$ |
| $B_{13}$ | 0 | 6 | $n-12$ | 6 | $\frac{1}{2}n+2$ | $B_{38}$ | 1 | 9 | $n-21$ | 11 | $\frac{1}{2}n+\frac{15}{4}$ |
| $B_{14}$ | 1 | 4 | $n-11$ | 6 | $\frac{1}{2}n+\frac{25}{12}$ | $B_{39}$ | 2 | 7 | $n-20$ | 11 | $\frac{1}{2}n+\frac{23}{6}$ |
| $B_{15}$ | 2 | 2 | $n-10$ | 6 | $\frac{1}{2}n+\frac{13}{6}$ | $B_{40}$ | 3 | 5 | $n-19$ | 11 | $\frac{1}{2}n+\frac{47}{12}$ |
| $B_{16}$ | 3 | 0 | $n-9$ | 6 | $\frac{1}{2}n+\frac{9}{4}$ | $B_{41}$ | 4 | 3 | $n-18$ | 11 | $\frac{1}{2}n+4$ |
| $B_{17}$ | 0 | 7 | $n-14$ | 7 | $\frac{1}{2}n+\frac{7}{3}$ | $B_{42}$ | 5 | 1 | $n-17$ | 11 | $\frac{1}{2}n+\frac{49}{12}$ |
| $B_{18}$ | 1 | 5 | $n-13$ | 7 | $\frac{1}{2}n+\frac{29}{12}$ | $B_{43}$ | 0 | 12 | $n-24$ | 12 | $\frac{1}{2}n+4$ |
| $B_{19}$ | 2 | 3 | $n-12$ | 7 | $\frac{1}{2}n+\frac{5}{2}$ | $B_{44}$ | 1 | 10 | $n-23$ | 12 | $\frac{1}{2}n+\frac{49}{12}$ |
| $B_{20}$ | 3 | 1 | $n-11$ | 7 | $\frac{1}{2}n+\frac{31}{12}$ | $B_{45}$ | 2 | 8 | $n-22$ | 12 | $\frac{1}{2}n+\frac{25}{6}$ |
| $B_{21}$ | 0 | 8 | $n-16$ | 8 | $\frac{1}{2}n+\frac{8}{3}$ | $B_{46}$ | 3 | 6 | $n-21$ | 12 | $\frac{1}{2}n+\frac{17}{4}$ |
| $B_{22}$ | 1 | 6 | $n-15$ | 8 | $\frac{1}{2}n+\frac{11}{4}$ | $B_{47}$ | 4 | 4 | $n-20$ | 12 | $\frac{1}{2}n+\frac{13}{3}$ |
| $B_{23}$ | 2 | 4 | $n-14$ | 8 | $\frac{1}{2}n+\frac{17}{6}$ | $B_{48}$ | 6 | 0 | $n-18$ | 12 | $\frac{1}{2}n+\frac{9}{2}$ |
| $B_{24}$ | 3 | 2 | $n-13$ | 8 | $\frac{1}{2}n+\frac{35}{12}$ | $B_{49}$ | 5 | 2 | $n-19$ | 12 | $\frac{1}{2}n+\frac{53}{12}$ |
| $B_{25}$ | 4 | 0 | $n-12$ | 8 | $\frac{1}{2}n+3$ | | | | | | |

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