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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 $\operatorname{diam}(G) = \max\{d_G(u, v) \mid u, v \in V(G)\}$.

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 $r=(r_1,r_2,\ldots,r_n)$ and $s=(s_1,s_2,\ldots,s_n)$ 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 $r \leq s$. Moreover, r < s means that $r \leq s$ and $r \neq s$, see [10] for details. The non-increasing sequence $d=(d_1,d_2,\ldots,d_n)$ of nonnegative integers is called a graphic sequence if we can find a simple graph G with the vertex set $V(G) = \{v_1,v_2,\ldots,v_n\}$ 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 γ , 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 $\gamma(G) = m \operatorname{diam}(G) n_1 + 2$.
- (2) If $G \not\cong P_n$, then $\gamma(G) < m \operatorname{diam}(G) n_1 + 1$.

Proof. It is clear that $\gamma(P_n) = m - \text{diam}(G) - n_1 + 2$. Let G be a graph such that $G \ncong P_n$. Suppose $u, v \in V(G), d_G(u, v) = \text{diam}(G)$ and $uw_1w_2 \dots w_{\text{diam}(G)-1}v$ is a shortest u - v path in G. Let $A = \{uw_1, w_1w_2, \dots, w_{\text{diam}(G)-2}w_{\text{diam}(G)-1}, w_{\text{diam}(G)-1}v\}$

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

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

Proof. By Proposition 2.2, we have $\operatorname{diam}(G) \leq n - n_1 + 1$ 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, $\operatorname{diam}(G) \leq 2n - \gamma(G) - \frac{5}{2}n_1 + 1$.

Theorem 2.4. Let G be a connected chemical graph with n vertices, m edges and cyclomatic number γ .

- (1) If $G \cong P_n$, then diam $(G) = 2R(G) n_1 1$.
- (2) If $G \ncong P_n$, then diam $(G) \le 4R(G) n_1$.

Proof. It is easy to see that $diam(P_n) = 2R(G) - n_1 - 1$. For $G \not\cong P_n$, by definition of R(G) and Lemma 2.1,

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

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

$$R(G) \ge n_1 - \frac{3}{2}n_2 - \frac{5}{3}n_3 - \frac{7}{4}n_4 + 2\operatorname{diam}(G)$$

$$= 2n_1 - \left(n_1 + \frac{3}{2}n_2 + \frac{5}{3}n_3 + \frac{7}{4}n_4\right) + 2\operatorname{diam}(G)$$

$$\ge 2n_1 - 7\left(n_1 + \frac{1}{2}n_2 + \frac{1}{3}n_3 + \frac{1}{4}n_4\right) + 2\operatorname{diam}(G).$$

Thus 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 $n_4 = 0$, diam $(G) \le 3R(G) - n_1$. Proof. By definition,

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

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), $R(G) \ge 2n_1 - (n_1 + \frac{3}{2}n_2 + \frac{5}{3}n_3) + 2\operatorname{diam}(G)$. Therefore, $\operatorname{diam}(G) \le 3R(G) - n_1$.

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 $n_4(G) \ge 1$, then $R(G) \ge \frac{1}{2}n - \frac{1}{4}$, 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 $n_3(G) \ge 3$, then $R(G) \ge \frac{1}{2}n$, proving the corollary.

For $n \geq 5$ we set

$$\Lambda_1 = \{G \mid G \text{ is a tricyclic graph, } n_3(G) = 4 \text{ and } n_2(G) = n - 4\},$$

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

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 $n_4(G) \ge 2$, $R(G) \ge \frac{1}{2}n + \frac{1}{2}$. If $n_4(G) = 1$ and $n_3(G) \le 1$, or $n_4(G) = 0$ and $n_3(G) \le 3$, 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 $n_3(G) \ge 5$, then $R(G) \ge \frac{1}{2}n + \frac{2}{3}$. If $n_4(G) = 1$ and $n_3(G) \ge 3$, then $R(G) \ge \frac{1}{2}n + \frac{3}{4}$, 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 φ defined on a set $\Lambda \subset \mathbb{R}^n$ is said to be Schurconvex on Λ if for all $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n) \in \Lambda$, if $x \leq y$, then $\varphi(x) \leq \varphi(y)$. In addition, φ is said to be strictly Schur-convex on Λ 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 φ 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 $d(G) \leq d(G')$, then $R(G) \leq R(G')$, with equality if and only if d(G) = d(G').

Proof. Let $\alpha:(0,\infty) \to \mathbb{R}$ 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, α 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 γ ($1 \le \gamma \le n-2$), a graph G^1_{γ} with the degree sequence

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

has the maximal inverse degree and a graph G^2_{γ} with the degree sequence

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

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 γ $(1 \le \gamma \le n-2)$ which is different from G^1_{γ} and G^2_{γ} . 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 $1 \le i \le 31$ (See Table 1). If $n \ge 22$ and T is a tree such that $T \notin \bigcup_{i=1}^{31} A_i$, then $R(T_i) < R(T_{i+1})$ for $i \in \{1, 2, ..., 29\} \setminus \{25\}$, $R(T_{25}) = R(T_{26})$, $R(T_{30}) = R(T_{31})$ 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 $i ∈ \{1, 2, ..., 29\} \setminus \{25\}$, $R(T_{25}) = R(T_{26})$, $R(T_{30}) = R(T_{31})$ and $R(T_{31}) < R(T)$ for $T ∈ \bigcup_{i=32}^{36} A_i$. 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 $1 \le n_1(T) \le n_1(T) \le n_1(T)$ and only if $1 \le n_1(T) \le n_1(T)$ is given in Table 1. Therefore, by Table 1, $1 \le n_1(T_l) \le n_1(T_l) < n_1(T_l)$ and this completes the proof. $1 \le n_1(T_l) < n_1(T_l)$

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

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

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

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

Proof. By Table 2, we can see that, for $i \in \{1, 2, ..., 40\} \setminus \{25, 30, 36\}$, $R(U_i) < R(U_{i+1})$ 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 $1 \le n_1(U) \le 12$ if and only if U is given in Table 2. Therefore, by Table 2, $R(U_{42}) \le R(U_l) < R(U)$ and this completes the proof. \square

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 $0 \le n_1 \le 12$.

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	$\frac{1}{2}n + \frac{17}{4}$
					$\frac{1}{2}n + \frac{11}{4}$						
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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References

- [1] X. Chen and S. Fujita, On diameter and inverse degree of chemical graphs, Appl. Anal. Discrete Math., 7(2013), 83–93.
- [2] K. C. Das, K. Xu and J. Wang, On inverse degree and topological indices of graphs, Filomat, 30(8)(2016), 2111–2120.
- [3] D. Dimitrov and A. Ali, On the extremal graphs with respect to variable sum exdeg index, Discrete Math. Lett., 1(2019), 42–48.
- [4] R. Entringer, Bounds for the average distance-inverse degree product in trees, Combinatorics, Graph Theory, and Algorithms I, II, 335–352, New Issues Press, Kalamazoo, MI, 1999.
- [5] P. Erdös, J. Pach and J. Spencer, On the mean distance between points of a graph, Congr. Numer., 64(1988), 121–124.
- [6] S. Fajtlowicz, On conjectures of graffiti II, Congr. Numer., 60(1987), 189–197.
- [7] A. Ghalavand and A. R. Ashrafi, Extremal graphs with respect to variable sum exdeg index via majorization, Appl. Math. Comput., 303(2017), 19–23.
- [8] A. Ghalavand, A. R. Ashrafi and I. Gutman, Extremal graphs for the second multiplicative Zagreb index, Bull. Int. Math. Virtual Inst., 8(2)(2018), 369–383.
- [9] L. B. Kier and L. H. Hall, The nature of structure-activity relationships and their relation to molecular connectivity, European J. Med. Chem., 12(1977), 307–312.
- [10] A. W. Marshall and I. Olkin, *Inequalities: Theory of majorization and its applications*, Mathematics in Science and Engineering **143**, Academic Press, Inc. New York-London, 1979.
- [11] K. Xu, Kexiang, and K. Ch. Das, Some extremal graphs with respect to inverse degree, Discrete Appl. Math., 203(2016), 171–183.
- [12] Z. Zhang, J. Zhang and X. Lu, The relation of matching with inverse degree of a graph, Discrete Math., **301**(2005), 243–246.