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NEW BOUNDS ON RECENT TOPOLOGICAL INDICES OF GRAPHS

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ABSTRACT. The Geometric-Harmonic index $GH(\zeta)$ of a simple graph ζ is defined as the sum of the terms $\frac{(d_\zeta(f)+d_\zeta(g))\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}$ over all edges fg of ζ and the modified first Kulli-Basava index KB_1^* of a simple graph ζ is defined as the sum of the terms $S_e(f)^2$ over all vertices f of ζ. Using several molecular structural parameters, we establish some new bounds on the Geometric-harmonic index and the modified first Kulli-Basava index in this study and connect these indices to a number of well-known molecular descriptors.

Keywords: The Geometric-Harmonic index, the modified first Kulli-Basava index, maximum vertex degree, minimum vertex degree.

AMS Subject Classification : 05C09, 05C12, 05C35, 05C90.

1. Introduction

Under the graph isomorphism condition, topological indices are graph invariants. Chemical graph theory uses these indices in a few different applications. For instance, see [3, 5, 6, 7, 9]. The bounds of a topological index are crucial data for a molecular graph because they define the topological indices approximative range in terms of molecular structural characteristics. Recent reports on the research of bounds can be found in [15, 17, 8]. In this study, we only take into account simple, undirected, finite graphs. Let $\zeta = (V, E)$ be a simple graph of order n size m, with vertex set $V(\zeta)$ and edge set $E(\zeta)$. The Δ and δ stand for the maximum and minimum degrees of ζ, respectively. The δ_1 represents the minimum non-pendent vertex degree of the graph ζ. Additionally, p stands for the number of pendent vertices in ζ. The degree $d_\zeta(f)$ of a vertex f is the number of vertices adjacent to $f \in V(\zeta)$. The degree of an edge $e = fg$ in ζ in defined by $d_\zeta(e) = d_\zeta(f) + d_\zeta(g) - 2$. Let $S_e(f)$ denote the sum of the degrees of all edges incident to $f \in V(\zeta)$ [2]. We provide a list of additional degree-based topological indices that are utilised throughout the sections.

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The below is a definition of the first Zagreb index [10].

$$M_1(\zeta) = \sum_{f\in V(\zeta)} d_\zeta(f)^2 = \sum_{fg\in E(\zeta)} (d_\zeta(f) + d_\zeta(g)).$$

The below is a definition of the second Zagreb index [11].

$$M_2(\zeta) = \sum_{fg\in E(\zeta)} (d_\zeta(f) \cdot d_\zeta(g)).$$

The below is a definition of the Airthmetic-Geometric index [19].

$$AG(\zeta) = \sum_{fg\in E(\zeta)} \frac{d_\zeta(f) + d_\zeta(g)}{2\sqrt{d_\zeta(f) \cdot d_\zeta(g)}}.$$

The below is a definition of the Randić connectivity index [16].

$$R(\zeta) = \sum_{fg\in E(\zeta)} \frac{1}{\sqrt{d_\zeta(f) \cdot d_\zeta(g)}}.$$

The below is a definition of the general Randić index (or product-connectivity index) [1].

$$R_\alpha(\zeta) = \sum_{fg\in E(\zeta)} (d_\zeta(f) \cdot d_\zeta(g))^\alpha.$$

Where α is a real number, $R_{-\frac{1}{2}}$ is the classical Randić connectivity index.
The below is a definition of the Hyper-Zagreb index [18] as

$$HM(\zeta) = \sum_{fg\in E(\zeta)} (d_\zeta(f) + d_\zeta(g))^2.$$

The below is a definition of the Geometric-Harmonic index [20].

$$GH(\zeta) = \sum_{fg\in E(\zeta)} \frac{(d_\zeta(f) + d_\zeta(g))\sqrt{d_\zeta(f) \cdot d_\zeta(g)}}{2}.$$

The below is a definition of the modified first Kulli-Basava index [2].

$$KB_1^*(\zeta) = \sum_{f\in V(\zeta)} S_e(f)^2.$$

2. Bounds on Geometric-Harmonic index of connected graphs

In this section, we establish some fresh bounds for the Geometric-Harmonic index of a connected graph G in terms of certain values of some graph parameters and other topological indices.

Lemma 2.1. [14] *Suppose r_i and s_i, $1 \le i \le n$ are positive real numbers, then*

$$\left| n\sum_{i=1}^{n} r_i s_i - \sum_{i=1}^{n} r_i \sum_{i=1}^{n} s_i \right| \le \alpha(n)(R-r)(S-s).$$

Where r, s, R and S are real constants, such that for each i, $1 \le i \le n, r \le r_i \le R$ and $s \le s_i \le S$. Further, $\alpha(n) = n\lceil \frac{n}{2} \rceil \left(1 - \frac{1}{n}\lceil \frac{n}{2} \rceil\right)$.

Theorem 2.2. *If ζ is a graph with n vertices and m edges, then*

$$GH(\zeta) \leq \frac{\alpha(m)(\Delta-\delta)^2}{m} + \frac{M_1(\zeta)R_{\frac{1}{2}}(\zeta)}{2m}.$$

Where $\alpha(m) = m\lceil \frac{m}{2} \rceil \left(1 - \frac{1}{m}\lceil \frac{m}{2} \rceil\right)$ with equality if and only if ζ is regular.

Proof. We choose $r_i = \frac{(d_\zeta(f)+d_\zeta(g))}{2}$, $s_i = \sqrt{d_\zeta(f) \cdot d_\zeta(g)}$, $r = \delta$, $R = \Delta$, $s = \delta$ and $S = \Delta$ in Lemma 2.1, we obtain

$$\left| m \sum_{fg\in E(\zeta)} \frac{(d_\zeta(f)+d_\zeta(g))\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2} - \sum_{fg\in E(\zeta)} \frac{(d_\zeta(f)+d_\zeta(g))}{2} \sum_{fg\in E(\zeta)} \sqrt{d_\zeta(f)\cdot d_\zeta(g)} \right| \leq \alpha(m)\left(\Delta-\delta\right)\left(\Delta-\delta\right)$$

$$\left| m \sum_{fg\in E(\zeta)} \frac{(d_\zeta(f)+d_\zeta(g))\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2} - \sum_{fg\in E(\zeta)} \frac{(d_\zeta(f)+d_\zeta(g))}{2} \sum_{fg\in E(\zeta)} \sqrt{d_\zeta(f)\cdot d_\zeta(g)} \right| \leq \alpha(m)\left(\Delta-\delta\right)^2$$

From the definition of the Geometric-Harmonic index $GH(\zeta)$, the general Randić index $R_\alpha(\zeta)$ and the first Zagreb index $M_1(\zeta)$, we have

$$mGH(\zeta) - \frac{M_1(\zeta)R_{\frac{1}{2}}(\zeta)}{2} \leq \alpha(m)(\Delta-\delta)^2$$

$$mGH(\zeta) \leq \alpha(m)(\Delta-\delta)^2 + \frac{M_1(\zeta)R_{\frac{1}{2}}(\zeta)}{2}$$

$$GH(\zeta) \leq \frac{\alpha(m)(\Delta-\delta)^2}{m} + \frac{M_1(\zeta)R_{\frac{1}{2}}(\zeta)}{2m}.$$

The equality hold if and only if $\delta = \Delta$. Thus ζ is regular. □

Lemma 2.3. *(Pólya-Szego Inequality [13]). Let $0 < m_1 \leq r_i \leq M_1$ and $0 < m_2 \leq s_i \leq M_2$ for $1 \leq i \leq n$, then*

$$\sum_{i=1}^n r_i^2 \sum_{i=1}^n s_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^n r_is_i\right)^2.$$

Lemma 2.4. *(Cauchy-Schwarz Inequality [13]). Let $R = \{r_1, r_2, \cdots, r_n\}$ and $S = \{s_1, s_2, \cdots, s_n\}$ be two sequences of real numbers. then*

$$\left(\sum_{i=1}^n r_is_i\right)^2 \leq \sum_{i=1}^n r_i^2 \sum_{i=1}^n s_i^2.$$

With equality if and only if the sequences R and S are proportional, i.e., there exists a constant c such that $r_i = cs_i$, for each $1 \leq i \leq n$.

Corollary 2.5. [15] *Let $r_1, r_2, \cdots, r_n$ be a real numbers. Then $\left(\sum_{i=1}^n r_i\right)^2 \leq n\sum_{i=1}^n r_i^2$, with equality if and only $r_1 = r_2 = \cdots = r_n$.*

Theorem 2.6. *If ζ is a graph with n vertices, m edges, and p, Δ, δ_1 stands for the number of pendent vertices, the maximum vertex degree, and the minimum non-pendent vertex degree, respectively, then*

$$GH(\zeta) \geq \frac{2\delta_1^3\Delta(m-p)}{\delta_1^2+\Delta^2} + \frac{p(\delta_1+1)\sqrt{\delta_1}}{2}.$$

Proof. For $2 \leq \delta_1 \leq d_\zeta(f) \leq \Delta$, we have $\delta_1^2 \leq \frac{d_\zeta(f)+d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2} \leq \Delta^2$ for any edge fg in ζ. Setting $m_1 = \delta_1^2, r_i = \left(\frac{(d_\zeta(f)+d_\zeta(g))\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2, 1 \leq i \leq m, M_1 = \Delta^2$ and $m_2 = s_i = M_2 = 1$, $1 \leq i \leq m$ in Pólya-Szego Inequality (Lemma 2.3), we obtain

$$\sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\left(\frac{(d_\zeta(f)+d_\zeta(g))\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2\sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}(1)^2$$

$$\leq \frac{1}{4}\left(\sqrt{\frac{\Delta^2}{\delta_1^2}}+\sqrt{\frac{\delta_1^2}{\Delta^2}}\right)^2\left(\sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\frac{d_\zeta(f)+d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2.$$

$$4(m-p)^2\left(\frac{\delta_1^2\Delta^2}{\delta_1^4+\Delta^4+2\delta_1^2\Delta^2}\right)\sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\left(\frac{(d_\zeta(f)+d_\zeta(g))^2 d_\zeta(f)\cdot d_\zeta(g)}{4}\right)$$

$$\leq \left(\sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\frac{d_\zeta(f)+d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2$$

Thus,

$$4(m-p)^2\left(\frac{\delta_1^2\Delta^2}{\delta_1^4+\Delta^4+2\delta_1^2\Delta^2}\right)(\delta_1^4) \leq \left(\sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\frac{d_\zeta(f)+d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2.$$

$$\left(\sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\frac{d_\zeta(f)+d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2 \geq 4(m-p)^2\left(\frac{\delta_1^6\Delta^2}{\delta_1^4+\Delta^4+2\delta_1^2\Delta^2}\right). \quad (1)$$

It is easy to see that as (1).

$$\begin{aligned} GH(\zeta) &= \sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\frac{d_\zeta(f)+d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2} \\ &\quad + \sum_{fg\in E(\zeta),d_\zeta(g)=1}\frac{d_\zeta(f)+1\sqrt{d_\zeta(f)}}{2} \\ &\geq \sum_{fg\in E(\zeta),d_\zeta(f)d_\zeta(g)\neq 1}\frac{d_\zeta(f)+d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}+\frac{p(\delta_1+1)\sqrt{\delta_1}}{2} \quad (2)\end{aligned}$$

From the inequalities (1) and (2), we have

$$GH(\zeta) \geq \frac{2\delta_1^3\Delta(m-p)}{\delta_1^2+\Delta^2}+\frac{p(\delta_1+1)\sqrt{\delta_1}}{2}.$$

With equality if and only if ζ is regular. □

Theorem 2.7. *If ζ is a graph with n vertices and m edges, then*

$$\frac{\delta\Delta M_1(\zeta)R_{\frac{1}{2}}(\zeta)}{m(\Delta^2+\delta^2)} \leq GH(\zeta).$$

With equality if and only if ζ is regular.

Proof. One can observe that $2\delta \leq d_\zeta(f) + d_\zeta(g) \leq \Delta$ for any edge fg in ζ and setting $m_1 = 2\delta$, $r_i = d_\zeta(f) + d_\zeta(g)$, $1 \leq i \leq m$, $M_1 = 2\Delta$ and $m_2 = \frac{\delta}{2}$, $r_i = \frac{\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}$, $1 \leq i \leq m$, $M_2 = \frac{\Delta}{2}$ in Pólya-Szego Inequality (Lemma 2.3), we obtain

$$\sum_{fg\in E(\zeta)} (d_\zeta(f) + d_\zeta(g))^2 \sum_{fg\in E(\zeta)} \left(\frac{\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2 \leq \frac{1}{4}\left(\sqrt{\frac{\Delta^2}{\delta^2}} + \sqrt{\frac{\delta^2}{\Delta^2}}\right)^2 \cdot \left(\frac{(d_\zeta(f) + d_\zeta(g))\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2$$

By using Cauchy inequality, we have

$$\sum_{fg\in E(\zeta)} (d_\zeta(f) + d_\zeta(g))^2 \sum_{fg\in E(\zeta)} \left(\frac{\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2 \geq \frac{1}{m^2}\left(\sum_{fg\in E(\zeta)} (d_\zeta(f) + d_\zeta(g))\right)^2 \cdot \left(\sum_{fg\in E(\zeta)} \frac{\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2$$

Combining the above two inequalities, we obtain

$$\frac{1}{m^2}\left(\sum_{fg\in E(\zeta)} (d_\zeta(f) + d_\zeta(g))\right)^2 \left(\sum_{fg\in E(\zeta)} \frac{\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2 \leq \frac{1}{4}\left(\sqrt{\frac{\Delta^2}{\delta^2}} + \sqrt{\frac{\delta^2}{\Delta^2}}\right)^2 \cdot \left(\frac{(d_\zeta(f) + d_\zeta(g))\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2$$

Thus,

$$\frac{(M_1(\zeta))^2(R_{\frac{1}{2}}(\zeta))^2}{4m^2} \leq \frac{(\Delta^2 + \delta^2)^2}{4\Delta^2\delta^2}(GH(\zeta))^2.$$
$$\frac{4\Delta^2\delta^2}{(\Delta^2 + \delta^2)^2}\left(\frac{(M_1(\zeta))^2(R_{\frac{1}{2}}(\zeta))^2}{4m^2}\right) \leq (GH(\zeta))^2.$$

Therefore,

$$\frac{\delta\Delta M_1(\zeta)R_{\frac{1}{2}}(\zeta)}{m(\Delta^2 + \delta^2)} \leq GH(\zeta).$$

The equality holds if and only if $d_\zeta(f) = d_\zeta(g) = \delta = \Delta$ for each $fg \in E(\zeta)$ which implies that ζ is regular. □

Definition 1. [13] *Let $t_1, t_2, \cdots, t_n$ be positive real numbers.*

i. *The arithmetic mean of $t_1, t_2, \cdots, t_n$ is equal to*

$$AM(t_1, t_2, \cdots, t_n) = \frac{t_1 + t_2 + \cdots + t_n}{n}.$$

ii. *The geometric mean of $t_1, t_2, \cdots, t_n$ is equal to*

$$GM(t_1, t_2, \cdots, r_n) = \sqrt[n]{t_1, t_2, \cdots, t_n}.$$

iii. *The harmonic mean of $t_1, t_2, \cdots, t_n$ is equal to*

$$HM(t_1, t_2, \cdots, t_n) = \frac{n}{\frac{1}{t_1} + \frac{1}{t_2} + \cdots + \frac{1}{t_n}}.$$

Lemma 2.8. *(AM-GM Inequality* [13]*). Let $t_1, t_2, \cdots, t_n$ be positive real numbers. Then, $AM(t_1, t_2, \cdots, t_n) \geq GM(t_1, t_2, \cdots, t_n)$, with equality if and only if $t_1 = t_2 = \cdots = t_n$.*

Lemma 2.9. *(AM-HM Inequality [13]). Let $t_1, t_2, \cdots, t_n$ be positive real numbers. Then, $AM(t_1, t_2, \cdots, t_n) \geq HM(t_1, t_2, \cdots, t_n)$, with equality if and only if $t_1 = t_2 = \cdots = t_n$.*

Lemma 2.10. *(AM-GM-HM Inequality [13]). Let $t_1, t_2, \cdots, t_n$ be positive real numbers. Then, $AM(t_1, t_2, \cdots, t_n) \geq GM(t_1, t_2, \cdots, t_n) \geq HM(t_1, t_2, \cdots, t_n)$, with equality if and only if $t_1 = t_2 = \cdots = t_n$.*

Theorem 2.11. *For any graph ζ with m edges, then*

$$M_2(\zeta) \leq GH(\zeta).$$

With equality if and only if ζ is regular.

Proof. By the definition of first Zagreb index,

$$\frac{M_1(\zeta)}{2} = \sum_{fg\in E(\zeta)} \frac{d_\zeta(f) + d_\zeta(g)}{2}$$

By Lemma 2.10 (AM-GM-HM Inequality), we get

$$\frac{M_1(\zeta)}{2} = \sum_{fg\in E(\zeta)} \frac{d_\zeta(f) + d_\zeta(g)}{2} \geq \sum_{fg\in E(\zeta)} \sqrt{d_\zeta(f) \cdot d_\zeta(g)} \geq \sum_{fg\in E(\zeta)} \frac{2}{\frac{1}{d_\zeta(f)} + \frac{1}{d_\zeta(g)}}.$$

By taking last two expressions, we obtain

$$\begin{aligned}
\sum_{fg\in E(\zeta)} \sqrt{d_\zeta(f) \cdot d_\zeta(g)} &\geq \sum_{fg\in E(\zeta)} \frac{2}{\frac{1}{d_\zeta(f)} + \frac{1}{d_\zeta(g)}} \\
\sum_{fg\in E(\zeta)} \sqrt{d_\zeta(f) \cdot d_\zeta(g)} &\geq \sum_{fg\in E(\zeta)} \frac{2d_\zeta(f)d_\zeta(g)}{d_\zeta(f) + d_\zeta(g)} \\
\sum_{fg\in E(\zeta)} \frac{d_\zeta(f) + d_\zeta(g)\sqrt{d_\zeta(f) \cdot d_\zeta(g)}}{2} &\geq \sum_{fg\in E(\zeta)} d_\zeta(f) \cdot d_\zeta(g) \\
\sum_{fg\in E(\zeta)} d_\zeta(f) \cdot d_\zeta(g) &\leq \sum_{fg\in E(\zeta)} \frac{d_\zeta(f) + d_\zeta(g)\sqrt{d_\zeta(f) \cdot d_\zeta(g)}}{2}
\end{aligned}$$

Therefore,

$$M_2(\zeta) \leq GH(\zeta).$$

With equality if and only if ζ is regular. □

Theorem 2.12. *Let $\zeta = (V, E)$ be a graph with $|V| = n$ and $|E| = m$, then*

$$GH(\zeta) \leq \frac{\sqrt{HM(\zeta) \cdot M_2(\zeta)}}{2}.$$

Further, equality holds if and only if ζ is regular graph.

Proof. By setting $r_i = d_\zeta(f) + d_\zeta(g)$, $s_i = \frac{\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}$ in Lemma 2.4, we get

$$\begin{aligned}
\left(\sum_{fg\in E(\zeta)} \frac{d_\zeta(f) + d_\zeta(g)\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2 &\leq \sum_{fg\in E(\zeta)} (d_\zeta(f) + d_\zeta(g))^2 \\
&\quad \cdot \sum_{fg\in E(\zeta)} \left(\frac{\sqrt{d_\zeta(f)\cdot d_\zeta(g)}}{2}\right)^2 \\
(GH(\zeta))^2 &\leq \frac{HM(\zeta)\cdot M_2(\zeta)}{4} \\
GH(\zeta) &\leq \frac{\sqrt{HM(\zeta)\cdot M_2(\zeta)}}{2}.
\end{aligned}$$

The equality holds in the above inequality if and only if ζ is regular graph. □

3. Bound on modified first Kulli-Basava index of connected graphs

In this section we obtain bound on the modified first Kulli-Basava index of graphs.

Lemma 3.1. [4] *Let ζ be a graph of order n and size m. Then*

$$M_1(\zeta) \geq 2m(2p+1) - pn(1+p) \text{ where } p = \left\lfloor \frac{2m}{n} \right\rfloor.$$

and the equality holds if and only if the difference of the degrees of any two vertices of graph ζ is at most one.

Lemma 3.2. [2] *If ζ is a (n, m) graph, then*
(i) $\sum_{f\in V(\zeta)} S_e(f) = 2(M_1(\zeta) - 2m)$.
(ii) $\sum_{f\in V(\zeta)} S_e(f) \leq 2\Delta(\zeta)(2m - n)$, *equality holds if and only if ζ is regular.*

Theorem 3.3. *Let ζ be the graph with n vertices and m edges. Then*

$$KB_1^*(\zeta) \geq \frac{4(M_1(\zeta) - 2m)^2}{n}$$

Equality holds if and only if ζ is a regular graph with $n \geq 2$.

Proof. By setting $r_i = 1$, $s_i = S_e(f)$ in Corollory 2.5, we get

$$\begin{aligned}
\left(\sum_{f\in V(\zeta)} S_e(f)\right)^2 &\leq n \cdot \sum_{f\in V(\zeta)} S_e(f)^2 \\
\left(\sum_{f\in V(\zeta)} S_e(f)\right)^2 &\leq n \cdot KB_1^*(\zeta) \\
\left(\sum_{f\in V(\zeta)} S_e(f)\right) &\leq \sqrt{n \cdot KB_1^*(\zeta)} \qquad (3)
\end{aligned}$$

By Lemma 3.2 and Eq. (3), we get

$$\begin{aligned}
\sum_{f\in V(\zeta)} S_e(f) = 2(M_1(\zeta) - 2m) &\leq \sqrt{nKB_1^*(\zeta)} \\
KB_1^*(\zeta) &\geq \frac{4(M_1(\zeta) - 2m)^2}{n}.
\end{aligned}$$

□

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