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Research Article

On Harary-Sombor index of graphs

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Abstract: Let G be an arbitrary simple connected graph. In this paper, we introduce Harary-Sombor index of G and denote it by $HSO(G)$. Then we calculate its values for several familiar classes of graphs. Also, we state an upper bound for the Harary-Sombor index of bipartite graphs. Moreover, we determine the extremum values of the Harary-Sombor index of trees.

Keywords: bipartite graph, Harary-Sombor index, path, star, tree.

AMS Subject classification: 92E10, 05C05, 05C12

1. Introduction

Let $G = (V(G), E(G))$ be a simple connected graph where $V(G)$ is the set of vertices and $E(G)$ is the set of edges of G. The *order* (*size*) of G refers to the number of vertices (edges) in the graph. Throughout this paper, d_v denotes the degree of vertex v in G and $d(u, v)$ represents the distance between vertices u and v in G. The maximum degree of G is denoted by Δ.
In mathematical chemistry, the topological index of a structural graph of a molecule (i.e. molecular structure descriptor) is a real number related to a structural graph of a molecule. Topological indices are used to investigate the correlation between chemical structure and various physical properties, biological activities or chemical reactivity. Also, topological indices do not depend on the labeling of the vertices and hence isomorphic graphs have the same topological indices. Until now, many different distance-based and degree-based topological indices have been investigated

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and employed in quantitative structure activity (property) relationship studies, with various rate of success.
The most well-known of these indices is the distance-based Wiener index, which is introduced in 1947 by Harry Wiener [15, 16] in an effort to analyze the boiling points of a group of alkanes called paraffin. The *Wiener index* of a graph G is defined as follows and is denoted by $W(G)$,

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u,v).$$

Another well-known distance-based index is the *Harary index*, which is defined as follows:

$$H(G) = \frac{1}{2} \sum_{\substack{u,v \in V(G) \\ u \neq v}} \frac{1}{d(u,v)},$$

for more details, you can refer to [3, 10, 12, 17].
Among degree-based topological indices, the *first* and the *second Zagreb indices* are well-known. They are introduced in 1972 by Gutman and Trinajstić [9] to approximate the π-electron energy, as shown in the following formulas:

$$M_1(G) = \sum_{v \in V(G)} d_v^2 = \sum_{uv \in E(G)} d_v + d_u \quad , \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

Next, in 2021 Gutman [7] defined the Sombor index of a graph G as follows:

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}.$$

Nowadays, studying on Sombor index of graphs attracted the attention of many researchers (see [4–6, 8, 13, 14]).
In [1] Alizadeh et al. introduced another new index that is called the *additively weighted Harary index*, by using the first Zagreb index and the Harary index as follows:

$$H_A(G) = \frac{1}{2} \sum_{u \neq v} \frac{d_u + d_v}{d(u,v)}.$$

They also calculated the values of this index for famous graphs and subsequently derived bounds for it. Additionally, they computed the exact value of this index for some graph composition operations.
In [2], An and Xiong introduced another index called the *multiplicatively weighted Harary index* by replacing the additive weighting of vertices with multiplicative

weighting. They also calculated its values for some graphs, including their compositions.

$$H_M(G) = \frac{1}{2}\sum_{u\neq v}\frac{d_u.d_v}{d(u,v)}.$$

Lin in [11] introduced the Harary-Albertson index and analyzed its application in quantitative structure property relationship. He also, derived relationships between this index and other topological indices and calculated its value for trees of a given order.

In this paper, we introduce Harary-Sombor index and calculate its values for some well-known graphs. Also, we state an upper bound for the Harary-Sombor index of bipartite graphs. Furthermore, we determine the extremum values of the Harary-Sombor index of trees.

2. Basic properties of the Harary-Sombor index

In this paper we introduce the new topological index of connected graphs that defined as

$$HSO(G) = \frac{1}{2}\sum_{\substack{u,v\in V(G)\\ u\neq v}}\frac{\sqrt{d_u^2+d_v^2}}{d(u,v)}$$

and called *Harary-Sombor index.* Clearly, $HSO(G) \geq SO(G)$ and equality holds if and only if $G = K_n$. Also, for a graph G of order n and size m, we have $HSO(G) \leq SO(G) + \frac{\sqrt{2}}{2}\Delta\left(\binom{n}{2} - m\right)$ and equality holds if and only if $G \cong K_n$. So, we have the following lemma.

Lemma 1. *For a graph G of order n and size m,*

$$SO(G) \leq HSO(G) \leq SO(G) + \frac{\Delta(n^2-n-2m)}{2\sqrt{2}}$$

and each equality holds if and only if $G \cong K_n$. In this case,

$$HSO(K_n) = SO(K_n) = \frac{n(n-1)^2}{\sqrt{2}}.$$

In the following, we calculate the values of the Harary-Sombor index of some familiar classes of graphs.

Lemma 2. *Let S_n, C_n and P_n be the star, the cycle and the path graph of order n, respectively. We have the following statements:*
(i) $HSO(S_n) = (n-1)\sqrt{n^2-2n+2} + \frac{\sqrt{2}}{4}(n-1)(n-2)$;

(ii) $HSO(C_n) = \begin{cases} 2\sqrt{2}nH_{\frac{n-1}{2}} & n \text{ is odd} \\ 2\sqrt{2}(nH_{\frac{n}{2}} - 1) & n \text{ is even} \end{cases}$;

(iii) $HSO(P_n) = 2\sqrt{5}H_{n-2} + \sqrt{8}(n-2)H_{n-3} - \sqrt{8}(n-3) + \frac{\sqrt{2}}{n-1}$;

where the n-th harmonic number H_n is defined as the n-th partial sum of the harmonic series, $\sum_{k=1}^{n} \frac{1}{k}$.

Proof. (i) Let $V(S_n) = \{u, v_1, \ldots, v_{n-1}\}$ and $d_u = n-1$. Since $d(u, v_i) = 1$ and $d(v_i, v_j) = 2$ we have:

$$\begin{aligned} HSO(S_n) &= (n-1)\sqrt{1+(n-1)^2} + \frac{\sqrt{2}}{2}\binom{n-1}{2} \\ &= (n-1)\sqrt{n^2-2n+2} + \frac{\sqrt{2}}{4}(n-1)(n-2). \end{aligned}$$

(ii) For the cycle C_n, distance of any two arbitrary vertices are from 1 to $\lfloor \frac{n}{2} \rfloor$. Also, $d_v = 2$ for every vertex $v \in V(C_n)$. If n is odd, then each number from 1 to $\frac{n-1}{2}$ appears in the denominator of n summands in $HSO(C_n)$. So,

$$HSO(C_n) = n\sqrt{8}\left(1 + \frac{1}{2} + \cdots + \frac{1}{\frac{n-1}{2}}\right) = 2\sqrt{2}nH_{\frac{n-1}{2}}.$$

Else, each number from 1 to $\frac{n}{2} - 1$ appears in the denominator of n summands and $\frac{n}{2}$ appears in the denominator of $\frac{n}{2}$ summands in $HSO(C_n)$. Thus,

$$\begin{aligned} HSO(C_n) &= \sqrt{8}\left(n\left(1 + \frac{1}{2} + \cdots + \frac{1}{\frac{n}{2}-1}\right) + \frac{n}{2} \times \frac{1}{\frac{n}{2}}\right) \\ &= \sqrt{8}\left(n\left(1 + \frac{1}{2} + \cdots + \frac{1}{\frac{n}{2}}\right) - 1\right) \\ &= 2\sqrt{2}(nH_{\frac{n}{2}} - 1). \end{aligned}$$

(iii) Let $P_n = v_1 \cdots v_n$. We have:

$$\begin{aligned} HSO(P_n) &= \sum_{k=2}^{n-1} \frac{\sqrt{1+4}}{d(v_1, v_k)} + \sum_{k=2}^{n-1} \frac{\sqrt{1+4}}{d(v_n, v_k)} + \sum_{i=2}^{n-2} \sum_{j=i+1}^{n-1} \frac{\sqrt{4+4}}{d(v_i, v_j)} + \frac{\sqrt{2}}{n-1} \\ &= 2\sqrt{5}H_{n-2} + \sqrt{8}\sum_{k=1}^{n-3} H_k + \frac{\sqrt{2}}{n-1}. \end{aligned}$$

On the other hand, $\sum_{k=1}^{n-3} H_k = (n-2)H_{n-3} - (n-3)$. So,

$$HSO(P_n) = 2\sqrt{5}H_{n-2} + \sqrt{8}(n-2)H_{n-3} - \sqrt{8}(n-3) + \frac{\sqrt{2}}{n-1}$$

and the proof is complete. □

Let $p \geq q \geq 2$ be positive integer numbers. The double star $DS_{p,q}$ is a tree obtained from S_p and S_q by connecting the center of S_p with that of S_q. One can calculate that

$$\begin{aligned} HSO(DS_{p,q}) &= \sqrt{p^2+q^2} + \frac{2p+q-3}{2}\sqrt{1+p^2} + \frac{2q+p-3}{2}\sqrt{1+q^2} \\ &+ \frac{3p^2+3q^2+4pq-13p-13q+16}{6\sqrt{2}}. \end{aligned}$$

Lemma 3. *Let $K_{p,q}$ be the complete bipartite graph. Then*

$$HSO(K_{p,q}) = \frac{1}{2\sqrt{2}}pq\left(\sqrt{8p^2+8q^2} + p + q - 2\right).$$

In particular if $p = q$, then $HSO(K_{p,p}) = \frac{1}{\sqrt{2}}p^2(3p-1)$.

Proof. Let $V(K_{p,q}) = X \cup Y$ with $|X| = p$ and $|Y| = q$. Therefore $d(u,v) = 1$ for any $u \in X$ and $v \in Y$ and vice versa; and $d(u,v) = 2$ otherwise. Hence

$$\begin{aligned} HSO(K_{p,q}) &= pq\sqrt{p^2+q^2} + \binom{p}{2}\frac{\sqrt{q^2+q^2}}{2} + \binom{q}{2}\frac{\sqrt{p^2+p^2}}{2} \\ &= pq\sqrt{p^2+q^2} + \frac{pq(p-1)}{2\sqrt{2}} + \frac{pq(q-1)}{2\sqrt{2}} \\ &= \frac{pq}{2\sqrt{2}}(\sqrt{8p^2+8q^2} + p + q - 2) \end{aligned}$$

and we are done. □

Now, we state the following upper bound for the Harary-Sombor index of bipartite graphs.

Theorem 1. *If G is a bipartite graph of order n, then*

$$HSO(G) \leq \begin{cases} \dfrac{n^2(3n-2)}{8\sqrt{2}} & n \text{ is even} \\ \dfrac{n^2-1}{8\sqrt{2}}\left(n-2+2\sqrt{n^2+1}\right) & n \text{ is odd} \end{cases}$$

with equality if and only if $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Proof. Let $G = G(X,Y)$ be a bipartite graph with $X = p$, $|Y| = q$, $p+q = n$ and $p \geq q$. It is clear that $HSO(G) \leq HSO(K_{p,q})$. So, by Lemma 3 we have:

$$HSO(G) = \frac{p(n-p)}{2\sqrt{2}}\left(\sqrt{8p^2 + 8(n-p)^2} + n - 2\right).$$

We define the function $f(x)$ on $[\lceil \frac{n}{2} \rceil, n-1]$, as follows:

$$f(x) = x(n-x)\left(n - 2 + \sqrt{16x^2 - 16nx + 8n^2}\right).$$

Thus

$$f'(x)\sqrt{16x^2 - 16nx + 8n^2} = g_1(x) + g_2(x), \qquad (\dagger)$$

where

$$g_1(x) = (n-2)(n-2x)\sqrt{16x^2 - 16nx + 8n^2}$$

and

$$g_2(x) = -48x^3 + 72nx^2 - 40n^2x + 8n^3.$$

Clearly,

$$g_1'(x)\sqrt{16x^2 - 16nx + 8n^2} = -2(n-2)(32x^2 - 32nx + 12n^2).$$

Thus $g_1'(x)\sqrt{16x^2 - 16nx + 8n^2}$ and consequently $g_1'(x)$ are negative functions and hence $g_1(x)$ is decreasing. Also, $g_2'(x)$ is negative and consequently $g_2(x)$ is decreasing. These imply that $f'(x)\sqrt{16x^2 - 16nx + 8n^2}$ is decreasing. On the other hand, $\sqrt{16x^2 - 16nx + 8n^2}$ is increasing on $[\frac{n}{2}, \infty]$. So, $f'(x)$ is decreasing on $[\lceil \frac{n}{2} \rceil, n-1]$. Moreover, $f'(\frac{n}{2}) = 0$, by Eq. $(\dagger)$. Thus $f'(x) < 0$ on $[\lceil \frac{n}{2} \rceil, n-1]$ and hence $f(x)$ is decreasing on this interval. Therefore maximum of $f(x)$ occurs at $\lceil \frac{n}{2} \rceil$ and the result follows. □

3. On the Harary-Sombor index of trees

In this section, we show that P_n and S_n have the minimum and maximum value of the Harary-Sombor index among all trees of order n, respectively.

Theorem 2. *Let G be a graph of order n and T ba an arbitrary spanning tree of G. Then*

$$HSO(P_n) \leq HSO(T) \leq HSO(G) \leq HSO(K_n).$$

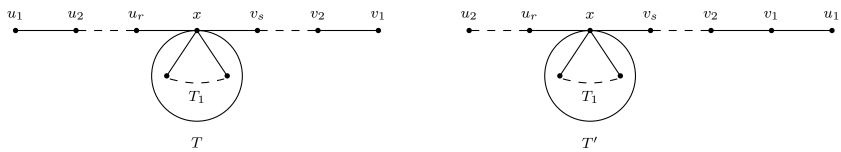

Figure 1. **The graphs T and T'.**

Proof. It is enough to show that $HSO(P_n) \leq HSO(T)$. If $T = P_n$, then the proof is straightforward. Else, there exists a vertex x in T with degree at least 3 such that at least two components of $T - x$ are paths. Suppose these paths have lengths $r - 1$ and $s - 1$, where $r \leq s$. Thus $T - x = P_r \cup P_s \cup T_1$, where T_1 is the subgraph induced by the vertices not included in these two paths. Now, we remove the end vertex of the path with the smaller size and add it to the end vertex of the path with the larger size and denote the resulting graph by T' (see Fig. 1).
If $r \geq 2$, then due to the differences of the summands related to u_1 and $V(T_1)$, u_2 and $V(T_1)$; and v_1 and $V(T_1)$ in the calculation of $HSO(T)$ and $HSO(T')$ we have:

$$\begin{aligned} HSO(T') = HSO(T) &- \sum_{y \in V(T_1)} \frac{\sqrt{1 + d_y^2}}{r + d(x,y)} + \sum_{y \in V(T_1)} \frac{\sqrt{1 + d_y^2}}{s + 1 + d(x,y)} \\ &- \sum_{y \in V(T_1)} \frac{\sqrt{4 + d_y^2}}{r - 1 + d(x,y)} + \sum_{y \in V(T_1)} \frac{\sqrt{1 + d_y^2}}{r - 1 + d(x,y)} \\ &- \sum_{y \in V(T_1)} \frac{\sqrt{1 + d_y^2}}{s + d(x,y)} + \sum_{y \in V(T_1)} \frac{\sqrt{4 + d_y^2}}{s + d(x,y)}. \end{aligned}$$

Now, by considering $r \leq s$ we get:

$$HSO(T') < HSO(T) - \left(\frac{1}{r - 1 + d(x,y)} - \frac{1}{s + d(x,y)}\right) \sum_{y \in V(T_1)} \left(\sqrt{4 + d_y^2} - \sqrt{1 + d_y^2}\right) < HSO(T).$$

Next, suppose $r = 1$. In order to the differences of the summands related to u_1 and $V(T_1) - \{x\}$, v_1 and $V(T_1) - \{x\}$, x and other vertices of T_1, x and v_i $(i = 2, \ldots, s)$, x and u_1; and x and v_1 in the calculation of $HSO(T)$ and $HSO(T')$ we obtain:

$$HSO(T') = HSO(T) - \sum_{\substack{y \in V(T_1) \\ y \neq x}} \frac{\sqrt{1 + d_y^2}}{1 + d(x,y)} + \sum_{\substack{y \in V(T_1) \\ y \neq x}} \frac{\sqrt{1 + d_y^2}}{s + 1 + d(x,y)}$$

$$
\begin{aligned}
&- \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{1+d_y^2}}{s+d(x,y)} + \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{4+d_y^2}}{s+d(x,y)}\\
&- \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{d_x^2+d_y^2}}{d(x,y)} + \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{(d_x-1)^2+d_y^2}}{d(x,y)}\\
&- \sum_{i=2}^{s} \frac{\sqrt{d_x^2+4}}{d(x,v_i)} + \sum_{i=2}^{s} \frac{\sqrt{(d_x-1)^2+4}}{d(x,v_i)}\\
&- \sqrt{d_x^2+1} + \frac{\sqrt{(d_x-1)^2+1}}{s+1}\\
&- \frac{\sqrt{d_x^2+1}}{s} + \frac{\sqrt{(d_x-1)^2+4}}{s}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
HSO(T') < HSO(T) &- \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{1+d_y^2}}{s+d(x,y)} + \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{4+d_y^2}}{s+d(x,y)}\\
&- \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{d_x^2+d_y^2}}{d(x,y)} + \sum_{\substack{y\in V(T_1)\\ y\neq x}} \frac{\sqrt{(d_x-1)^2+d_y^2}}{d(x,y)}\\
&- \sqrt{d_x^2+1} + \frac{\sqrt{(d_x-1)^2+1}}{s+1}\\
&- \frac{\sqrt{d_x^2+1}}{s} + \frac{\sqrt{(d_x-1)^2+4}}{s}.
\end{aligned}
$$

Also,

$$
\sqrt{d_x^2+d_y^2} - \sqrt{(d_x-1)^2+d_y^2} > \sqrt{4+d_y^2} - \sqrt{1+d_y^2},
$$

since $d_x \geq 3$. Moreover,

$$
d_x^2+1 > (d_x-1)^2+4.
$$

Thus $HSO(T') < HSO(T)$.

If $T' = P_n$, the proof is complete; otherwise, by repeating the above process as many times as necessary, P_n is finally reached and the proof is complete. □

Theorem 3. *For a tree T of order n, $HSO(T) \leq HSO(S_n)$.*

Proof. Let $T \neq S_n$ be an arbitrary tree. So, G has a diagonal path of length at least 3. Let v and w be the second and the third vertices of such a path, respectively and

$u_1, \ldots, u_r$ be leaves of T adjacent to v. We remove edge vw and matching the vertices v and w together; and add a new leaf adjacent to $u = w$ and denote the resulting tree by T' (see Fig. 2).

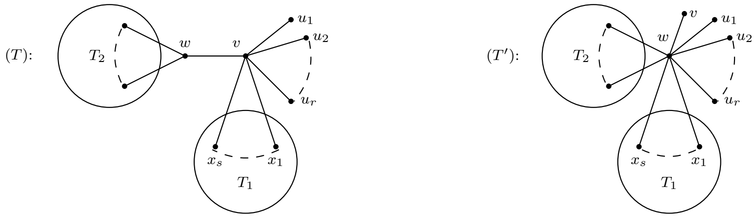

Figure 2. **The graphs T and T'.**

Due to the differences of the summands related to u_i's and v, u_i's and w, v and w, v and $V(T_1)$, w and $V(T_1)$, u_i's and $V(T_2)$, v and $V(T_2)$, w and $V(T_2)$; and $V(T_1)$ and $V(T_2)$ in the calculation of $HSO(T)$ and $HSO(T')$ we have:

$$
\begin{aligned}
HSO(T') = HSO(T) &- r\sqrt{1+(r+s+1)^2} + \frac{\sqrt{2}}{2}r \\
&- r\frac{\sqrt{1+d_w^2}}{2} + r\sqrt{1+(d_w+r+s)^2} \\
&- \sqrt{d_w^2+(r+s+1)^2} + \sqrt{(d_w+r+s)^2+1} \\
&- \sum_{x\in V(T_1)} \frac{\sqrt{(r+s+1)^2+d_x^2}}{d(v,x)} + \sum_{x\in V(T_1)} \frac{\sqrt{1+d_x^2}}{d(v,x)+1} \\
&- \sum_{x\in V(T_1)} \frac{\sqrt{d_w^2+d_x^2}}{d(v,x)+1} + \sum_{x\in V(T_1)} \frac{\sqrt{(d_w+r+s)^2+d_x^2}}{d(v,x)} \\
&- r\sum_{y\in V(T_2)} \frac{\sqrt{1+d_y^2}}{d(w,y)+2} + r\sum_{y\in V(T_2)} \frac{\sqrt{1+d_y^2}}{d(w,y)+1} \\
&- \sum_{y\in V(T_2)} \frac{\sqrt{(r+s+1)^2+d_y^2}}{d(w,y)+1} + \sum_{y\in V(T_2)} \frac{\sqrt{1+d_y^2}}{d(w,y)+1} \\
&- \sum_{y\in V(T_2)} \frac{\sqrt{d_w^2+d_y^2}}{d(w,y)} + \sum_{y\in V(T_2)} \frac{\sqrt{(d_w+r+s)^2+d_y^2}}{d(w,y)} \\
&- \sum_{x\in V(T_1),y\in V(T_2)} \frac{\sqrt{d_x^2+d_y^2}}{d(x,v)+d(w,y)+1} + \sum_{x\in V(T_1),y\in V(T_2)} \frac{\sqrt{d_x^2+d_y^2}}{d(x,v)+d(w,y)}.
\end{aligned}
$$

Note that $f(X) = \sqrt{1+(X+r+s)^2} - \frac{1}{2}\sqrt{1+X^2}$ is an increasing function for $X > 0$.

So,

$$\sqrt{1+(d_w+r+s)^2}-\frac{\sqrt{1+d_w^2}}{2}\geq\sqrt{1+(1+r+s)^2}-\frac{\sqrt{2}}{2},$$

since $d_w \geq 2$. Also, for arbitrary positive real numbers a and b, $g(X) = \frac{1}{b}\sqrt{(X+r+s)^2+a^2} - \frac{1}{b+1}\sqrt{X^2+a^2}$ is an increasing function for $X > 0$. So, for any $x \in V(T_1)$ we have

$$\frac{1}{d(v,x)}\sqrt{(d_w+r+s)^2+d_x^2}-\frac{1}{d(v,x)+1}\sqrt{d_w^2+d_x^2}\geq\frac{1}{d(v,x)}\sqrt{(1+r+s)^2+d_x^2}-\frac{1}{d(v,x)+1}\sqrt{1+d_x^2}.$$

Moreover, $h(X) = \sqrt{(X+r+s)^2+a^2} - \sqrt{X^2+a^2}$ is an increasing function for $X > 0$. So, for any $y \in V(T_2)$ we have

$$\sqrt{(d_w+r+s)^2+d_y^2}-\sqrt{d_w^2+d_y^2}\geq\sqrt{(1+r+s)^2+d_y^2}-\sqrt{1+d_y^2}.$$

Furthermore, $\frac{1}{d(w,y)+1} \leq \frac{1}{d(w,y)}$. Therefore, $HSO(T') > HSO(T)$. If $T' = S_n$, the proof is complete. Else, by repeating the above process as many times as necessary, S_n is finally reached and we are done. □

Declarations

Ethical Approval. Not Applicable.
Competing interests. The authors declare that there are no conflict of interests in the manuscript.
Authors' contributions. All authors contribute to finding and proving the results. The first author wrote the manuscript and the other authors proof read the manuscript.
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