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EXTREMAL VALUES ON THE MODIFIED SOMBOR INDEX OF TREES AND UNICYCLIC GRAPHS

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Abstract: Let $G=(V,E)$ be a simple connected graph. The modified Sombor index denoted by $mSo(G)$ is defined as

$$mSo(G)=\sum_{uv\in E}\frac{1}{\sqrt{d_u^2+d_v^2}},$$

where d_v denotes the degree of vertex v. In this paper we present extremal values of modified Sombor index over the set of trees and unicyclic graphs.

Keywords: Modified Sombor Index, Trees, Unicyclic graphs, Extremal values.

1. Introduction

A topological index is a real number derived from a structure of a graph that is not dependent on the way the vertices are labeled. A wide range of different topological indices have been employed in QSAR (Quantitative Structure – Activity Relationship) and QSPR (Quantitative Structure – Property Relationship) studies. Any topological indices belong to one of the two classes: they are either bond-additive, or distance based. Typical representation of bond-additive indices are two Zagreb indices, Harmonic index and Randić index.

Let $G=(V,E)$ be a simple connected graph. By the open neighborhood of a vertex v of G we mean the set

$$N_G(v)=\{u\in V: uv\in E\}$$

and by the closed neighborhood,

$$N_G[v]=N_G(v)\cup\{v\}.$$

The degree d_v of a vertex v is the cardinality of its open neighborhood. We denote by P_n and C_n a path and a cycle with n-vertices, respectively. A length of a cycle is the number of edges contained in the cycle. A star of order $n\geq 2$, denoted by S_n is a tree with at least $n-1$ leaves. A contraction of an edge $e=uv$ is the replacement of u and v with a single vertex such that edges incident to the new vertex are the edges other than e that were incident with u or v and the resulting graph is denoted by $G.uv$.

Recently, a degree based topological index called the Sombor index was introduced by Ivan Gutman in [4]. It is defined as

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

and further studied in [1–3, 6, 9, 10]. A variant of Sombor index namely, modified Sombor index, denoted by $mSo(G)$, is defined as

$$mSo(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u^2 + d_v^2}}.$$

In [8], a lower bound on a Modified Sombor index of unicyclic graphs with a given diameter is presented. In [7], bounds of modified Sombor index in terms of spectral radius and energy is given. A study on modified Sombor index matrix is done in [11]. An extreme value of the product of the Sombor index and the modified Sombor index is studied in [5].

In [7], to determine the extremal trees, unicyclic graphs, bicyclic graphs with respect to modified Sombor index were proposed. We determine the extremal graphs for the class of trees and unicyclic graphs, which answers the problem posed in [7]. In particular, we show that star and paths are the graphs with minimum and maximum modified Sombor index among all trees, and for unicyclic graphs we show that $U_n(n-1,2,2)$ and cycle are the graphs with minimum and maximum modified Sombor index.

2. Graph transformations

To begin with we present some graph transformations which will be useful to determine the extremal trees and unicyclic graphs.

Transformation A (*see Fig. 1*). Let G be a nontrivial connected graph and $u, v \in V(G)$, such that $d(v) \geq 3$ in G and $P_1 : uu_1u_2 \ldots u_r$ and $P_2 : vv_1v_2 \ldots v_s$ be two paths in G. Now we denote the graph H obtained from G by concatenating the paths P_1 and P_2.

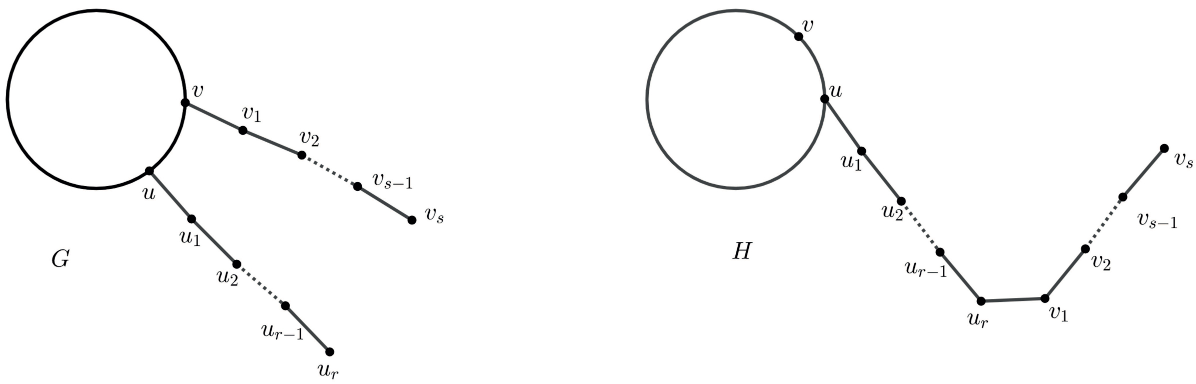

Figure 1. Transformation A.

Theorem 1. *Let H be the graph obtained from G using Transformation A, then $mSo(G) \leq mSo(H)$.*

P r o o f. The vertex v_1 in path P_2 is made adjacent to vertex u_r. Then

$$mSo(H) = mSo(G) - \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{8}} - \frac{1}{\sqrt{d_v^2 + 4}}$$
$$- \sum_{\alpha \in N(v) \setminus v_1} \frac{1}{\sqrt{d_v^2 + d_\alpha^2}} + \sum_{\alpha \in N(v) \setminus v_1} \frac{1}{\sqrt{(d_v - 1)^2 + d_\alpha^2}}$$

$$= mSo(G) - \frac{1}{\sqrt{5}} + \frac{2}{\sqrt{8}} - \frac{1}{\sqrt{d_v^2+4}} + \sum_{\alpha \in N(v)\setminus v_1} \left(\frac{1}{\sqrt{(d_v-1)^2+d_\alpha^2}} - \frac{1}{\sqrt{d_v^2+d_\alpha^2}} \right)$$

$$mSo(H) \geq mSo(G) - \frac{1}{\sqrt{5}} + \frac{2}{\sqrt{8}} - \frac{1}{\sqrt{13}} + \sum_{\alpha \in N(v)\setminus v_1} \left(\frac{1}{\sqrt{(d_v-1)^2+d_\alpha^2}} - \frac{1}{\sqrt{d_v^2+d_\alpha^2}} \right)$$

$$mSo(H) \geq mSo(G) - \frac{1}{\sqrt{5}} + \frac{2}{\sqrt{8}} - \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{10}} > mSo(G).$$

□

Transformation B (see Fig. 2). Let G be a nontrivial connected graph and $u \in V(G)$, such that $d(u) \geq 3$ in G and $P : uu_1u_2 \ldots u_t$ be the path in G. The H is constructed from G by removing the leaf u_t in the path P and attaching it to the vertex u by an edge uu_t.

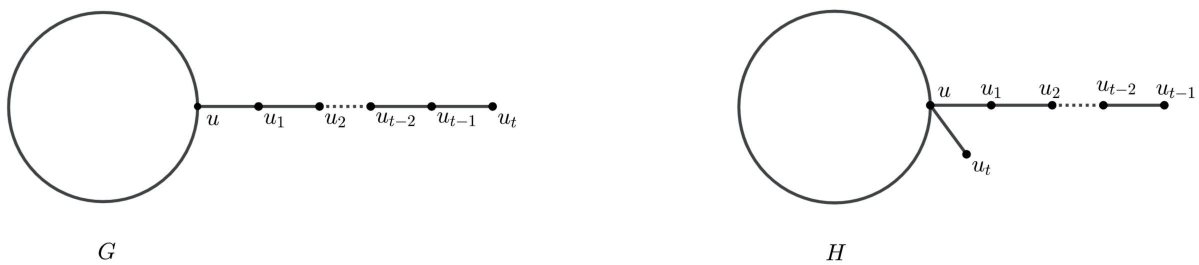

Figure 2. Transformation B.

Theorem 2. *Let H be the graph obtained from G using transformation B, then $mSo(H) \leq mSo(G)$.*

P r o o f. Applying Transformation B to graph G, we have

$$mSo(H) = mSo(G) - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{(d_u+1)^2+1}}$$

$$- \sum_{\alpha \in N(u)} \frac{1}{\sqrt{d_u^2+d_\alpha^2}} + \sum_{\alpha \in N(u)} \frac{1}{\sqrt{(d_u+1)^2+d_\alpha^2}}$$

$$= mSo(G) - \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{(d_u+1)^2+1}} + \sum_{\alpha \in N(u)} \left(\frac{1}{\sqrt{(d_u-1)^2+d_\alpha^2}} - \frac{1}{\sqrt{d_u^2+d_\alpha^2}} \right)$$

$$mSo(H) \leq mSo(G) - \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{17}} < mSo(G).$$

□

Transformation C (see Fig. 3). Let G be a nontrivial connected graph, $uv \in E(G)$ with $N(v) \cap N(u) = \emptyset$. We denote the graph H obtained from $G.uv$ and making the vertex v adjacent to u by an edge uv.

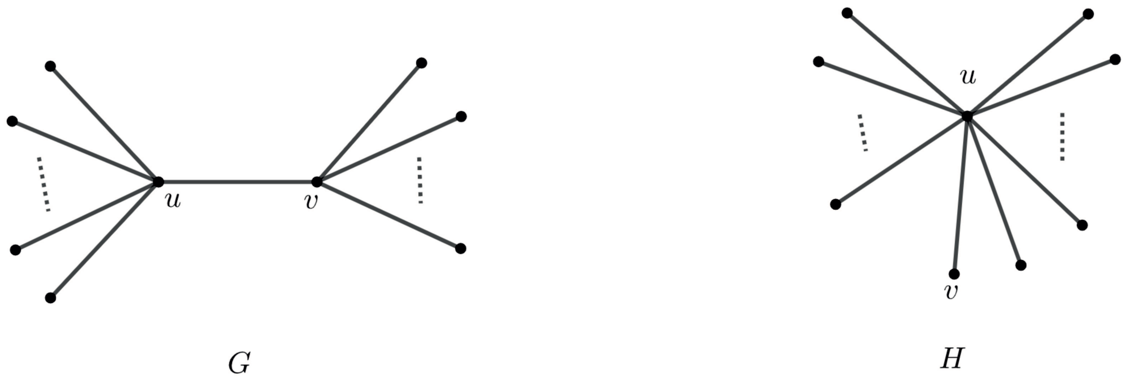

Figure 3. Transformation C.

Theorem 3. *Let H be the graph obtained from G using transformation C, then $mSo(H) \leq mSo(G)$.*

P r o o f. From the definition of Transformation C, we have $d_u, d_v \geq 2$. Then

$$mSo(H) = mSo(G) - \frac{1}{\sqrt{d_u^2 + d_v^2}} - \sum_{\alpha \in N(u)\backslash v} \frac{1}{\sqrt{d_u^2 + d_\alpha^2}} - \sum_{\alpha \in N(v)\backslash u} \frac{1}{\sqrt{d_v^2 + d_\alpha^2}}$$
$$+ \sum_{\alpha \in N(v)\cup N(u)\backslash\{u,v\}} \frac{1}{\sqrt{(d_v + d_u - 1)^2 + d_\alpha^2}} + \frac{1}{\sqrt{(d_v + d_u - 1)^2 + 1}}.$$

Since,

$$-\sum_{\alpha \in N(u)\backslash v} \frac{1}{\sqrt{d_u^2 + d_\alpha^2}} - \sum_{\alpha \in N(v)\backslash u} \frac{1}{\sqrt{d_v^2 + d_\alpha^2}} + \sum_{\alpha \in N(v)\cup N(u)\backslash\{u,v\}} \frac{1}{\sqrt{(d_v + d_u - 1)^2 + d_\alpha^2}} \leq 0,$$
$$-\frac{1}{\sqrt{d_u^2 + d_v^2}} + \frac{1}{\sqrt{(d_v + d_u - 1)^2 + 1}} \leq 0 \quad \text{for any} \quad d_u, d_v \geq 2.$$

Thus $mSo(H) \leq mSo(G)$. □

Transformation D (see Fig. 4). Let G be a unicyclic graph with cycle of length α, denoted by C_α and $u \in C_\alpha$, such that $d(u) = 3$ in G and $P : uu_1u_2 \ldots u_t$ $(t \neq 2)$ be the path in G. Let w be the neighbour of u in C_α. The graph H is constructed from G by removing the leaf v_t and including it in the cycle C_α between the vertices u, w.

Theorem 4. *Let H be the graph obtained from G using transformation D, then $mSo(G) \leq mSo(H)$.*

P r o o f. From Transformation D, we have $d_u = 3$. Then
Case 1: $t \geq 3$

$$mSo(H) = mSo(G) - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{8}} = mSo(G).$$

Case 2: $t = 1$

$$mSo(H) = mSo(G) - \frac{1}{\sqrt{10}} - \frac{2}{\sqrt{13}} + \frac{3}{\sqrt{8}} \geq mSo(G).$$

□

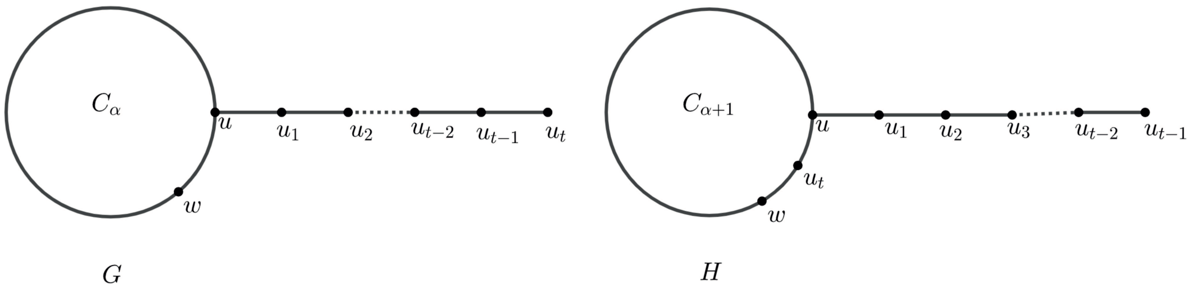

Figure 4. Transformation D.

Lemma 1. *Let G be a unicyclic path with cycle of length $n-2$, say C_{n-2} and $u \in C_{n-2}$ with a path uu_1u_2. Let H be the graph obtained from G by removing the vertices u_1 and u_2 and included in the cycle $C_{n-\alpha}$. Then $mSo(G) < mSo(H)$.*

P r o o f. Let the $d_u = 3$ in $V(G)$. Then,

$$mSo(H) = mSo(G) - \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{8}} - \frac{3}{\sqrt{13}} + \frac{5}{\sqrt{8}} > mSo(G).$$

□

Let $U_n(n_1, n_2, n_3)$ be the family of n-vertex unicyclic graph obtained from attaching n_1-2, n_2-2 and n_3-2 pendent vertices to the three vertices of a triangle respectively, where $n_1+n_2+n_3 = n+3$ and $n_1 \geq n_2 \geq n_3 \geq 2$.

Lemma 2. *For any $n \geq 5$, $n_1 + n_2 + n_3 = n + 3$ and $n_1 \geq n_2 \geq n_3 \geq 3$,*

$$mSo(U_n(n-1, 2, 2)) \leq mSo(U_n(n_1, n_2, n_3)).$$

P r o o f. Since $n_1 \geq n_2 \geq n_3 \geq 3$, we need to prove

$$mSo(U_n(n+1, n_2-1, n_3)) < mSo(U_n(n_1, n_2, n_3))$$

for $n_2 \geq 3$. Let

$$f(x) = \frac{x-2}{\sqrt{x^2+1}}, \quad x \geq 3.$$

Then

$$f''(x) = \frac{-4x^2-3x+2}{(x^2+1)^{5/2}} < 0$$

implies that $f(x+1) - f(x)$ is decreasing function for $x \geq 3$. Thus

$$\begin{gathered} mSo(U_n(n_1+1, n_2-1, n_3)) - mSo(U_n(n_1, n_2, n_3)) \\ = mSo(U_n(n_1+1, n_2-1, n_3)) - mSo(U_{n-1}(n_1, n_2-1, n_3)) \\ -(mSo(U_n(n_1, n_2, n_3)) - mSo(U_{n-1}(n_1, n_2-1, n_3))) \end{gathered}$$

$$\begin{gathered} = \frac{n_2-2}{\sqrt{n_2^2+1}} - \frac{n_2-3}{\sqrt{(n_2-1)^2+1}} + \frac{1}{\sqrt{n_1^2+n_2^2}} - \frac{1}{\sqrt{n_1^2+(n_2-1)^2}} + \frac{1}{\sqrt{n_2^2+n_3^2}} - \frac{1}{\sqrt{(n_2-1)^2+n_3^2}} \\ -(\frac{n_1-1}{\sqrt{(n_1+1)^2+1}} - \frac{n_1-2}{\sqrt{n_1^2+1}} + \frac{1}{\sqrt{(n_1+1)^2+n_3^2}} - \frac{1}{\sqrt{n_1^2+n_3^2}} + \\ \frac{1}{\sqrt{(n_1+1)^2+(n_2-1)^2}} - \frac{1}{\sqrt{n_1^2+(n_2-1)^2}}). \end{gathered}$$

Since

$$\frac{1}{\sqrt{n_1^2+n_2^2}} - \frac{1}{\sqrt{n_1^2+(n_2-1)^2}} < 0,$$
$$\frac{1}{\sqrt{n_2^2+n_3^2}} - \frac{1}{\sqrt{(n_2-1)^2+n_3^2}} < 0,$$
$$\frac{1}{\sqrt{(n_1+1)^2+n_3^2}} - \frac{1}{\sqrt{n_1^2+n_3^2}} < 0$$
$$\frac{1}{\sqrt{(n_1+1)^2+(n_2-1)^2}} - \frac{1}{\sqrt{n_1^2+(n_2-1)^2}} < 0,$$

then

$$\begin{aligned} &mSo(U_n(n_1+1, n_2-1, n_3)) - mSo(U_n(n_1, n_2, n_3)) \\ &\le f(n_2) - f(n_2-1) - (f(n_1+1) - f(n_1)) < 0. \end{aligned}$$

□

3. Extremal trees and unicyclic graphs

In this section, we determine the extremal values of the modified Sombor index on the class of trees and unicyclic graphs.

Theorem 5. *Let T be a tree with n-vertices, where $n \ge 3$. Then*

$$mSo(S_n) \le mSo(T) \le mSo(P_n).$$

P r o o f. By repeated use of the Transformation A, any tree T can be transformed into a path. Thus by Theorem 1, $mSo(T) \le mSo(P_n)$.

Now by repeated use of the Transformation C on T, we obtain a star. Thus by Theorem 3, $mSo(T) \ge mSo(S_n)$. □

Corollary 1. *Let T be a tree on n vertices, where $n \ge 3$, then*

$$\frac{n-1}{\sqrt{n^2-2n+2}} \le mSo(T) \le \frac{2}{\sqrt{5}} + \frac{n-2}{\sqrt{8}}.$$

Theorem 6. *Let G be an unicyclic graph with n-vertices, where $n \ge 4$. Then*

$$mSo(U_n(n-1, 2, 2)) \le mSo(G) \le mSo(C_n).$$

P r o o f. By repeated use of the transformation A, any unicyclic graph G can be transformed into a comet. Thus by Theorem 1, $mSo(G) \le mSo(CO_{n-\alpha,\alpha})$. Furthermore by using Theorem 4 and Lemma 1, we get $mSo(CO_{n-\alpha,\alpha}) \le mSo(C_n)$.

Now by repeated use of the Transformation B on G, we obtain a unicyclic graph G' with a cycle and remaining vertices as leaves. Thus by Theorem 2, $mSo(G) \ge mSo(G')$. Furthermore repeating the transformation C on G' we get $U_n(n_1, n_2, n_3)$. By Theorem 3, $mSo(G') \ge mSo(U_n(n_1, n_2, n_3))$. Furthermore using Lemma 2, we get $mSo(U_n(n_1, n_2, n_3)) \ge mSo(U_n(n-1, 2, 2))$. □

Corollary 2. *Let G be an unicyclic graph on n vertices, where $n \ge 4$, then*

$$\frac{n-3}{\sqrt{n^2-2n+2}} + \frac{2}{\sqrt{n^2-2n+5}} + \frac{1}{\sqrt{8}} \le mSo(G) \le \frac{n}{\sqrt{8}}.$$

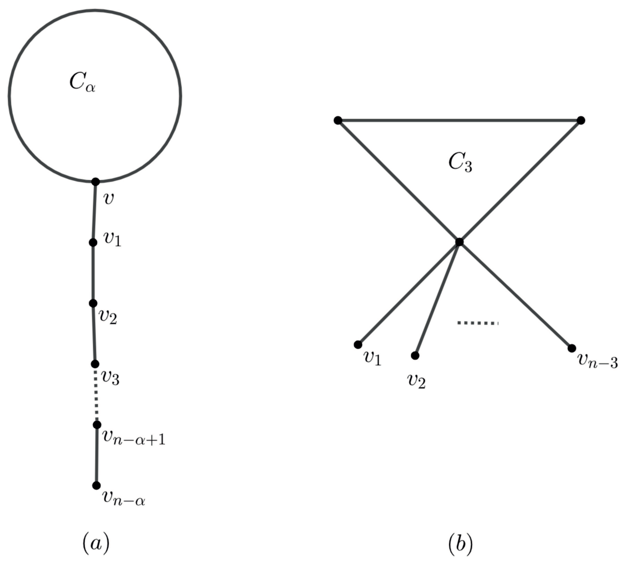

Figure 5. (a) Comet $CO_{n-\alpha,\alpha}$ (b) $U_n(n-1,2,2)$.

4. Conclusion

Bounds on modified Sombor index in terms of graph parameters are determined and various topological indices are compared with modified Sombor index in [7]. In [7] an open problem was proposed to determine the extremal trees, unicyclic graphs and bicyclic graphs with respect to modified Sombor index. Extremal trees and unicyclic graphs are determined here, which answers a part on the problem.

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REFERENCES

1. Cruz R., Gutman I., Rada J. Sombor index of chemical graphs. *Appl. Math. Comput.*, 2021. Vol. 399. Art. no. 126018. DOI: 10.1016/j.amc.2021.126018
2. Cruz R., Rada J. The path and the star as extremal values of vertex-degree-based topological indices among trees. *MATCH Commun. Math. Comput. Chem.*, 2019. Vol. 82. P. 715–732.
3. Deng H., Tang Z., Wu R. Molecular trees with extremal values of Sombor indices. *Int. J. Quantum Chem.*, 2021. Vol. 121, No. 11. Art. no. 26622. DOI: 10.1002/qua.26622
4. Gutman I. Geometric approach to degree-based topological indices: Sombor indices. *MATCH Commun. Math. Comput. Chem.*, 2021. Vol. 86. P. 11–16.
5. Gutman I., Redžepović I., Furtula B. On the product of Sombor and modified Sombor indices. *Open J. Discrete Appl. Math.*, 2023. Vol. 6, No. 2. P. 1–6.
6. Hernández J. C., Rodríguez J. M., Rosario O., Sigarreta J. M. Extremal problems on the general Sombor index of a graph. *AIMS Mathematics*, 2022. Vol. 7. No. 5. P. 8330–8343. DOI: 10.3934/math.2022464
7. Huang Y., Liu H. Bounds of modified Sombor index, spectral radius and energy. *AIMS Mathematics*, 2021. Vol. 6, No. 10. P. 11263–11274. DOI: 10.3934/math.2021653

8. Shooshtari H., Sheikholeslami S. M., Amjadi J. Modified Sombor index of unicyclic graphs with a given diameter. *Asian-Eur. J. Math.*, 2023. Vol. 16, No. 06. Art. no. 2350098. DOI: 10.1142/S1793557123500985
9. Wu F., An X., Wu B. Sombor indices of cacti. *AIMS Mathematics*, 2023. Vol. 8. No. 1. P. 1550–1565. DOI: 10.3934/math.2023078
10. Yang Ch., Ji M., Das K.C., Mao Y. Extreme graphs on the Sombor indices. *AIMS Mathematics*, 2022. Vol. 7, No. 10. P. 19126–19146. DOI: 10.3934/math.20221050
11. Zuo X., Rather B. A., Imran M., Ali A. On some topological indices defined via the modified Sombor matrix. *Molecules*, 2022. Vol. 27. No. 19. Art. no. 6772. DOI: 10.3390/molecules27196772