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# TEMO theorem for Sombor index

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**Abstract:** TEMO = topological effect on molecular orbitals was discovered by Polansky and Zander in 1982, in connection with the eigenvalues of molecular graphs. Eventually, analogous regularities were established for a variety of other topological indices. We now show that a TEMO-type regularity also holds for the Sombor index ($SO$): For the graphs $S$ and $T$, constructed by connecting a pair of vertex-disjoint graphs by two edges, $SO(S) < SO(T)$ holds. Analogous relations are verified for several other degree-based graph invariants.

**Keywords:** Sombor index; TEMO; Degree (of vertex); Vertex-degree-based graph invariant.

**MSC:** 05C07; 05C09.

## 1. Introduction

In this paper, we consider a pair of graphs that traditionally are denoted by $S$ and $T$. These are constructed by starting with any two vertex-disjoint graphs $G_1$ and $G_2$. Let $a$ and $b$ be two distinct vertices of $G_1$, and let $c$ and $d$ be two distinct vertices of $G_2$. Then $S$ is the graph obtained from $G_1$ and $G_2$ by connecting $a$ with $c$ and $b$ with $d$. The graph $T$ is obtained analogously, by connecting $a$ with $d$ and $b$ with $c$, see Figure 1.

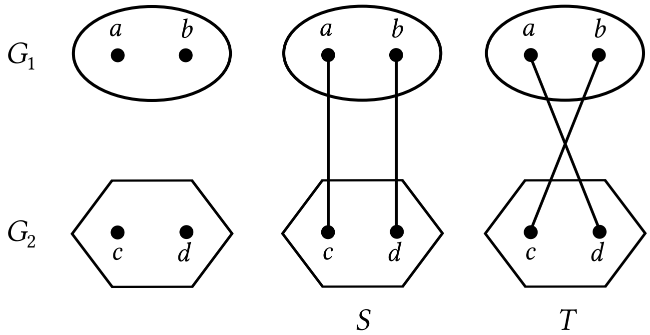


**Figure 1.** The structure of the graphs $S$ and $T$ and the labeling of their vertices.

In 1982, Polansky and Zander discovered a remarkable property of the graphs $S$ and $T$ [1]. They established that the characteristic polynomials of $S$ and $T$ are related as

$$\phi(T,\lambda) - \phi(S,\lambda) = \big[\phi(G_1-a,\lambda) - \phi(G_1-b,\lambda)\big]\big[\phi(G_2-c,\lambda) - \phi(G_2-d,\lambda)\big].$$

In the special case when $G_1 \cong G_2$,

$$\phi(T,\lambda) - \phi(S,\lambda) = \big[\phi(G_1-a,\lambda) - \phi(G_1-b,\lambda)\big]^2,$$

which means that the inequality

$$\phi(T,\lambda) \geq \phi(S,\lambda) \tag{1}$$

holds for all real values of the variable $\lambda$.

The inequality (1) implies certain regularities for the distribution of the eigenvalues of $S$ and $T$ [2–4] and have appropriate (experimentally verifiable) consequences on the distribution of the molecular orbital energy levels [5]. The authors of [1] called this a "*topological effect on molecular orbitals*" and used the acronym TEMO. Eventually, TEMO was extensively investigated; a detailed bibliography of this research can be found in the books [6,7].

After the discovery of the regularities between the eigenvalues of $S$ and $T$, a number of other TEMO-like relations for these pairs of graphs was discovered [8–16].

## 2. TEMO for Sombor index

The Sombor index ($SO$) is a recently conceived vertex-degree-based graph invariant [17], that already attracted much attention (see, e.g. [18–22]). It is defined as

$$SO = SO(G) = \sum_{uv\in \mathbf{E}(G)} \sqrt{\delta_u^2 + \delta_v^2}\,, \tag{2}$$

where $\delta_u$ is the degree (= number of first neighbors) of the vertex $u$, $uv$ denotes the edge connecting the vertices $u$ and $v$, and the summation goes over all edges of the underlying graph $G$.

In what follows, we establish a TEMO-like property of the Sombor index, i.e., investigate the relation between $SO(S)$ and $SO(T)$.

Denote by $\delta_a, \delta_b, \delta_c, \delta_d$ the degrees of the vertices $a, b, c, d$ of the graphs $S$ and $T$ (see Fig. 1). It is obvious that if either $\delta_a = \delta_b$ or $\delta_c = \delta_d$ or both, then $SO(S) = SO(T)$. Therefore, we consider the case $\delta_a \neq \delta_b$ and $\delta_c \neq \delta_d$. Without loss of generality, we may assume that $\delta_a > \delta_b$ and $\delta_c > \delta_d$.

**Theorem 1.** *Let $G_1$ and $G_2$ be arbitrary vertex-disjoint graphs and $a, b, c, d$ their vertices as indicated in Figure 1. If $\delta_a > \delta_b$ and $\delta_c > \delta_d$, then $SO(S) < SO(T)$.*

Note that the degree of the vertex $a$ in the graph $G_1$ is $\delta_a - 1$, etc.

**Proof.** Observe first that

$$\begin{aligned} SO(S) &= \sqrt{\delta_a^2 + \delta_c^2} + \sqrt{\delta_b^2 + \delta_d^2} + SO^*\,, \\ SO(T) &= \sqrt{\delta_a^2 + \delta_d^2} + \sqrt{\delta_b^2 + \delta_c^2} + SO^*\,, \end{aligned}$$

where $SO^*$ is the sum of the terms $\sqrt{\delta_u^2 + \delta_v^2}$ over other edges of $S$ or $T$. Thus,

$$SO(S) - SO(T) = \sqrt{\delta_a^2 + \delta_c^2} + \sqrt{\delta_b^2 + \delta_d^2} - \sqrt{\delta_a^2 + \delta_d^2} - \sqrt{\delta_b^2 + \delta_c^2}\,.$$

It needs to be demonstrated that

$$\sqrt{\delta_a^2 + \delta_d^2} + \sqrt{\delta_b^2 + \delta_c^2} > \sqrt{\delta_a^2 + \delta_c^2} + \sqrt{\delta_b^2 + \delta_d^2}\,. \tag{3}$$

In order to achieve this goal, consider

$$Q = \left(\delta_a^2 - \delta_b^2\right)\left(\delta_c^2 - \delta_d^2\right),$$

which by the assumptions made in the statement of Theorem 1 is evidently positive-valued.

$$\begin{aligned} Q > 0 &\iff \delta_a^2\,\delta_c^2 + \delta_b^2\,\delta_d^2 > \delta_a^2\,\delta_d^2 + \delta_b^2\,\delta_c^2 \\ &\iff \delta_a^2\,\delta_b^2 + \delta_c^2\,\delta_d^2 + \delta_a^2\,\delta_c^2 + \delta_b^2\,\delta_d^2 > \delta_a^2\,\delta_b^2 + \delta_c^2\,\delta_d^2 + \delta_a^2\,\delta_d^2 + \delta_b^2\,\delta_c^2 \\ &\iff \left(\delta_a^2 + \delta_d^2\right)\left(\delta_b^2 + \delta_c^2\right) > \left(\delta_a^2 + \delta_c^2\right)\left(\delta_b^2 + \delta_d^2\right) \\ &\iff 2\sqrt{\left(\delta_a^2 + \delta_d^2\right)\left(\delta_b^2 + \delta_c^2\right)} > 2\sqrt{\left(\delta_a^2 + \delta_c^2\right)\left(\delta_b^2 + \delta_d^2\right)} \\ &\iff \left(\delta_a^2 + \delta_d^2\right) + \left(\delta_b^2 + \delta_c^2\right) + 2\sqrt{\left(\delta_a^2 + \delta_d^2\right)\left(\delta_b^2 + \delta_c^2\right)} > \left(\delta_a^2 + \delta_c^2\right) + \left(\delta_b^2 + \delta_d^2\right) + 2\sqrt{\left(\delta_a^2 + \delta_c^2\right)\left(\delta_b^2 + \delta_d^2\right)} \\ &\iff \left(\sqrt{\delta_a^2 + \delta_d^2} + \sqrt{\delta_b^2 + \delta_c^2}\right)^2 > \left(\sqrt{\delta_a^2 + \delta_c^2} + \sqrt{\delta_b^2 + \delta_d^2}\right)^2 \end{aligned}$$

which directly implies the inequality (3). □

## 3. More TEMO-type relations

In an analogous, yet slightly easier, manner, we can verify the following TEMO-type results.

Using the notation of Eq. (2), the second Zagreb index $M_2$, the Randić index $R$, the reciprocal Randić index $RR$, and the nirmala index $N$ are, respectively, defined as [23–26]

$$\begin{aligned} M_2 = M_2(G) &= \sum_{uv\in \mathbf{E}(G)} \delta_u\, \delta_v\,, \\ R = R(G) &= \sum_{uv\in \mathbf{E}(G)} \frac{1}{\sqrt{\delta_u\, \delta_v}}\,, \\ RR = RR(G) &= \sum_{uv\in \mathbf{E}(G)} \sqrt{\delta_u\, \delta_v}\,, \\ N = N(G) &= \sum_{uv\in \mathbf{E}(G)} \sqrt{\delta_u + \delta_v}\,. \end{aligned}$$

**Theorem 2.** *Let $G_1$ and $G_2$ be arbitrary vertex-disjoint graphs and $a,b,c,d$ their vertices as indicated in Figure 1. If $\delta_a > \delta_b$ and $\delta_c > \delta_d$, then*

*(a)* $M_2(S) > M_2(T)$,
*(b)* $R(S) > R(T)$,
*(c)* $RR(S) > RR(T)$,
*(d)* $N(S) < N(T)$.

Analogous relations hold also for the reduced versions of these indices, in which $\delta$ is replaced by $\delta - 1$.

**Conflicts of Interest:** "The author declares no conflict of interest."

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