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Research Article

Sombor energy and Hückel rule

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Abstract

The Sombor index, a recently invented vertex-degree-based graph invariant, is insensitive to the size of cycles contained in a graph. In contrast to this, the Sombor energy, the sum of absolute values of the Sombor matrix, is found to have a significant cycle-size dependence. In the case of bipartite graphs, this dependence is analogous to the Hückel $(4n+2)$-rule: cycles of size $4, 8, 12, \ldots$ decrease, and cycles of size $6, 10, 12, \ldots$ increase the Sombor energy. A theorem corroborating this empirical observation is offered.

Keywords: energy (of a graph); Sombor index; Sombor energy; graph energy; topological index; degree (of a vertex).

2020 Mathematics Subject Classification: 05C07, 05C09, 05C50.

1. Introduction

Since the introduction of the concept of *Sombor index* [10], its chemical applications were extensively studied [1,2,6,24,28,29]. However, one chemically important property of the Sombor index, namely its dependence on the size of the cycles contained in a (molecular) graph, was never examined. The reason for this is evident: It is easy to recognize that neither the Sombor index nor any of the numerous other vertex-degree-based topological indices have any noteworthy cycle-size dependence. The examples depicted in Figure 1 may suffice to corroborate this conclusion.

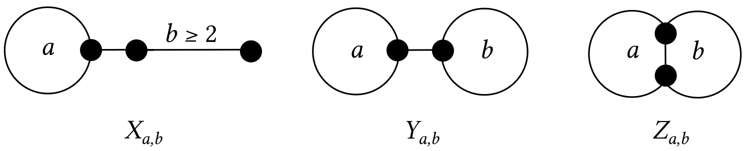

Figure 1: Examples of molecular graphs whose Sombor index is independent of the size (a,b) of their cycles; n = number of vertices; $SO(X_{a,b}) = \sqrt{5} + 3\sqrt{13} + (n-4)\sqrt{8}$; $SO(Y_{a,b}) = \sqrt{18} + 4\sqrt{13} + (n-4)\sqrt{8}$; $SO(Z_{a,b}) = \sqrt{18} + 4\sqrt{13} + (n-4)\sqrt{8}$.

Recently, a detailed theory of degree-based matrices and the respective degree-based energies was elaborated [4,11,13,17,23,32]. Within this theory, also the concept of *Sombor matrix* and *Sombor energy* was introduced [7,12,15,19,34]. In this paper, we show that, in contrast to the Sombor index, the Sombor energy possesses a pronounced cycle-size dependence. In particular, we establish the existence of a Hückel-rule-type regularity for the Sombor energy.

Recall that the famous Hückel $(4n+2)$-rule claims that cycles of size 6, 10, 14, ... stabilize, whereas cycles of size 4, 8, 12, ... destabilize a cyclic conjugated π-electron system [8,18,20,21,27]. In terms of graph energy [5,14,22] or other eigenvalue-based topological indices [30], cycles of size 4, 8, 12, ... have a positive (increasing) effect on graph energy, whereas the effect of 4, 8, 12, ... cycles is negative. In what follows, we demonstrate that an analogous regularity holds for the Sombor energy. A characteristic example is shown in Figure 2.

2. Mathematical introduction

Let G be a simple graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. Because we are interested in effects caused by even cycles, it will be assumed that G is connected and bipartite and, of course, contains at least one cycle. Recall that in bipartite graphs, the size of all cycles is even.

If the vertices $u, v \in \mathbf{V}(G)$ are adjacent, then the edge connecting them is denoted by uv. The number of edges incident to a vertex v is the degree of vertex v, and is denoted by d_v.

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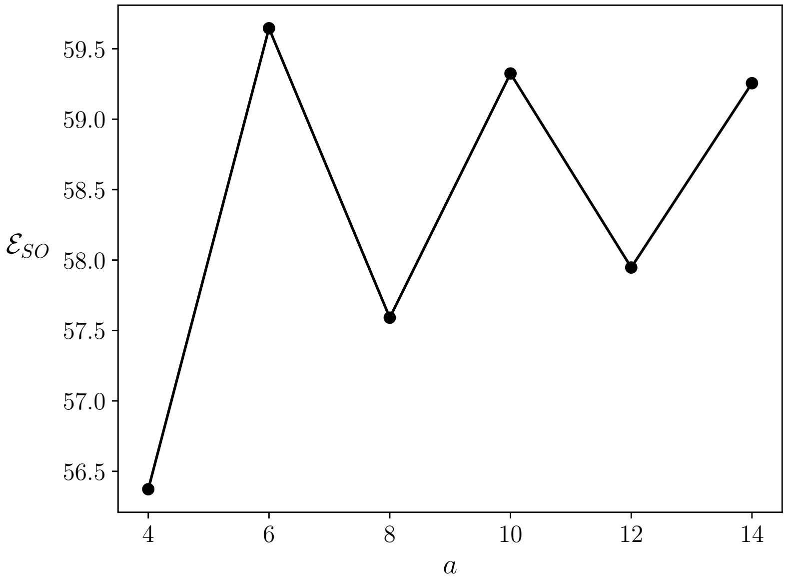

Figure 2: The Sombor energy of the unicyclic graph $X_{a,b}$, $a + b = 16$, plotted versus the size a of its cycle.

The Sombor index is defined as [10]

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

Bearing this in mind, if $\mathbf{V}(G) = \{v_1, v_2, \dots, v_n\}$ is the vertex set of the graph G, then its Sombor matrix $\mathbf{A}_{SO}(G) = (a_{SO})_{ij}$ is the symmetric matrix of order n, whose elements are

$$(a_{SO})_{ij} = \begin{cases} \sqrt{d_{v_i}^2 + d_{v_j}^2} & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{if } v_i v_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases}$$

If the eigenvalues of $\mathbf{A}_{SO}(G)$ are $\lambda_1, \lambda_2, \dots, \lambda_n$, then the Sombor energy of the graph G is defined as

$$\mathcal{E}_{SO} = \mathcal{E}_{SO}(G) = \sum_{i=1}^{n} |\lambda_i|\,.$$

For the hitherto established properties of the Sombor energy see [7, 12, 15, 19, 34].

3. Numerical work

In order to get an idea on the cycle-size dependence of the Sombor energy, we calculated the $\mathcal{E}_{SO}$-values of several classes of molecular graphs, in which the size of the cycles varies. In Tables 1 and 2 are presented such results for the graphs X, Y, and Z, depicted in Figure 1.

Table 1: Sombor energies of the unicyclic graphs $X_{a,b}$ whose structure is found in Figure 1. The Hückel-rule-type dependence on cycle size is clearly visible.

number of vertices	size of cycle	$\mathcal{E}_{SO}(X)$	number of vertices	size of cycle	$\mathcal{E}_{SO}(X)$
8	4	27.392	12	8	43.132
8	6	30.984	12	10	45.006
10	4	34.662	14	4	49.145
10	6	38.121	14	6	52.462
10	8	35.895	14	8	50.365
12	4	41.910	14	10	52.154
12	6	45.285	14	12	50.737

Table 2: Sombor energies of bicyclic graphs $Y_{a,b}$ and $Z_{a,b}$ whose structure is found in Figure 1. A Hückel-rule-type dependence can be envisaged, but is somewhat less pronounced than in the case of $X_{a,b}$.

number of vertices	sizes of cycles	$\mathcal{E}_{SO}(Y)$	number of vertices	sizes of cycles	$\mathcal{E}_{SO}(Z)$
8	4,4	30.658	8	4,6	33.914
10	4,6	40.038	10	4,8	40.986
12	4,8	46.162	10	6,6	43.638
12	6,6	51.284	12	4,10	48.165
14	4,10	54.172	12	6,8	49.260
14	6,8	56.018	14	4,12	55.394
			14	6,10	57.670
			14	8,8	56.028

4. A theorem on cycle dependence of Sombor energy

The Sombor matrix $\mathbf{A}_{SO}(G)$ can be viewed as the adjacency matrix of an ordinary graph with appropriately weighted edges. Let, thus, G be a bipartite graph, such that its edge $e = uv$ has a weight $w(e) = w(uv)$. Recall that in our case, $w(uv) = \sqrt{d_u^2 + d_v^2} > 0$.

Since G is bipartite, its characteristic polynomial of G has the form [3, 19]

$$\phi(G, \lambda) = \sum_{k \geq 0} (-1)^k \, b(G, k) \, \lambda^{n-2k}$$

so that all its coefficients $b(G, k)$ are non-negative. According to the Sachs theorem [3, 19, 25, 31]

$$(-1)^k \, b(G, k) = \sum_{\sigma \in \mathcal{S}_{2k}(G)} (-1)^{p(\sigma)} \, 2^{c(\sigma)} \, w(\sigma) \tag{1}$$

where $\mathcal{S}_k(G)$ is the set of all Sachs graphs of G possessing exactly $2k$ vertices, and where σ is an element of $\mathcal{S}_{2k}(G)$, containing $p(\sigma)$ components, of which $c(\sigma)$ are cycles. The weight $w(\sigma)$ of the Sachs graph σ is equal to the product of the weights of its components. If the isolated edge uv (consisting of two vertices) is a component of σ, then its weight is w_{uv}^2. If a cycle Z is a component of σ, then its weight is the product of weights of its edges [21, 31].

The energy of the weighted bipartite graph G, i.e., the sum of the absolute values of its eigenvalues, is related with the coefficients of the characteristic polynomial by means of the Coulson integral formula [9, 22]

$$\mathcal{E}(G) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \sum_{k \geq 0} b(G, k) \, x^{2k} \tag{2}$$

which means that the energy is a monotonically increasing function of each of the coefficients.

Let Z be a cycle of the graph G, and let its size be h, an even number. Label the edges of Z consecutively by $e_1, e_2, \ldots, e_h$. We are interested in the effect of the cycle Z on the energy of the graph G. In view of the Sachs and Coulson formulas (1) and (2), this effect will manifest itself via the Sachs graphs which contain Z.

Let $\sigma_1 \in \mathcal{S}_{2k}(G)$ be a Sachs graph containing the cycle Z. Then the components of σ_1, other than Z form a Sachs graph $\sigma^* \in \mathcal{S}_{2k-h}(G - Z)$. It holds,

$$\begin{aligned} p(\sigma_1) &= 1 + p(\sigma^*) \\ c(\sigma_1) &= 1 + c(\sigma^*) \\ w(\sigma_1) &= w(Z) \cdot w(\sigma^*) \end{aligned}$$

which by Equation (1) yields

$$\sum_{\sigma_1} (-1)^{p(\sigma)} \, 2^{c(\sigma)} \, w(\sigma) = -2 \, w(Z) \sum_{\sigma^*} (-1)^{p(\sigma)} \, 2^{c(\sigma)} \, w(\sigma) = -2 \, w(Z) \, (-1)^{k-h/2} \, b(G - Z, k - h/2) \, . \tag{3}$$

If there is a Sachs graph σ_1, then there must exist another Sachs graph σ_2 which instead of the cycle Z contains the edges $e_1, e_3, \ldots, e_{h-1}$. There also must exist a Sachs graph σ_3 containing the edges $e_2, e_4, \ldots, e_h$. For them,

$$p(\sigma_2) = h/2 + p(\sigma^*)$$

$$\begin{aligned} c(\sigma_2) &= c(\sigma^*) \\ w(\sigma_2) &= w(e_1)^2\, w(e_3)^2 \cdots w(e_{h-1})^2 \cdot w(\sigma^*) \\ p(\sigma_3) &= h/2 + p(\sigma^*) \\ c(\sigma_3) &= c(\sigma^*) \\ w(\sigma_3) &= w(e_2)^2\, w(e_4)^2 \cdots w(e_h)^2 \cdot w(\sigma^*) \end{aligned}$$

and, in an analogous manner as above

$$\sum_{\sigma_2} (-1)^{p(\sigma)}\, 2^{c(\sigma)}\, w(\sigma) = (-1)^{h/2}\, w(e_1)^2\, w(e_3)^2 \cdots w(e_{h-1})^2\, (-1)^{k-h/2}\, b(G-Z, k-h/2) \tag{4}$$

and

$$\sum_{\sigma_3} (-1)^{p(\sigma)}\, 2^{c(\sigma)}\, w(\sigma) = (-1)^{h/2}\, w(e_2)^2\, w(e_4)^2 \cdots w(e_h)^2\, (-1)^{k-h/2}\, b(G-Z, k-h/2)\,. \tag{5}$$

The total effect of the cycle Z on the coefficient $b(G,k)$ is thus

$$ef(G,Z) = (-1)^k \sum_{\sigma_1,\sigma_2,\sigma_3} (-1)^{p(\sigma)}\, 2^{c(\sigma)}\, w(\sigma)$$

which by taking into account Equations (3)–(5) yields

$$ef(G,Z) = \Big[w(e_1)^2\, w(e_3)^2 \cdots w(e_{h-1})^2 + w(e_2)^2\, w(e_4)^2 \cdots w(e_h)^2 - 2(-1)^{h/2}\, w(Z) \Big] b(G-Z, k-h/2)\,.$$

Bearing in mind that $w(Z) = w(e_1)w(e_2)\cdots w(e_{h-1})w(e_h)$,

$$\begin{aligned} ef(G,Z) &= \left[\Big(w(e_1)w(e_3)\cdots w(e_{h-1}) \Big)^2 + \Big(w(e_2)w(e_4)\cdots w(e_h) \Big)^2 \pm 2\, w(e_1)w(e_2)\cdots w(e_h) \right] b(G-Z, k-h/2) \\ &= \Big[w(e_1)w(e_3)\cdots w(e_{h-1}) \pm w(e_2)w(e_4)\cdots w(e_h) \Big]^2\, b(G-Z, k-h/2)\,. \end{aligned}$$

We now arrive at our main result:

Theorem 4.1. *(a) If the size h of the cycle Z contained in the bipartite graph G is divisible by 4, i.e., if $h/2$ is even, then the respective energy effect is*

$$ef(G,Z) = \Big[w(e_1)w(e_3)\cdots w(e_{h-1}) - w(e_2)w(e_4)\cdots w(e_h) \Big]^2\, b(G-Z, k-h/2)\,.$$

(b) If the size h of the cycle Z contained in the bipartite graph G is not divisible by 4, i.e., if $h/2$ is odd, then the respective energy effect is

$$ef(G,Z) = \Big[w(e_1)w(e_3)\cdots w(e_{h-1}) + w(e_2)w(e_4)\cdots w(e_h) \Big]^2\, b(G-Z, k-h/2)\,.$$

By Theorem 4.1, $ef(G,Z) \geq 0$ for all edge-weighted bipartite graphs G and all their cycles Z. This means that all cycles increase the value of the coefficients $b(G,k)$ and thus, by Equation (2), increase the value of $\mathcal{E}(G)$. However, in the case of cycles of size 4, 8, 12, … , this increasing effect is smaller than for the cycles of size 6, 10, 14, … , and may be equal to zero. Needless to say that these conclusions apply also to the Sombor energy $\mathcal{E}_{SO}$.

One should note that the validity of both Theorem 4.1 and its proof are restricted to bipartite graphs. Their extension to even cycles in non-bipartite graphs seems to be not easy and remains a task for the future.

Since the term $b(G-Z, k-h/2)$ is non-negative, and since (in our case) all edge-weights are positive-valued, Theorem 4.1 is in good agreement with the empirically observed fact that the Sombor energy has a Hückel-rule-type cycle-dependence. Yet, it should not be considered as a proper proof of this Hückel-rule-type cycle-dependence.

5. A historical remark

This paper is dedicated to Professor Nenad Trinajstić. Therefore, it should be noted that studies related to the Hückel rule were the topics of Trinajstić's earliest researches, published exactly half a century ago [16, 26]. Also later, he remained interested in problems of this kind (e.g., [8, 20, 33]). The paper [16] happens to be the first scientific publication of one of the present authors (I.G.), who then was one of Professor Trinajstić's first students.

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