MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **88** (2022) 133-140
ISSN: 0340-6253
doi: 10.46793/match.88-1.133R

Comparing Energy and Sombor Energy – An Empirical Study

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(Received December 3, 2021)

Abstract

The Sombor index is a recently invented vertex-degree-based topological index, to which a matrix – called Sombor matrix – is associated in a natural manner. The graph energy $\mathcal{E}(G)$ is the sum of absolute values of the eigenvalues of the adjacency matrix of the graph G. Analogously, the Sombor energy $\mathcal{E}_{SO}(G)$ is the sum of absolute values of the eigenvalues of the Sombor matrix. In this paper, we present computational results on the relations between $\mathcal{E}_{SO}(G)$ and $\mathcal{E}(G)$ for various classes of (molecular) graphs, and establish the respective regularities. The correlation between $\mathcal{E}_{SO}(G)$ and $\mathcal{E}(G)$ if found to be much more perplexed than earlier reported.

1 Introduction

In this paper, we consider simple (molecular) graphs. Let G be such a graph, with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. If two vertices have a common edge then they are said to be adjacent. If the vertices u and v are adjacent, then the edge connecting them is denoted by uv. The number of edges incident to a vertex v is called the degree of that vertex v, and is denoted by d_v.

In the chemical and mathematical literature, a great number of vertex-degree-based (VDB) topological indices of the form

$$TI = TI(G) = \sum_{uv \in \mathbf{E}(G)} F(d_u, d_v) \tag{1}$$

have been and are currently considered, where F is a suitably chosen function, with property $F(x, y) = F(y, x)$ [15, 25, 26, 30]. Among them is the *Sombor index* [8], for which $F(x, y) = \sqrt{x^2 + y^2}$.

The adjacency matrix $\mathbf{A}(G) = \big[a_{ij}\big]$ of the graph G, with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$, is the symmetric matrix of order n, whose elements are defined as [3]

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{if } v_i v_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases} \tag{2}$$

In analogy to Eq. (2), bearing in mind Eq. (1), one defines the matrix $\mathbf{A}_{TI}(G) = \big[(a_{TI})_{ij}\big]$ as

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

The (ordinary) graph energy $\mathcal{E}(G)$ is the sum of absolute values of the eigenvalues of the adjacency matrix $\mathbf{A}(G)$. The theory of this graph–spectral invariant is nowadays much studied and elaborated in full detail [12, 17, 22]. The "energy" associated with the topological index TI, Eq. (1), is the sum of absolute values of the eigenvalues of the matrix $\mathbf{A}_{TI}(G)$ [4, 18, 24]. Since the Sombor index is defined as

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

the *Sombor energy* $\mathcal{E}_{SO}(G)$ is the sum of absolute values of the eigenvalues of the Sombor matrix $\mathbf{A}_{SO}(G)$, whose elements are

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

The Sombor index SO is a recently designed VDB molecular structure descriptor, conceived by means of geometric considerations [8]. It promptly attracted much attention and its chemical applications (e.g., [1, 2, 20, 23]) and mathematical properties (e.g., [5, 16, 21, 29]) are being studied in a remarkably large number of papers (over 70 by the end of 2021). Also promptly, the concept of Sombor index was extended to Sombor energy and other spectral properties of the Sombor matrix [6, 7, 9, 13, 19, 31]. Relations between Sombor index and graph energy were studied [27, 28]. Curiously, however, the relation between graph energy and Sombor energy was so far not investigated. Exceptionally, in Ref. [7], $\mathcal{E}_{SO}$ was correlated with the total π-electron energy of a set of aza-derivatives of benzenoid hydrocarbons. Since these benzenoids had different number of carbon atoms,

an artificial increasing, nearly linear correlation was found. The authors of [7] have ignored the long known fact that such correlations need to be studied only within classes of isomers or – equivalently – within classes of (molecular) graphs with fixed number of vertices and number of edges. Otherwise, since the respective quantities (in this case, $\mathcal{E}_{SO}$ and $\mathcal{E}$) both significantly increase with the size of the underlying graphs, any "correlation" thus obtained is apparent and artificial.

In this paper, we report our studies of the correlations between $\mathcal{E}_{SO}(G)$ and $\mathcal{E}(G)$ for the graphs G belonging to the class of trees with fixed number of vertices, and to the class of catacondensed benzenoids with fixed number of hexagons. As will be seen, our results are completely different from those in [7], and are somewhat surprising.

2 Comparing energy and Sombor energy of trees

Our calculations were done for the class of all trees and, separately, for all chemical trees with a fixed number n of vertices, $n = 4, 5, \ldots, 15$. Without a single exception, we observed the following regularities:

- The data pairs $(\mathcal{E}, \mathcal{E}_{SO})$ are grouped into mutually separated clusters. On each cluster the data points form a (nearly) straight line.
- The slopes of lines are negative, indicating that in the case of trees, there is a decreasing linear correlations between the Sombor energy and graph energy.
- The slopes of the lines are nearly equal, i.e., the lines are nearly parallel. The distances between lines are also nearly equal.
- Trees with equal nullity n_0 (equal number of zero eigenvalues [3]) belong to the same cluster. Trees with different nullity belong to different clusters.

In Tables 1 and 2 are collected some representative data for chemical trees and all trees. Fig. 1 provides an illustrative example for the case of all trees ($n = 8$).

n	A	B	C	R
8	-7.01	-3.00	93.03	0.881
9	-6.70	-3.03	102.93	0.855
10	-6.71	-2.79	114.89	0.861
11	-6.89	-2.99	130.02	0.866
12	-6.60	-2.73	138.05	0.851
13	-6.76	-2.86	152.98	0.856
14	-6.59	-2.71	162.41	0.850
15	-6.70	-2.78	176.68	0.852

Table 1. The parameters in the approximate formula $\mathcal{E}_{SO} = A\,\mathcal{E} + B\,n_0 + C$ for chemical trees with n vertices. Note that A and B are both negative-valued and almost independent of n, whereas C increases with n. R = correlation coefficient.

n	A	B	C	R
8	-7.21	-3.14	95.01	0.967
9	-8.16	-3.84	118.93	0.965
10	-8.01	-3.53	130.77	0.960
11	-8.52	-3.91	152.00	0.957
12	-8.38	-3.71	164.28	0.952
13	-8.64	-3.90	183.05	0.951
14	-8.53	-3.77	195.83	0.947
15	-8.65	-3.85	212.85	0.946

Table 2. Same data as in Table 1 for all trees with n vertices.

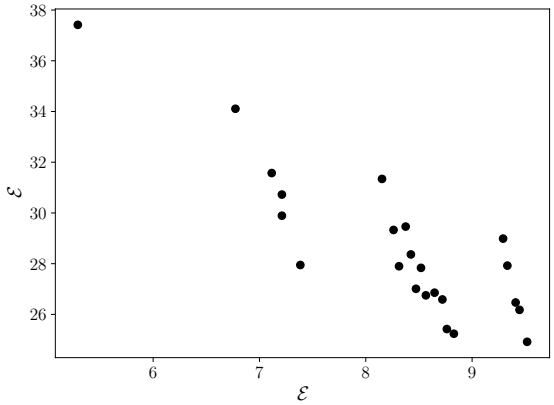

Fig. 1. Sombor energy plotted versus energy for the set of trees with 8 vertices. Each line pertains to trees with equal nullity $n_0 = 4, 2, 0$ from left to right. The outlier in the upper left corner corresponds to the star (whose nullity is 6).

3 Comparing energy and Sombor energy of catacondensed benzenoids

Our calculations were done for the class of all catacondensed benzenoid systems with a fixed number h of hexagons, $h = 6, 7, \ldots, 10$. Recall that these have $4h + 2$ vertices and $5h + 1$ edges [11]. Without a single exception, we observed the following regularities:

- The data pairs $(\mathcal{E}, \mathcal{E}_{SO})$ are grouped into mutually separated clusters. On each cluster the data points form a (nearly) straight line.
- The slopes of lines are positive, indicating that in the case of benzenoids, there is an increasing linear correlation between the Sombor energy and graph energy.
- The slopes of the lines are nearly equal, i.e., the lines are nearly parallel. However, the distances between lines are not equal.
- Catacondensed benzenoids belonging to the same cluster have equal bay numbers b (= number of edges on the boundary, connecting two vertices of degree 3 [11]). However, there exist several clusters, pertaining to the same bay number.
- In the examples studied by us, we find that not more than two clusters pertain to the same bay number. Nevertheless, it may be that for larger h-values, the number of such clusters will be greater than two.
- The clusters with equal b-value lie close to each other. The structural parameter determining to which cluster a catacondensed species belongs seems to be the existence and number of branching hexagons (hexagons attached to three other hexagons [11]).
- We thus conjecture that each cluster contains catacondensed benzenoids with equal b-value and equal number of branching hexagons. In addition, it may be that there will be no two clusters containing species with equal b-value and equal number of branching hexagons.
- In harmony with the previous conjecture, the cluster (line) with greater $\mathcal{E}$-value consists of maximally branched catacondensed benzenoid systems (which, in the same time, have maximal number of Kekulé structures [10, 14]).

Fig. 2 provides an illustrative example for the above stated regularities ($h = 8$).

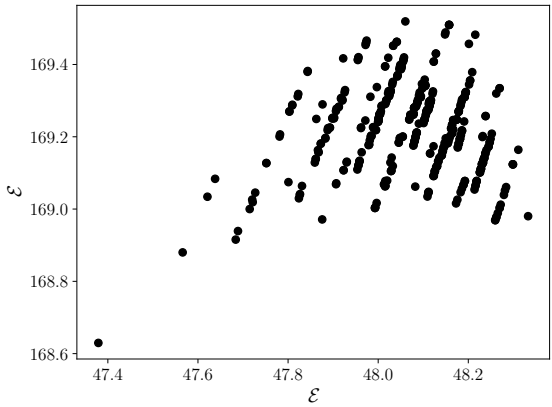

Fig. 2. Sombor energy plotted versus energy for the set of catacondensed benzenoid molecules with 8 hexagons. Each line pertains to systems with equal number of bay regions. The bay numbers assume ten different values $0, 1, 2, \ldots, 9$ whereas there are 15 lines (of which the most right one consists of a single point), and one outlier. The outlier in the lower left corner corresponds to the linear polyacene (whose bay number is zero). The isolated point on the right–hand side corresponds to the (unique) species with three branching hexagons.

4 Concluding remarks

The observations presented in the previous two sections show that the relation between energy and Sombor energy is completely different for trees and for (polycyclic) benzenoid molecules.

Rationalizing this relation in the case of trees is relatively straightforward. It is known that energy decreases with increasing branching, whereas by increasing branching the vertex degrees increase and therefore both the Sombor index and the Sombor energy increase. In addition, the energy is known to decrease with increasing nullity, whereas there is no reason why the Sombor index and its energy should be sensitive to the n_0-value.

To case of catacondensed benzenoids seems to be more perplexed. One should first observe (and it is easy to prove) that all catacondensed benzenoids with fixed h and b values, have same Sombor indices. Thus, the species belong to the same cluster have equal SO-value.

That the E_{SO}-value depends on the bay number (and increases with it) is related to the fact that the number of (3-3)-type edges is equal to $h + b - 1$ [11], and these edges contribute most to E_{SO}. The fact that species with equal b-value still may have

quite different Sombor energies is less easy to understand. Since the energy of benzenoid molecules (linearly) increases with the number of Kekulé structure [11], we arrive at a surprising conclusion that also the Sombor energy of catacondensed benzenoid molecules depends on, and increases with, their Kekulé structure count.

All conclusions and conjectures stated in this paper are based on our numerical studies and are purely empirical. We invite colleagues to prove mathematical confirmations (or refutations) for our claims, and trust that this will happen soon.

Acknowledgement. Izudin Redžepović was supported by the Serbian Ministry of Education, Science and Technological Development (Grant No. 451-03-9/2021-14/200122).

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