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Sombor Energy of Hexacyclic Systems

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Abstract

The paper is concerned with hexacyclic systems (F_n) and their Möbius counterparts (M_n). Continuing the studies in *MATCH Commun. Math. Comput. Chem.* **94** (2025) 477, the characteristic polynomial and the eigenvalues of the Sombor matrix of F_n and M_n, and the respective Sombor energies are determined. Upper and lower bounds for the Sombor energy in terms of the number of hexagons are also obtained.

1 Introduction

Let G be a simple graph with vertex set $\mathbf{V}(G)$ and edges set $\mathbf{E}(G)$, and let $uv \in \mathbf{E}(G)$ be the edge connecting the vertices $u, v \in \mathbf{V}(G)$. Let $d(u)$ be the degree (= number of first neighbors) of the vertex $u \in \mathbf{V}(G)$.

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In present-day mathematical chemistry, a large number of graph invariants of the form

$$TI = TI(G) = \sum_{uv \in \mathbf{E}(G)} \varphi\big(d(u), d(v)\big) \tag{1}$$

is being studied, where φ is an appropriately chosen function. These are referred to as *vertex-degree-based* (VDB) or *bond incidence degree* (BID) topological indices [17,19,34]. Among them, the recently conceived *Sombor index*, defined as [9]

$$SO = SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d(u)^2 + d(v)^2}$$

attracted much attention. This VDB molecular structure descriptor is based on geometric considerations [9, 12, 16, 21]. Of its several noteworthy applications we mention here just a few [1, 2, 15, 30–33]. Results of its mathematical investigations are found in the review [22].

The structure of the molecular graphs called here hexacyclic systems (F_n) and their Möbius counterparts (M_n) was described in detail in the preceding paper [26], and illustrated in its Figure 1. The underlying benzenoid systems are usually referred to as cylindrical (Hückel) and Möbius polyacenes. The Hückel molecular orbital theory of these conjugated species was studied in detail in the early days of mathematical chemistry. The adjacency spectrum of F_n was first determined by Derflinger and Sofer [5] (see also [8, 23, 28]), whereas that of M_n by Polansky [28]. The Laplacian and signless Laplacian spectra of F_n and M_n were recently studied by the present authors in [26]. For some earlier work along the same lines see [24].

If n denotes the number of hexagons of F_n and M_n, then it is easy to see that $|\mathbf{V}(F_n)| = |\mathbf{V}(M_n)| = 4n$ and $|\mathbf{E}(F_n)| = |\mathbf{E}(M_n)| = 5n$. Both F_n and M_n possess only vertices of degree 2 and 3. Of their edges, $4n$ connect vertices of degree 2 and 3, and n connect two vertices of degree 3. Therefore, for any VDB topological index of type (1),

$$TI(F_n) = TI(M_n) = 4n\,\varphi(2,3) + n\,\varphi(3,3)$$

and thus

$$SO(F_n) = SO(M_n) = 4n\sqrt{2^2+3^2} + n\sqrt{3^2+3^2}\,.$$

This means that VDB topological indices cannot distinguish between a hexacyclic system and its Möbuis counterpart. As will be seen below, this is not the case with the spectra of VDB matrices. For this reason, in this paper we study the spectrum of the Sombor matrix of F_n and M_n, which encodes the structural differences between these molecular graphs.

Let the vertices of the graph G be labeled by $v_1, v_2, \ldots, v_N$. Then the matrix pertaining to the VDB topological matrix $TI(G)$, given by Eq. (1), is the square matrix of order N, whose (i,j)-element is defined as

$$\begin{cases} \varphi\big(d(v_i), d(v_j)\big) & \text{if } \; v_iv_j \in \mathbf{E}(G) \\ 0 & \text{if } \; v_iv_j \notin \mathbf{E}(G) \\ 0 & \text{if } \; i=j\,. \end{cases}$$

Then the *Sombor matrix* $\mathbf{SO} = \mathbf{SO}(G)$ is defined via its (i,j)-elements as

$$\begin{cases} \sqrt{d(v_i)^2 + d(v_j)^2} & \text{if } \; v_iv_j \in \mathbf{E}(G) \\ 0 & \text{if } \; v_iv_j \notin \mathbf{E}(G) \\ 0 & \text{if } \; i=j\,. \end{cases}$$

The concept of Sombor matrix was put forward soon after the Sombor topological index was introduced [6,10,35], and was eventually investigated by numerous authors, see e.g., [20,27,29]. In all those papers the emphasis was put on its spectral properties, eigenvalues and energy in particular.

2 Spectral properties of the Sombor matrix of hexacyclic systems

Our main result is computation of the characteristic polynomial of the Sombor matrix of hexacyclic systems, which is different for F_n and M_n. It is given in the following theorem.

Theorem 1. *(i) The characteristic polynomial of the Sombor matrix of the hexacyclic system F_n with $n > 1$ hexagons is given by*

$$P_{F_n}(\mu) = \prod_{j=1}^{n} \left(\left(\mu^2 - 3\sqrt{2}\mu - 26 - 26\cos\left(\frac{2\pi j}{n}\right) \right) \times \right.$$
$$\left. \times \left(\mu^2 + 3\sqrt{2}\mu - 26 - 26\cos\left(\frac{2\pi j}{n}\right) \right) \right).$$

(ii) The characteristic polynomial of the Sombor matrix of the Möbius hexacyclic system M_n with $n > 1$ hexagons is given by

$$P_{M_n}(\nu) = \prod_{j=0}^{2n-1} \left(\nu^2 - (-1)^j \, 3\sqrt{2}\nu - 26 - 26\cos\frac{\pi j}{n} \right).$$

From the characteristic polynomials $P_{F_n}(\mu)$ and $P_{M_n}(\nu)$, the spectrum of matrices $\mathbf{SO}(F_n)$ and $\mathbf{SO}(M_n)$ follows immediately:

Corollary 1. *The spectrum of the Sombor matrix of F_n is given by $S = S_1 \cup S_2$, where*

$$S_1 = \left\{ \mu_{1,j}^{\pm} = \frac{\sqrt{2}}{2} \left(3 \pm \sqrt{61 + 52\cos\left(\frac{2\pi j}{n}\right)} \right) : j = 1, \ldots, n \right\},$$
$$S_2 = \left\{ \mu_{2,j}^{\pm} = \frac{\sqrt{2}}{2} \left(-3 \pm \sqrt{61 + 52\cos\left(\frac{2\pi j}{n}\right)} \right) : j = 1, \ldots, n \right\}.$$

Corollary 2. *The spectrum of the Sombor matrix of M_n is given by $T = T_1 \cup T_2$, where*

$$T_1 = \left\{ \nu_{1,j}^{\pm} = \frac{\sqrt{2}}{2} \left(3 \pm \sqrt{61 + 52\cos\left(\frac{2\pi j}{n}\right)} \right) : j = 0, \ldots, n-1 \right\},$$
$$T_2 = \left\{ \nu_{2,j}^{\pm} = \frac{\sqrt{2}}{2} \left(-3 \pm \sqrt{61 + 52\cos\left(\frac{(2j+1)\pi}{n}\right)} \right) : j = 0, \ldots, n-1 \right\}.$$

In what follows, using the spectra of $\mathbf{SO}(F_n)$ and $\mathbf{SO}(M_n)$, we compute the respective Sombor energies, which happen to have different values. In addition, we will deduce upper and lower bounds for the Sombor energy of F_n and M_n in terms of number n of hexagons. We conclude the paper with numerical calculations of these energies.

In order to prove Theorem 1, some preparation is needed.

3 Preparatory notes

We start by recalling the vertex labeling of the graphs F_n and M_n, described in [23] (see also Figure 1 in [26]).

The number of vertices of F_n and M_n is $4n$ and the number of edges is $5n$. The set of vertices $\mathbf{V}(F_n)$ is written as $\mathbf{V}(F_n) = X_1 \cup X_2 \cup Y_1 \cup Y_2$, where

$$X_1 = \{1, 3, 5, \ldots, 2n-1\}, \quad X_2 = \{1', 3', 5', \ldots, (2n-1)'\},$$
$$Y_1 = \{2, 4, 6, \ldots, 2n\}, \qquad Y_2 = \{2', 4', 6', \ldots, (2n)'\}.$$

Therefore, the adjacency matrix of F_n is given by

$$A(F_n) = \begin{pmatrix} \mathbf{0} & \mathbf{I}_n & \mathbf{C}^T & \mathbf{0} \\ \mathbf{I}_n & \mathbf{0} & \mathbf{0} & \mathbf{C}^T \\ \mathbf{C} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C} & \mathbf{0} & \mathbf{0} \end{pmatrix},$$

where the matrix $\mathbf{C}$ is such that $\mathbf{C}^T$ is the incidence matrix of the cycle C_n. The degree of all vertices in $X_1 \cup X_2$ is 3, whereas the degree of vertices in $Y_1 \cup Y_2$ is 2. Hence

$$\mathbf{SO}(F_n) = \begin{pmatrix} \mathbf{0} & 3\sqrt{2}\mathbf{I}_n & \sqrt{13}\mathbf{C}^T & \mathbf{0} \\ 3\sqrt{2}\mathbf{I}_n & \mathbf{0} & \mathbf{0} & \sqrt{13}\mathbf{C}^T \\ \sqrt{13}\mathbf{C} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \sqrt{13}\mathbf{C} & \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

By using the same vertex labeling as in the case of F_n, the adjacency matrix of M_n can be written as

$$A(M_n) = \begin{pmatrix} \mathbf{0}_n & \mathbf{I}_n & \mathbf{D}^T \\ \mathbf{I}_n & \mathbf{0}_n & \\ \mathbf{D} & & \mathbf{0}_{2n} \end{pmatrix},$$

where

$$\mathbf{D}^T = \begin{pmatrix} 1 & 0 & 0 & & & 1 \\ 1 & 1 & 0 & & & \\ 0 & 1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & 1 & 1 & 0 \\ 0 & & & 0 & 1 & 1 \end{pmatrix}_{2n}.$$

Using the values for degrees, it follows that

$$\mathbf{SO}(M_n) = \begin{pmatrix} \mathbf{0}_n & 3\sqrt{2}\mathbf{I}_n & \sqrt{13}\mathbf{D}^T \\ 3\sqrt{2}\mathbf{I}_n & \mathbf{0}_n & \\ \sqrt{13}\mathbf{D} & & \mathbf{0}_{2n} \end{pmatrix}.$$

3.1 Circulant matrices

Circulant matrices of order n are matrices of the type

$$S = \begin{pmatrix} s_0 & s_1 & \dots & s_{n-2} & s_{n-1} \\ s_{n-1} & s_0 & \dots & s_{n-3} & s_{n-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ s_2 & s_3 & \dots & s_0 & s_1 \\ s_1 & s_2 & \dots & s_{n-1} & s_0 \end{pmatrix}. \qquad (2)$$

Their eigenvalues are well-known and are described by the following Lemma [4].

Lemma 1. *Let S be a circulant matrix of order n. Then its eigenvalues are*

$$\lambda_j = s_0 + s_1\omega_j + s_2\omega_j^2 + \cdots + s_{n-1}\omega_j^{n-1},$$

for $j = 0, 1, \ldots, n-1$, *and*

$$\det(S) = \prod_{j=0}^{n-1} \left(s_0 + s_1\omega_j + s_2\omega_j^2 + \cdots + s_{n-1}\omega_j^{n-1} \right),$$

where $\omega_j = e^{\frac{2\pi i j}{n}}$ *is the* n*-th root of unity.*

4 Proof of Theorem 1

In this section we prove our main result. This will be done in two parts. In Section 4.1 we evaluate the characteristic polynomial of the matrix $\mathbf{SO}(F_n)$, whereas in Section 4.2 we compute the characteristic polynomial od the matrix $\mathbf{SO}(M_n)$.

4.1 The spectrum of the Sombor matrix of F_n

From the definition of the characteristic polynomial of $\mathbf{SO}(F_n)$ we have

$$P_{F_n}(\mu) = \det(\mu\, \mathbf{I}_{4n} - \mathbf{SO}(F_n)),$$

hence

$$\begin{aligned} P_{F_n}(\mu) &= \det \begin{pmatrix} \mu\mathbf{I}_n & -3\sqrt{2}\mathbf{I}_n & -\sqrt{13}\mathbf{C}^T & \mathbf{0} \\ -3\sqrt{2}\mathbf{I}_n & \mu\mathbf{I}_n & \mathbf{0} & -\sqrt{13}\mathbf{C}^T \\ -\sqrt{13}\mathbf{C} & \mathbf{0} & \mu\mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & -\sqrt{13}\mathbf{C} & \mathbf{0} & \mu\mathbf{I}_n \end{pmatrix} \\ &= \det \begin{pmatrix} -\mu\mathbf{I}_n & 3\sqrt{2}\mathbf{I}_n & \sqrt{13}\mathbf{C}^T & \mathbf{0} \\ 3\sqrt{2}\mathbf{I}_n & -\mu\mathbf{I}_n & \mathbf{0} & \sqrt{13}\mathbf{C}^T \\ \sqrt{13}\mathbf{C} & \mathbf{0} & -\mu\mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & \sqrt{13}\mathbf{C} & \mathbf{0} & -\mu\mathbf{I}_n \end{pmatrix}. \end{aligned}$$

Using the following property of the determinant of the block matrix consisting of four matrices A_j, $j = 1, 2, 3, 4$

$$\det\left(\begin{pmatrix} A_1 & A_2 \\ A_3 & A_4 \end{pmatrix}\right) = \det\left(A_1 - A_2A_4^{-1}A_3\right)\det(A_4) \tag{3}$$

we deduce that

$$P_{F_n}(\mu) = \det\left(\begin{pmatrix} -\mu\mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & -\mu\mathbf{I}_n \end{pmatrix}\right) \det\left(\begin{pmatrix} -\mu\mathbf{I}_n & 3\sqrt{2}\mathbf{I}_n \\ 3\sqrt{2}\mathbf{I}_n & -\mu\mathbf{I}_n \end{pmatrix}\right.$$

$$\left. -13\begin{pmatrix} \mathbf{C}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^T \end{pmatrix}\begin{pmatrix} -\mu\mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & -\mu\mathbf{I}_n \end{pmatrix}^{-1}\begin{pmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{C} \end{pmatrix}\right).$$

By performing simple calculations using properties of determinants, we get

$$\begin{aligned}
P_{F_n}(\mu) =& \mu^{2n} \det\left(\begin{pmatrix} -\mu\mathbf{I}_n & 3\sqrt{2}\mathbf{I}_n \\ 3\sqrt{2}\mathbf{I}_n & -\mu\mathbf{I}_n \end{pmatrix} + \frac{13}{\mu}\begin{pmatrix} \mathbf{C}^T\mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^T\mathbf{C} \end{pmatrix}\right) \\
=& \mu^{2n} \det\left(\begin{pmatrix} -\mu\mathbf{I}_n + \frac{13}{\mu}\mathbf{C}^T\mathbf{C} & 3\sqrt{2}\mathbf{I}_n \\ 3\sqrt{2}\mathbf{I}_n & -\mu\mathbf{I}_n + \frac{13}{\mu}\mathbf{C}^T\mathbf{C} \end{pmatrix}\right) \\
=& \mu^{2n} \det\left(\left(\mu - 3\sqrt{2}\right)\mathbf{I}_n - \frac{13}{\mu}\mathbf{C}^T\mathbf{C}\right) \times \\
& \times \det\left(\left(\mu + 3\sqrt{2}\right)\mathbf{I}_n - \frac{13}{\mu}\mathbf{C}^T\mathbf{C}\right) \\
=& 13^{2n} \det\left(\frac{1}{13}\mu\left(\mu - 3\sqrt{2}\right)\mathbf{I}_n - \mathbf{C}^T\mathbf{C}\right) \times \\
& \times \det\left(\frac{1}{13}\mu\left(\mu + 3\sqrt{2}\right)\mathbf{I}_n - \mathbf{C}^T\mathbf{C}\right).
\end{aligned}$$

Now, we recall a result from [3], in which it is proved that the signless Laplacian matrix $Q(C_n)$ associated to the cycle C_n with n vertices can be expressed as

$$Q(C_n) = \mathbf{C}^T\mathbf{C}, \tag{4}$$

where $\mathbf{C}$ is such that $\mathbf{C}^T$ is the incidence matrix of the cycle C_n. Therefore,

$$P_{F_n}(\mu) = 13^{2n} \det\left(\frac{1}{13}\mu\left(\mu - 3\sqrt{2}\right)\mathbf{I}_n - Q(C_n)\right) \times$$

$$\times \det\left(\frac{1}{13}\mu\left(\mu + 3\sqrt{2}\right)\mathbf{I}_n - Q(C_n)\right)$$

$$= 13^{2n} Q_{C_n}\left(\frac{1}{13}\mu\left(\mu - 3\sqrt{2}\right)\right) Q_{C_n}\left(\frac{1}{13}\mu\left(\mu + 3\sqrt{2}\right)\right).$$

According to [23, Lemma 2.3.], the characteristic polynomial of $Q(C_n)$ is of the form

$$Q_{C_n}(\lambda) = \det(\lambda \mathbf{I}_n - Q(C_n)) = \prod_{j=1}^{n}\left(\lambda - 2 - 2\cos\left(\frac{2\pi j}{n}\right)\right), \qquad (5)$$

which implies

$$P_{F_n}(\mu) = \prod_{j=1}^{n}\left(\mu\left(\mu - 3\sqrt{2}\right) - 2 - 2\cos\left(\frac{2\pi j}{n}\right)\right) \times$$

$$\times \left(\mu\left(\mu + 3\sqrt{2}\right) - 2 - 2\cos\left(\frac{2\pi j}{n}\right)\right).$$

This proves the first part of Theorem 1.

4.2 The spectrum of the Sombor matrix of M_n

The characteristic polynomial of the Sombor matrix of M_n is

$$P_{M_n}(\nu) = \det(\nu\,\mathbf{I}_{4n} - \mathbf{SO}(M_n)). \qquad (6)$$

In order to compute $P_{M_n}(\nu)$, we will use properties of circulant matrices. Namely, by definition

$$P_{M_n}(\nu) = \det\begin{pmatrix} \nu\mathbf{I}_n & -3\sqrt{2}\mathbf{I}_n & \multicolumn{2}{c}{-\sqrt{13}\mathbf{D}^T} \\ -3\sqrt{2}\mathbf{I}_n & \nu\mathbf{I}_n & & \\ \multicolumn{2}{c}{-\sqrt{13}\mathbf{D}} & \multicolumn{2}{c}{\nu\mathbf{I}_{2n}} \end{pmatrix}.$$

Using the identity (3), it follows that

$$
\begin{aligned}
P_{M_n}(\nu) &= \nu^{2n}\det\left(\begin{pmatrix} \nu\mathbf{I}_n & -3\sqrt{2}\mathbf{I}_n \\ -3\sqrt{2}\mathbf{I}_n & \nu\mathbf{I}_n \end{pmatrix} - \frac{13}{\nu}\mathbf{D}^T\mathbf{D}\right) \\
&= 13^{2n}\det\left(\begin{pmatrix} \frac{1}{13}\nu^2\mathbf{I}_n & \frac{-3\sqrt{2}}{13}\nu\mathbf{I}_n \\ \frac{-3\sqrt{2}}{13}\nu\mathbf{I}_n & \frac{1}{13}\nu^2\mathbf{I}_n \end{pmatrix} - \mathbf{D}^T\mathbf{D}\right).
\end{aligned}
$$

It is straightforward to see that the matrix $\mathbf{D}^T\mathbf{D}$ is a circulant matrix of order $2n$, as well as the matrix

$$
\begin{pmatrix} \frac{1}{13}\nu^2\mathbf{I}_n & \frac{-3\sqrt{2}}{13}\nu\mathbf{I}_n \\ \frac{-3\sqrt{2}}{13}\nu\mathbf{I}_n & \frac{1}{13}\nu^2\mathbf{I}_n \end{pmatrix}.
$$

Thus, their difference is also a circulant matrix, equal to

$$
\begin{pmatrix}
\frac{\nu^2}{13}-2 & -1 & 0 & & 0 & \frac{-3\sqrt{2}\nu}{13} & & & -1 \\
-1 & \frac{\nu^2}{13}-2 & -1 & & 0 & 0 & \frac{-3\sqrt{2}\nu}{13} & & 0 \\
 & & \ddots & \ddots & & & & \ddots & \\
0 & & -1 & \frac{\nu^2}{13}-2 & -1 & & & 0 & \frac{-3\sqrt{2}\nu}{13} \\
\frac{-3\sqrt{2}\nu}{13} & & & -1 & \frac{\nu^2}{13}-2 & -1 & & & 0 \\
 & \frac{-3\sqrt{2}\nu}{13} & & & -1 & \frac{\nu^2}{13}-2 & -1 & & \\
 & & \ddots & & & & \ddots & \ddots & \\
0 & & & \frac{-3\sqrt{2}\nu}{13} & & & -1 & \frac{\nu^2}{13}-2 & -1 \\
-1 & & & & \frac{-3\sqrt{2}\nu}{13} & & & -1 & \frac{\nu^2}{13}-2
\end{pmatrix}.
$$

This is the circulant matrix of the form (2) with $s_0 = \frac{\nu^2}{13} - 2$, $s_1 = -1$, $s_n = \frac{-3\sqrt{2}\nu}{13}$, $s_{2n-1} = -1$ and $s_j = 0$ for all $j \neq 0, 1, n, 2n-1$. Therefore, Lemma 1 yields that

$$
\begin{aligned}
P_{M_n}(\nu) &= 13^{2n}\prod_{j=0}^{2n-1}\left(\frac{1}{13}\nu^2 - 2 - \frac{3\sqrt{2}}{13}(-1)^j\nu - 2\cos\frac{\pi j}{n}\right) \\
&= \prod_{j=0}^{2n-1}\left(\nu^2 - (-1)^j 3\sqrt{2}\nu - 26 - 26\cos\frac{\pi j}{n}\right).
\end{aligned}
$$

This completes the proof of the second part of Theorem 1.

5 Sombor energy of F_n and M_n

In this section, we derive expressions for the Sombor energy of hexacyclic systems F_n and M_n and provide upper and lower bounds for their values, depending on the number n of hexagons.

Recall that the ordinary energy of a graph G, introduced in 1978 [7], is the sum of absolute values of the eigenvalues of the adjacency matrix of G [18]. Eventually, the concept of graph energy was extended to other graph matrices. Thus, the energy of the graph matrix $\mathbf{M}(G)$ is defined as the sum of the absolute values of the eigenvalues of $\mathbf{M}(G)$ [11, 14]. More generally, the energy of the graph matrix $\mathbf{M}(G)$ is the sum of singular values of $\mathbf{M}(G)$ [25].

Therefore, the Sombor energy of F_n and M_n are given by

$$E_{SO}(F_n) = \sum_{k=1}^{4n} |\mu_k|$$

and

$$E_{SO}(M_n) = \sum_{k=1}^{4n} |\nu_k|$$

where μ_k and ν_k are the eigenvalues of the matrices $\mathbf{SO}(F_n)$ and $\mathbf{SO}(M_n)$, specified in Corollaries 1 and 2.

Corollary 3. *The Sombor energy of the hexacyclic system graph F_n is given by*

$$E_{SO}(F_n) = 2\sqrt{2}\sum_{j=1}^{n} \sqrt{61 + 52\cos\left(\frac{2\pi j}{n}\right)}. \tag{7}$$

Proof. The proof follows from the expressions for the eigenvalues, Corollary 1, by paring the eigenvalues $\mu^+_{k,j}$ and $\mu^-_{k,j}$ for $k = 1, 2$ and $j = 1, \ldots, n$. ∎

In a fully analogous manner, using Corollary 2, we arrive at:

Corollary 4. *The Sombor energy of the hexacyclic system graph M_n is given by*

$$E_{SO}(M_n) = \sqrt{2} \sum_{j=0}^{2n-1} \sqrt{61 + 52\cos\left(\frac{\pi j}{n}\right)}. \tag{8}$$

We now derive upper and lower bounds for the energies $E_{SO}(F_n)$ and $E_{SO}(M_n)$. Our starting point is the following lemma.

Lemma 2. *For real numbers a,b, such that $a > b > 0$ and integers $n \geq 1$, we have the following upper and lower bounds*

$$\left(\sqrt{\frac{a-b}{2}} + \frac{2\sqrt{b}}{\pi}\right) - \frac{\sqrt{b}}{n} \leq \frac{1}{n} \sum_{j=0}^{n-1} \sqrt{a + b\cos\left(\frac{2\pi j}{n}\right)} \leq \sqrt{a} \tag{9}$$

and

$$\left(\sqrt{\frac{a-b}{2}} + \frac{2\sqrt{b}}{\pi}\right) - \frac{\sqrt{b}}{2n} \leq \frac{1}{2n} \sum_{j=0}^{2n-1} \sqrt{a + b\cos\left(\frac{\pi j}{n}\right)} \leq \sqrt{a}\,. \tag{10}$$

Proof. First, we prove the right–hand side of (9). The Cauchy–Schwarz inequality

$$\left(\sum_{i=1}^{n} a_i\, b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right),$$

directly implies

$$\left(\sum_{j=1}^{n} \sqrt{a + b\cos\left(\frac{2\pi j}{n}\right)}\right)^2 \leq n \sum_{j=1}^{n} \left(a + b\cos\left(\frac{2\pi j}{n}\right)\right).$$

Since

$$\sum_{j=1}^{n} \cos\left(\frac{2\pi j}{n}\right) = 0$$

it follows that

$$\left(\sum_{j=1}^{n} \sqrt{a + b\cos\left(\frac{2\pi j}{n}\right)}\right)^2 \leq an^2$$

which proves the right–hand side of (9).

In order to prove the lower bound in (9), we start with the inequality

$$\sqrt{x^2+y^2} \geq \frac{|x|+|y|}{\sqrt{2}}$$

between the quadratic and arithmetic means, from which it follows

$$\begin{aligned}\sqrt{a+b\cos\left(\frac{2\pi j}{n}\right)} &= \sqrt{a-b+2b\cos^2\left(\frac{\pi j}{n}\right)} \\ &\geq \frac{1}{\sqrt{2}}\left(\sqrt{a-b}+\sqrt{2b}\left|\cos\left(\frac{\pi j}{n}\right)\right|\right).\end{aligned}$$

Therefore,

$$\frac{1}{n}\sum_{j=0}^{n-1}\sqrt{a+b\cos\left(\frac{2\pi j}{n}\right)} \geq \sqrt{\frac{a-b}{2}}+\frac{\sqrt{b}}{n}\sum_{j=0}^{n-1}\left|\cos\left(\frac{\pi j}{n}\right)\right|. \qquad (11)$$

Next, using trigonometric identities, it is easy to establish that

$$\sum_{j=0}^{n-1}\left|\cos\left(\frac{\pi j}{n}\right)\right| = \sum_{j=0}^{n}\left|\cos\left(\frac{\pi j}{n}\right)\right| - 1 = 2\sum_{j=0}^{\lfloor (n-1)/2\rfloor}\cos\left(\frac{\pi j}{n}\right) - 1, \qquad (12)$$

where $\lfloor x\rfloor$ denotes the integer part of the real number x. Now, we use that

$$2\cos\left(\frac{\pi j}{n}\right) = e^{i\frac{\pi j}{n}} + e^{-i\frac{\pi j}{n}}$$

and use the formula for the geometric sequence partial sum to get

$$2\sum_{j=0}^{\lfloor (n-1)/2\rfloor}\cos\left(\frac{\pi j}{n}\right) = \frac{1-e^{i\frac{\pi}{n}(\lfloor (n-1)/2\rfloor+1)}}{1-e^{i\frac{\pi}{n}}} + \frac{1-e^{-i\frac{\pi}{n}(\lfloor (n-1)/2\rfloor+1)}}{1-e^{-i\frac{\pi}{n}}},$$

which is equivalent to

$$2\sum_{j=0}^{\lfloor (n-1)/2\rfloor} \cos\left(\frac{\pi j}{n}\right) = 1 - \frac{\cos\left(\frac{\pi}{n}\left(\lfloor\frac{n-1}{2}\rfloor+1\right)\right) - \cos\left(\frac{\pi}{n}\lfloor\frac{n-1}{2}\rfloor\right)}{1-\cos\left(\frac{\pi}{n}\right)}$$
$$= 1 + \frac{\sin\left(\frac{\pi}{2n}\left(2\lfloor\frac{n-1}{2}\rfloor+1\right)\right)}{\sin\left(\frac{\pi}{2n}\right)},$$

where the last identity was deduced by applying trigonometric identities.

When n is odd, it is easy to see that

$$\sin\left(\frac{\pi}{2n}\left(2\lfloor\tfrac{n-1}{2}\rfloor+1\right)\right) = \sin(\pi/2) = 1\,,$$

whereas for even n, one gets

$$\sin\left(\frac{\pi}{2n}\left(2\lfloor\tfrac{n-1}{2}\rfloor+1\right)\right) = \sin(\pi/2-\pi/(2n)) = \cos(\pi/(2n))\,.$$

Therefore, for all n, using the inequalities

$$\sin\left(\frac{\pi}{2n}\right) \le \frac{\pi}{2n} \quad , \quad \cos\left(\frac{\pi}{2n}\right) \ge 1 - \frac{1}{2}\left(\frac{\pi}{2n}\right)^2$$

and $1-\frac{\pi}{4n} \ge 0$, we get

$$2\sum_{j=0}^{\lfloor\frac{n-1}{2}\rfloor} \cos\left(\frac{\pi j}{n}\right) \ge 1 + \frac{\cos\left(\frac{\pi}{2n}\right)}{\sin\left(\frac{\pi}{2n}\right)} \ge 1 + \frac{2n}{\pi}\left(1-\frac{1}{2}\left(\frac{\pi}{2n}\right)^2\right) \ge \frac{2n}{\pi}.$$

Combining the above expression with (11) and (12) yields

$$\frac{1}{n}\sum_{j=0}^{n-1}\sqrt{a+b\cos\left(\frac{2\pi j}{n}\right)} \ge \sqrt{\frac{a-b}{2}} + \frac{\sqrt{b}}{n}\left(\frac{2n}{\pi}-1\right).$$

This proves the left–hand side of (9).

The proof of (10) is carried out in an analogous manner and will be omitted. ■

By setting $a=61$ and $b=52$ in the above lemma, in view of expressions (7) and (8), we arrive at the following corollary.

Corollary 5. *The Sombor energies of F_n and M_n are bounded as*

$$\left(6+\frac{4\sqrt{104}}{\pi}\right)n-\frac{4\sqrt{26}}{n}\leq E_{SO}(F_n)\leq 2\sqrt{122}\,n$$

and

$$\left(6+\frac{4\sqrt{104}}{\pi}\right)n-\frac{4\sqrt{26}}{2n}\leq E_{SO}(M_n)\leq 2\sqrt{122}\,n\,.$$

6 Numerical work

Based on the above established formulas, we calculated Sombor energies of F_n and M_n, as well as their bounds, for some selected values of n. The respective numerical values are given in Tables 1 and 2. We see that the relative errors of the upper and lower bounds are around 6.1% and 8.8%, respectively.

n	$E_{SO}(F_n)$	$E_{SO}(M_n)$
2	38.55187	41.36666
3	63.53299	62.39095
4	82.73332	83.25649
5	104.34040	104.08698
6	124.78190	124.90861
7	145.79251	145.72786
8	166.51298	166.54644
9	187.38234	187.36484
10	208.17396	208.18318
11	229.00640	229.00151
12	249.81722	249.81983
13	270.63955	270.63815
14	291.45572	291.45647
15	312.27519	312.27479
16	333.09289	333.09311
17	353.91154	353.91143
18	374.72968	374.72974
19	395.54810	395.54806
20	416.36636	416.36638

Table 1. Sombor energies of the hexacyclic systems F_n and M_n.

n	$\left(6+\frac{4\sqrt{104}}{\pi}\right)n-\frac{4\sqrt{26}}{n}$	$E_{SO}(F_n)$	$2\sqrt{122}\,n$
20	378.67113	416.36636	441.81444
25	473.79782	520.45798	552.26805
30	568.85653	624.54957	662.72166
35	663.87638	728.64117	773.17527
40	758.87196	832.73276	883.62888
45	853.85135	936.82436	994.08249
50	948.81941	1040.91596	1104.53610
55	1043.77922	1145.00755	1214.98971
60	1138.73286	1249.09915	1325.44332
65	1233.68174	1353.19074	1435.89693
70	1328.62689	1457.28234	1546.35054
75	1423.56904	1561.37393	1656.80415
80	1518.50877	1665.46553	1767.25776
85	1613.44650	1769.55713	1877.71137
90	1708.38257	1873.64872	1988.16498
95	1803.31723	1977.74032	2098.61859
100	1898.25070	2081.83191	2209.07220

Table 2. Sombor energy and its bounds for the hexacyclic system F_n.

From Table 1 we see that whenever the number of hexagons n is even, then the Sombor energy of the Möbius hexacyclic system M_n exceeds that of the ordinary hexacyclic system F_n, i.e., $E_{SO}(M_n) > E_{SO}(F_n)$. If n is odd, then the ordering of the Sombor energies is opposite, i.e., $E_{SO}(M_n) < E_{SO}(F_n)$.

In order to try to understand the cause of this regularity, note that the perimeter of M_n consists of a $(4n)$-sized cycle, whereas the perimeter of F_n is composed of two disjoint $(2n)$-cycles.

In the case of Sombor energy, certain Hückel-rule-type phenomena were established [13]. If the same apply also to the hexacyclic species, then the following situation could happen.

For odd $n = 2k+1$, the two perimeter cycles of F_n are of $(4k+2)$-type (that is, of size not divisible by 4), and therefore would have an increasing effect on Sombor energy. For even $n = 2k$, these cycles are of $(4k)$-type (that is, of size divisible by 4), having a decreasing effect on Sombor energy. The perimeter cycle of M_n is always of $(4k)$-type, but since its size is twice larger, its decreasing effect would be smaller.

It may be that such cyclic effects result in different ordering of Sombor energies of M_n and F_n for even and odd n. However, testing of this hypothesis would require more detailed, and more quantitative considerations, which remains a task for the future.

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