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Sombor Energy of a Graph with Self–Loops

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Abstract

This study aims to extend the notion of degree-based topological index, associated adjacency-type matrix and its energy from a simple graph to a graph with self-loops. Let G_S be a graph with k self-loops obtained from a simple graph G, we define Sombor index for G_S as $SO(G_S) = \sum_{v_i v_j \in X(G)} \sqrt{d_i^2(G_S) + d_j^2(G_S)} + \sqrt{2} \sum_{v_i \in S} d_i(G_S)$, where $S \subseteq V(G)$ having self-loop to each of its vertices in S. In addition we investigate some fundamental properties of Sombor eigenvalues, McClelland and Koolen-Moulton-type bound for Sombor energy of G_S. Also explores the correlation between Sombor energy of G_S and the total $\pi-$electron energies associated with the corresponding hetero-molecular systems.

1 Introduction

Let G be a simple connected graph of order n and size m with vertex set $V(G)$ and edge set $X(G)$. The degree d_i is the number of edges incident on the vertex v_i of G, for $1 \leq i \leq n$.

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Topological indices are graph invariants widely used for characterizing molecular graphs, predicting the biological activity of chemical compounds, establishing relationships between the structure and properties of molecules, and making their chemical applications. Any degree-based topological indices are of the form [9],

$$TI(G) = \sum_{v_i v_j \in X(G)} f(d_i, d_j). \tag{1}$$

where f is a suitably chosen symmetric function. In 2015, B. Furtula and I. Gutman defined a degree-based topological index called the forgotten index [5] as,

$$F(G) = \sum_{v_i v_j \in X(G)} [d_i^2 + d_j^2] = \sum_{v_i \in V(G)} d_i^3. \tag{2}$$

The Sombor matrix has its origin from the recently introduced topological index known as Sombor index [8], denoted by $SO(G)$, defined as,

$$SO(G) = \sum_{v_i v_j \in X(G)} \sqrt{d_i^2 + d_j^2}. \tag{3}$$

For the Sombor index, associated adjacency type matrix $A_F(G)$, called Sombor matrix [9] denoted as $A_{SO}(G)$, was defined by I. Gutman in 2021 as,

$$A_{SO}(G)_{ij} = \begin{cases} \sqrt{d_i^2 + d_j^2} & \text{if } v_i v_j \in X(G), \\ 0 & \text{if } v_i v_j \notin X(G), \\ 0 & \text{if } i = j. \end{cases}$$

Let $\sigma_1, \sigma_2, \ldots, \sigma_n$ be the eigenvalues of $A_{SO}(G)$, then the Sombor energy $En_{SO}(G)$ [9] is defined as,

$$En_{SO}(G) = \sum_{i=1}^{n} |\sigma_i|. \tag{4}$$

In the domain of spectral graph theory, energy of graph with self-loops was introduced recently by I. Gutman [12] in 2021. Let G_S be the graph with self-loops, obtained from a simple graph G, by attaching a self-loop to each of its vertices belonging to S, where $S \subseteq V(G)$ with $|S| = k$. Let $X(G_S)$ and $d_i(G_S)$ represent edge set of G_S and degree of vertex v_i in G_S, for $1 \leq i \leq n$ respectively. More on degree-based topological indices, energy of a graph with self-loops and terminologies refer [1,2,4,6,7,14–16].

Since self-loops distinguish hetero-atoms from carbon atoms in hetero-conjugated molecules [10, 11, 17, 18], the spectral aspect of a simple graph extended to a graph with self-loops opens up a new area of study for structural features and related chemical properties of molecules. Motivated by this, we now extend the degree-based topological index $TI(G)$ and associated matrix $A_F(G)$ from graph G to G_S.

In analogy with the degree-based topological index $TI(G)$ in Eq. (1), we define $TI(G_S)$ for G_S as,

$$TI(G_S) = \sum_{v_iv_j \in X(G)} f(d_i(G_S), d_j(G_S)) + \sum_{v_i \in S} f(d_i(G_S), d_i(G_S)). \tag{5}$$

Also define the matrix $A_F(G_S)$ associated with topological index $TI(G_S)$ as,

$$A_F(G_S)_{ij} = \begin{cases} f(d_i(G_S), d_j(G_S)) & \text{if } v_iv_j \in X(G), \\ 0 & \text{if } v_iv_j \notin X(G), \\ f(d_i(G_S), d_i(G_S)) & \text{if } i = j \text{ and } v_i \in S, \\ 0 & \text{if } i = j \text{ and } v_i \notin S. \end{cases}$$

From Eq. (5), forgotten index $F(G_S)$ and Sombor index $SO(G_S)$ for a graph G_S is defined as,

$$F(G_S) = \sum_{v_iv_j \in X(G)} [d_i^2(G_S) + d_j^2(G_S)] + 2 \sum_{v_i \in S} d_i^2(G_S) = \sum_{v_i \in V(G)} d_i^3(G_S). \tag{6}$$

$$SO(G_S) = \sum_{v_iv_j \in X(G)} \sqrt{d_i^2(G_S) + d_j^2(G_S)} + \sqrt{2}Q, \tag{7}$$

where $Q = \sum_{v_i \in S} d_i(G_S)$.

We define Sombor matrix $A_{SO}(G_S)$ as,

$$A_{SO}(G_S)_{ij} = \begin{cases} \sqrt{d_i^2(G_S) + d_j^2(G_S)} & \text{if } v_iv_j \in X(G), \\ 0 & \text{if } v_iv_j \notin X(G), \\ \sqrt{2}d_i(G_S) & \text{if } i = j \text{ and } v_i \in S, \\ 0 & \text{if } i = j \text{ and } v_i \notin S. \end{cases}$$

Let $\sigma_1(G_S), \sigma_2(G_S), \ldots, \sigma_n(G_S)$ be the eigenvalues of $A_{SO}(G_S)$. The Sombor energy of graph with self-loops is defined as,

$$En_{SO}(G_S) = \sum_{i=1}^{n} \left| \sigma_i(G_S) - \frac{\sqrt{2}Q}{n} \right|. \tag{8}$$

Let $t_i = \sigma_i(G_S) - \frac{\sqrt{2}Q}{n}$, $i = 1, 2, \ldots, n$, denote the auxiliary eigenvalues of $A_{SO}(G_S)$.

In section 2, 3, and 4 we discuss the properties of Sombor eigenvalues, Sombor energy, and its chemical applicability.

2 Sombor eigenvalues of graph G_S

The eigenvalues of $A_{SO}(G)$ satisfy the following relation [9]:

$$\sum_{i=1}^{n} \sigma_i = 0; \qquad \sum_{i=1}^{n} \sigma_i^2 = 2F(G). \tag{9}$$

Lemma 1. *Let $G(V, X)$ be a graph with n vertices and m edges. If $S \subseteq V(G)$, then the eigenvalues of $A_{SO}(G_S)$ satisfy,*

1. $\sum_{i=1}^{n} \sigma_i(G_S) = \sqrt{2}Q$

2. $\sum_{i=1}^{n} \sigma_i^2(G_S) = 2\left(F(G_S) - \sum_{v_i \in S} d_i^2(G_S)\right)$

Proof. 1. We have,

$$\sum_{i=1}^{n} \sigma_i(G_S) = \sum_{i=1}^{n} [A_{SO}(G_S)]_{ii} = \sum_{v_i \in S} \sqrt{2} d_i(G_S) = \sqrt{2} Q.$$

2. Also,

$$\begin{aligned}\sum_{i=1}^{n} \sigma_i^2(G_S) &= \sum_{i=1}^{n} [A_{SO}(G_S)^2]_{ii} \\ &= 2 \sum_{v_i v_j \in X(G)} [d_i^2(G_S) + d_j^2(G_S)] + 2 \sum_{v_i \in S} d_i^2(G_S) \\ &= 2 \left(F(G_S) - \sum_{v_i \in S} d_i^2(G_S) \right).\end{aligned}$$

■

Lemma 2. *Let $G(V, X)$ be a graph with n vertices and m edges. If $S \subseteq V(G)$, then the auxiliary eigenvalues $t_1, t_2, \ldots, t_n$ of $A_{SO}(G_S)$ satisfy,*

1. $\sum\limits_{i=1}^{n} t_i = 0$
2. $\sum\limits_{i=1}^{n} t_i^2 = 2R$

where $R = F(G_S) - \sum\limits_{v_i \in S} d_i^2(G_S) - \frac{Q^2}{n}$.

Proof. 1. We have,

$$\sum_{i=1}^{n} t_i = \sum_{i=1}^{n} \left(\sigma_i(G_S) - \frac{\sqrt{2}Q}{n} \right) = \sum_{i=1}^{n} \sigma_i(G_S) - \sum_{i=1}^{n} \frac{\sqrt{2}Q}{n} = 0.$$

2. Also,

$$\begin{aligned}\sum_{i=1}^{n} t_i^2 &= \sum_{i=1}^{n} \left(\sigma_i(G_S) - \frac{\sqrt{2}Q}{n} \right)^2 \\ &= \sum_{i=1}^{n} \sigma_i^2(G_S) + 2 \sum_{i=1}^{n} \left(\frac{Q}{n} \right)^2 - 2 \frac{\sqrt{2}Q}{n} \sum_{i=1}^{n} \sigma_i(G_S)\end{aligned}$$

$$= 2\left(F(G_S) - \sum_{v_i \in S} d_i^2(G_S) - \frac{Q^2}{n}\right) = 2R.$$

∎

Lemma 3. *Let $t_1, t_2, \ldots, t_n$ be the auxiliary eigenvalues of $A_{SO}(G_S)$. Then t_i, $1 \le i \le n$ are the eigenvalues of the matrix $A_{SO}(G_S) - \frac{\sqrt{2}Q}{n}I$.*

Proof. Let $t_1, t_2, \ldots, t_n$ be the auxiliary eigenvalues(e.v) of $A_{SO}(G_S)$. It is known that for scalar matrix $B = \alpha I$, in $A + B$, we write $e.v(A + \alpha I)$ as $e.v(A) + e.v(\alpha I)$, where α is a scalar.

Therefore, $e.v\left(A_{SO}(G_S) - \frac{\sqrt{2}Q}{n}I\right) = e.v\left(A_{SO}(G_S)\right) - e.v\left(\frac{\sqrt{2}Q}{n}I\right) = \sigma_i(G_S) - \frac{\sqrt{2}Q}{n} = t_i$, for $1 \le i \le n$. ∎

Lemma 4. *[13] Let $A \in M_n$ be Hermitian, and let the eigenvalues of A be ordered as $\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_n$. Then, $\sigma_n y^* y \le y^* A y \le \sigma_1 y^* y$ for all $y \in \boldsymbol{C}^n$.*

Lemma 5. *Let $\sigma_1(G_S) \ge \sigma_2(G_S) \ge \cdots \ge \sigma_n(G_S)$ and $t_1 \ge t_2 \ge \cdots \ge t_n$ be the eigenvalues and auxiliary eigenvalues of $A_{SO}(G_S)$ respectively. Then, $\sigma_1(G_S)$ and t_1 satisfy,*

1. $\sigma_n(G_S) \le \frac{2SO(G_S) - \sqrt{2}Q}{n} \le \sigma_1(G_S)$
2. $t_n \le \frac{2\left(SO(G_S) - \sqrt{2}Q\right)}{n} \le t_1$.

Proof. 1. Let $\sigma_1(G_S) \ge \sigma_2(G_S) \ge \cdots \ge \sigma_n(G_S)$ be the eigenvalues of $A_{SO}(G_S)$. Then, for $y = 1_n$ the $n \times 1$ vector having all its entry 1, we get,

$$\begin{aligned} y^T A_{SO}(G_S) y &= \sum_{i=1}^{n} \sum_{j=1}^{n} [A_{SO}(G_S)]_{ij} \\ &= 2 \sum_{v_i v_j \in X(G)} \sqrt{d_i^2(G_S) + d_j^2(G_S)} + \sqrt{2} \sum_{v_i \in S} d_i(G_S) \\ &= 2SO(G_S) - \sqrt{2}Q. \end{aligned}$$

Therefore, by Lemma 4, $\sigma_n(G_S) \le \frac{2SO(G_S) - \sqrt{2}Q}{n} \le \sigma_1(G_S)$.

2. Also, let $t_1 \geq t_2 \geq \cdots \geq t_n$ be the auxiliary eigenvalues of $A_{SO}(G_S)$. Then for $y = 1_n$ we get,

$$\begin{aligned} y^T\left(A_{SO}(G_S) - \frac{\sqrt{2}Q}{n}I\right)y &= \sum_{i=1}^{n}\sum_{j=1}^{n}\left[A_{SO}(G_S) - \frac{\sqrt{2}Q}{n}I\right]_{ij} \\ &= 2\sum_{v_iv_j\in X(G)}\sqrt{d_i^2(G_S)+d_j^2(G_S)}+ \\ &\qquad \sqrt{2}\sum_{v_i\in S} d_i(G_S) - \sqrt{2}Q \\ &= 2\left(SO(G_S) - \sqrt{2}Q\right). \end{aligned}$$

Therefore, by Lemma 3 and Lemma 4, $t_n \leq \frac{2\left(SO(G_S)-\sqrt{2}Q\right)}{n} \leq t_1$. ∎

3 Sombor energy of G_S

Theorem 1. *(McClelland-type bound) Let G_S be a graph of order n and $S \subseteq V(G)$. Then $En_{SO}(G_S) \leq \sqrt{2nR}$.*

Proof. Put $a_i = 1$ and $b_i = |t_i|$ in Cauchy–Schwarz inequality we get,

$$En_{SO}(G_S) = \sqrt{\left(\sum_{i=1}^{n}|t_i|\right)^2} \leq \sqrt{n\sum_{i=1}^{n}|t_i|^2} = \sqrt{2nR}.$$ ∎

Lemma 6. *Let G_S be a connected graph of order $n \geq 2$ and $S \subseteq V(G)$. Then,*

$$\sqrt{\frac{2R}{n}} \leq \frac{2\left(SO(G_S)-\sqrt{2}Q\right)}{n}$$

where $R = F(G_S) - \sum_{v_i\in S} d_i^2(G_S) - \frac{Q^2}{n}$.

Proof. Let G_S be a connected graph of order $n \geq 2$ and $S \subseteq V(G)$. Let e_i represents $n \times 1$ vector with all its entry zero except i^{th} entry 1. Then, by using Lemma 2 and Lemma 3,

$$\begin{aligned}
\sqrt{\frac{2R}{n}} &= \sqrt{\frac{\sum\limits_{i=1}^{n} t_i^2}{n}} = \sqrt{\frac{\sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n}\left[A_{SO}(G_S) - \frac{\sqrt{2}Q}{n}I\right]_{ij}^2}{n}} \\
&\leq \sqrt{\frac{\sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n}\left([A_{SO}(G_S)]_{ij}^2 - \left[\frac{\sqrt{2}Q}{n}I\right]_{ij}^2\right)}{n}} \\
&= \sqrt{\frac{\sum\limits_{\substack{i,j=1\\ i\neq j}}^{n}[A_{SO}(G_S)]_{ij}^2 + \sum\limits_{i=1}^{n}[A_{SO}(G_S)]_{ii}^2 - \left(\frac{\sqrt{2}Q}{n}\right)^2 n}{n}} \\
&\leq \frac{\sum\limits_{\substack{i,j=1\\ i\neq j}}^{n}[A_{SO}(G_S)]_{ij}}{n} + \frac{\sum\limits_{i=1}^{n}[A_{SO}(G_S)]_{ii}}{n} - \frac{\sqrt{2}Q}{n} \\
&= \frac{2\left(SO(G_S) - \sqrt{2}Q\right)}{n}.
\end{aligned}$$

Therefore, $\sqrt{\frac{2R}{n}} \leq \frac{2\left(SO(G_S)-\sqrt{2}Q\right)}{n}$. ■

Theorem 2. *(Koolen-Moulton-type bound) Let G_S be a connected graph of order $n \geq 2$ and $S \subseteq V(G)$. Then,*

$$En_{SO}(G_S) \leq \frac{2(SO(G_S)-\sqrt{2}Q)}{n} + \sqrt{(n-1)\left(2R - \left(\frac{2(SO(G_S)-\sqrt{2}Q)}{n}\right)^2\right)}.$$

Proof. Let G_S be a connected graph of order $n \geq 2$ and $S \subseteq V(G)$. Consider,

$$\begin{aligned}
&\sum_{i=2}^{n}\sum_{j=2}^{n}(|t_i| - |t_j|)^2 \geq 0 \\
&\sum_{i=2}^{n}\left(\sum_{j=2}^{n}|t_i|^2 + \sum_{j=2}^{n}|t_j|^2 - 2\sum_{j=2}^{n}|t_i||t_j|\right) \geq 0 \\
&2(n-1)\left(2R - |t_1|^2\right) - 2\left(En_{SO}(G_S) - |t_1|\right)^2 \geq 0
\end{aligned}$$

Further simplification results in,

$$En_{SO}(G_S) \leq |t_1| + \sqrt{(n-1)\left(2R - |t_1|^2\right)}. \tag{10}$$

Since $|t_1| > 0$, function in Eq. (10) is monotonically decreasing in the interval $\left(\sqrt{\frac{2R}{n}}, \sqrt{2R}\right)$. Then by using Lemma 5 and Lemma 6 in Eq. (10) results in,

$$En_{SO}(G_S) \leq \frac{2(SO(G_S)-\sqrt{2}Q)}{n} + \sqrt{(n-1)\left(2R - \left(\frac{2(SO(G_S)-\sqrt{2}Q)}{n}\right)^2\right)}.$$

■

Theorem 3. *For complete graph K_n with $k \geq 1$ self-loops. Then, the characteristic polynomial $p(x)$ is*

$$p(\sigma(G_S)) = (\sigma(G_S))^{k-1}\left(\sigma(G_S) + (n-1)\sqrt{2}\right)^{n-k-1}$$
$$\left(\sigma^2(G_S) - \sigma(G_S)\sqrt{2}(2k+n^2-2n+1) - 2k(n^2+2n-2k-1)\right).$$

Proof. For complete graph K_n with $k \geq 1$ self-loops, we have

$$A_{SO}((K_n)_S) = \begin{bmatrix} (n+1)\sqrt{2}I_k & \sqrt{2(n^2+1)}J_{k\times(n-k)} \\ \sqrt{2(n^2+1)}J_{(n-k)\times k} & (n-1)\sqrt{2}(J-I))_{n-k} \end{bmatrix}$$

Let $W = \begin{bmatrix} Y \\ Z \end{bmatrix}$ be an eigenvector of order n, such that vector Y be of order k and vector Z be of order $n-k$. If $\sigma(G_S)$ be a eigenvalue of $A_{SO}((K_n)_S)$. Then,

$$[\sigma(G_S)I - A_{SO}((K_n)_S)]\begin{bmatrix} X \\ Y \end{bmatrix} =$$

$$\begin{bmatrix} [\sigma(G_S)I_k - (n+1)\sqrt{2}J_k]Y_{k\times 1} + \sqrt{2(n^2+1)}J_{k\times(n-k)}Z_{(n-k)\times 1} \\ \sqrt{2(n^2+1)}J_{(n-k)\times k}Y_{k\times 1} + [\sigma(G_S)I - (n-1)\sqrt{2}(J-I)]_{(n-k)}Z_{(n-k)\times 1} \end{bmatrix} \tag{11}$$

Case 1: Let $Y = Y_j = e_1 - e_j$, $j = 2, 3, \ldots, k$. and $Z = O_{n-k\times 1}$

From Eq. (11),

$[\sigma(G_S)I_k - (n+1)\sqrt{2}J_k]Y_j = \sigma(G_S)Y_j$.

Which implies that, $\sigma(G_S) = 0$ is a eigenvalue with multiplicity of at least $k-1$ since there are $k-1$ linearly independent eigenvectors of the form Y_j.

Case 2: Let $Y = O_k$ and $Z = Z_j = e_1 - e_j$, $j = 2, 3, \ldots, n-k$.

From Eq. (11),

$[\sigma(G_S)I_{n-k} - (n-1)\sqrt{2}(J-I)_{(n-k)}]Z_j = \sigma(G_S)Z_j + (n-1)\sqrt{2}Z_j$.

So, $\sigma(G_S) = -(n-1)\sqrt{2}$ is an eigenvalue with multiplicity at least $(n-k-1)$ since there are $n-k-1$ linearly independent eigenvector of the form Z_j.

Case 3: Let $Y = 1_k$ and $Z = \frac{-k\sqrt{2(n^2+1)}}{\sigma(G_S)-(n-1)\sqrt{2}(n-k-1)}1_{n-k}$ where, $\sigma(G_S)$ be a root of the equation $\sigma^2(G_S) - \sqrt{2}(2k+n^2-2n+1)\sigma(G_S) - 2k(n^2+2n-2k-1) = 0$

$$\left[\sigma(G_S) - \frac{(n+1)\sqrt{2}k - 2(n^2+1)(n-k)k}{\sigma(G_S)-(n-1)\sqrt{2}(n-k-1)}\right]1_{n-k} = \frac{\sigma^2(G_S)-\sqrt{2}(2k+n^2-2n+1)\sigma(G_S)-2k(n^2+2n-2k-1)}{\sigma(G_S)-(n-1)\sqrt{2}(n-k-1)}$$

Thus, the characteristic polynomial is,

$$p(\sigma(G_S)) = (\sigma(G_S))^{k-1}(\sigma(G_S)+(n-1)\sqrt{2})^{n-k-1} \left(\sigma^2(G_S) - \sigma(G_S)\sqrt{2}(2k+n^2-2n+1) - 2k(n^2+2n-2k-1)\right).$$

■

4 Chemical applicability of $En_{SO}(G_S)$

Several topological indices have been studied extensively by chemists to correlate the structure of chemical compounds with empirically acquired data on their physico-chemical properties. In nature, along with hydrocarbon molecules (molecules containing only hydrogen and carbon), there are several other compounds in which different types of atoms replace carbon and hydrogen. Such molecules, referred as hetero-atomic molecules, have been focused on in recent years in graph theory. The graphs with self-loops enable the wide study range of hetero-molecules, where each self-loop replaces a hetero-atom.

It is well known that the total π-electron energy increases with the size (number of atoms) of the underlying conjugated molecule. The same holds for the Sombor energy. Therefore, when comparing the Sombor energy with total π-electron energy of molecules of different size, an artificially good (linear) correlation will be obtained. This was the case in Ref. [6] and also in Fig. 2 in this paper. In order to get a more realistic insight, sets of isomers should be considered. For more details on this matter see Ref. [20]

In this paper, hetero-molecular systems in Fig. 1, from Ref. [3], are interpreted as a graph with self-loops, where each hetero-atom 'x' is replaced by a self-loop. Solving secular determinant by taking appropriate values of Coulomb integral α and resonance integral β, we obtain the total π-electron energy. The equation $\alpha_{\mathrm{x}} = \alpha + h\beta$, $\beta_{\mathrm{xy}} = k\beta$ gives the Coulomb integral for atom x and resonance integral for bound xy, respectively. For a given hetero-molecular system, the different values for parameters h and k give different sets of total π-electron energies depending on which atom is in conjugation [19]. This study correlates $En_{SO}(G_S)$ with the total π-electron energy of hetero-molecular system for h=1 and k=1 [3, 19] and the graphs considered are G_{S_i}, $1 \leq i \leq 28$, where G_{S_1}=Venyl chloride like systems, G_{S_2}=Butadiene perturbed at C2, G_{S_3}=Acrolein like systems, G_{S_4}=1,1-Dichloro-ethylene like systems, G_{S_5}=Glyoxal like and 1,2-Dichloro-ethylene like systems, G_{S_6}=Pyrrole like systems, G_{S_7}=Pyridine like systems,
G_{S_8}=Pyridazine like systems, G_{S_9}=Pyrimidine like systems,
$G_{S_{10}}$=Pyrazine like systems, $G_{S_{11}}$=Triazene like systems, $G_{S_{12}}$=Aniline like systems, $G_{S_{13}}$=O-Phenylene-diamine like systems, $G_{S_{14}}$=m- Phenylene-diamine like systems, $G_{S_{15}}$=p-Phenylene-diamine like systems,
$G_{S_{16}}$=Benzaldehyde like systems, $G_{S_{17}}$=Quinoline like systems, $G_{S_{18}}$=Iso-quinoline like systems, $G_{S_{19}}$=1-Naphthalein like systems,
$G_{S_{20}}$=2-Naphthalein like systems, $G_{S_{21}}$=Iso-indole like systems,
$G_{S_{22}}$=Indole like systems, $G_{S_{23}}$=Benzylidine-aniline-like systems,
$G_{S_{24}}$=Azobenzene like systems, $G_{S_{25}}$=Acridine like systems,
$G_{S_{26}}$=Phenazine like systems, $G_{S_{27}}$=9,10-Anthraquinone like systems,
$G_{S_{28}}$=Carbazole like systems.

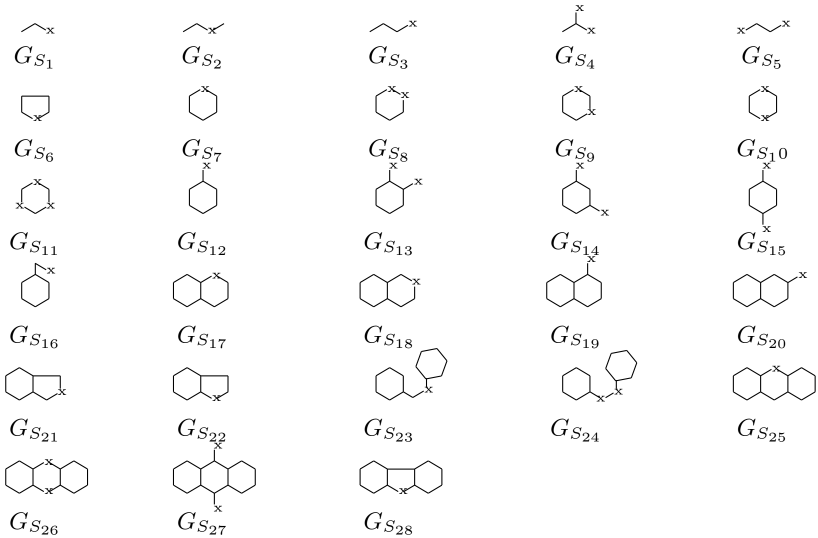

Figure 1. Hetero-moleclular systems

The scatter plot of the total π-electron energy for $h = 1$ and $k = 1$ against $En_{SO}(G_S)$ in Fig. 2 shows a strong correlation with the correlation coefficient 0.994.

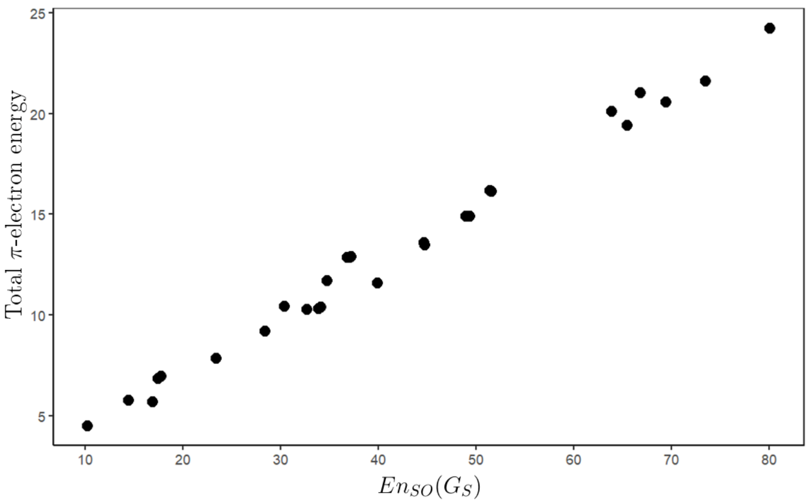

Figure 2. Scatter plot of $En_{SO}(G_S)$ with the total π-electron energies

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