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CENTROSYMMETRIC GRAPHS AND A LOWER BOUND FOR GRAPH ENERGY OF FULLERENES

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Abstract

The energy of a molecular graph G is defined as the summation of the absolute values of the eigenvalues of adjacency matrix of a graph G. In this paper, an infinite class of fullerene graphs with $10n$ vertices, $n \geq 2$, is considered. By proving centrosymmetricity of the adjacency matrix of these fullerene graphs, a lower bound for its energy is given. Our method is general and can be extended to other class of fullerene graphs.

Keywords: centrosymmetric matrix, fullerene graph, energy.

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1. Introduction

All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. Let $G = (V, E)$ be a simple graph and $W \subseteq V$. Then the induced subgraph by W is the subgraph of G obtained by taking the vertices in W and joining those pairs of vertices in W which are joined in G. The notation $G - \{v_1, v_2, \ldots, v_k\}$ stands for a graph obtained by removing the vertices $v_1, v_2, \ldots, v_k$ from G and all edges incident to any of them.

Suppose M is a molecule. A *molecular graph* for M is a graph for which atoms are vertices and chemical bonds are edges of the graph. From the chemical point of view, such a graph has vertices with degrees ≤ 4. It merits mention here that in the Hückel theory only pi electron molecular orbitals are included because these determine the general properties of these molecules and the sigma electrons are ignored. So, when we are talking about Hückel theory we need the molecule to have a pi system and therefore all chemical graphs should have max degree 3 or less - a vertex of degree 4 represents a saturated carbon atom that cannot be part of a pi system. The max degree 4 is for alkanes, which is not for the context required for the present paper.

The adjacency matrix of a graph G is denoted by $A(G)$. The *characteristic polynomial* of $A(G)$ is defined as $\Phi(G, x) = \det(A(G) - xI)$ and its roots are named the *eigenvalues* of $A(G)$ and form the spectrum of this graph. We encourage the interested readers to consult [2, 3]. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be eigenvalues of $A(G)$. Then the *graph energy* of G, $E(G)$, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$ [7, 8]. This graph parameter has important applications in Hückel theory and so it has some specific chemical interests and has been extensively studied. An extension of this graph invariant was done by Zhou and Gutman [9, 15].

A *fullerene graph* is a cubic planar and 3-connected graph such that its faces are pentagon and hexagon. Suppose p, h, n and m are the number of pentagons, hexagons, vertices and edges of a fullerene graph F, respectively. Since each vertex lies in exactly three faces and each edge lies in two faces, the number of vertices is $n = (5p + 6h)/3$, the number of edges is $m = (5p + 6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$ and so $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$. Therefore, $p = 12, v = 2h + 20$ and $e = 3h + 30$.

The fullerene graphs are models of fullerene molecules. Such molecules are constructed entirely from carbon atoms and has important applications in chemistry. These molecules found more interest from scientists after giving Nobel prize to discovers of buckminsterfullerene [12]. We encourage the interested readers to consult the famous book of Fowler and Manolopoulos [4] for more information on this topic.

For a matrix A of size $m \times n$, A^H denotes its conjugate transpose, i.e. $A^H = \bar{A}^T$, where A^T and $\bar{A}$ denote the transpose and conjugate of A, respectively. The square roots of the eigenvalues of $A^H A$ are called *singular values* of A. We denote the singular values of A by $s_1(A) \geq s_2(A) \geq \cdots \geq s_m(A)$. The *energy* of this matrix is defined by $\varepsilon(A) = \sum_{i=1}^{m} s_i(A)$.

The goal of this paper is to continue our earlier investigation on fullerene graphs [6] and compute a bound for its graph energy. It merits mention here that the energy of a fullerene is not the summation of the absolute values of the eigenvalues but twice the summation of the first $\frac{n}{2}$ eigenvalues in non-increasing order. Notice that by a result in the seminal paper of Gutman [7], the energy and graph energy for molecules with bipartite molecular graphs are the same, but fullerenes are not bipartite.

The following classical result in algebraic graph theory [2, 3] is critical throughout this paper:

Key Fan Theorem. *Let* $\mathbf{A}, \mathbf{B}$ *and* $\mathbf{C}$ *be square matrices of order* n. *If* $\mathbf{C} = \mathbf{A} + \mathbf{B}$, *then*

$$\sum s_i(\mathbf{A}) + \sum s_i(\mathbf{B}) \geq \sum s_i(\mathbf{C}).$$

Equality holds if and only if there exists an orthogonal matrix $\mathbf{P}$ *such that the matrices* $\mathbf{PA}$ *and* $\mathbf{PB}$ *are positive semidefinite.*

2. Definitions and Preliminaries

A matrix $A_{n\times n}$ is called *centrosymmetric* if $a_{ij} = a_{n-i+1,n-j+1}$, $1 \leq i, j \leq n$. The mathematical properties of this special class of matrices can be found in [13, 14, 16]. In general, if the matrix $A_{n\times n}$ is a centrosymmetric matrix with $n = 2m$, then A has the following form:

$$\mathbf{A} = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,m} & a_{1,m+1} & \cdots & a_{1,2m-1} & a_{1,2m} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,m} & a_{2,m+1} & \cdots & a_{2,2m-1} & a_{2,2m} \\ . & . & \cdots & . & . & \cdots & . & . \\ . & . & \cdots & . & . & \cdots & . & . \\ . & . & \cdots & . & . & \cdots & . & . \\ a_{m,1} & a_{m,2} & \cdots & a_{m,m} & a_{m,m+1} & \cdots & a_{m,2m-1} & a_{m,2m} \\ a_{m,2m} & a_{m,2m-1} & \cdots & a_{m,m+1} & a_{m,m} & \cdots & a_{m,2} & a_{m,1} \\ . & . & \cdots & . & . & \cdots & . & . \\ . & . & \cdots & . & . & \cdots & . & . \\ . & . & \cdots & . & . & \cdots & . & . \\ a_{2,2m} & a_{2,2m-1} & \cdots & a_{2,m+1} & a_{2,m} & \cdots & a_{2,2} & a_{2,1} \\ a_{1,2m} & a_{1,2m-1} & \cdots & a_{1,m+1} & a_{1,m} & \cdots & a_{1,2} & a_{1,1} \end{pmatrix}$$

and if $n = 2m + 1$ is an odd number, then

$$\mathbf{A}=\begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,m} & a_{1,m+1} & a_{1,m+2} & \cdots & a_{1,2m-1} & a_{1,2m} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,m} & a_{2,m+1} & a_{2,m+2} & \cdots & a_{2,2m-1} & a_{2,2m} \\ . & . & \cdots & \cdots & . & . & \cdots & . & . \\ . & . & \cdots & \cdots & . & . & \cdots & . & . \\ . & . & \cdots & \cdots & . & . & \cdots & . & . \\ a_{m,1} & a_{m,2} & \cdots & a_{m,m} & a_{m,m+1} & a_{m,m+2} & \cdots & a_{m,2m-1} & a_{m,2m} \\ a_{m+1,1} & a_{m+1,2} & \cdots & a_{m+1,m} & a_{m+1,m+1} & a_{m+1,m} & \cdots & a_{m+1,2} & a_{m+1,1} \\ a_{m,2m} & a_{m,2m-1} & \cdots & a_{m,m+2} & a_{m,m+1} & a_{m,m} & \cdots & a_{m,2} & a_{m,1} \\ . & . & \cdots & . & . & . & \cdots & . & . \\ . & . & \cdots & . & . & . & \cdots & . & . \\ . & . & \cdots & . & . & . & \cdots & . & . \\ a_{2,2m} & a_{2,2m-1} & \cdots & a_{2,m+2} & a_{2,m+1} & a_{2,m} & \cdots & a_{2,2} & a_{2,1} \\ a_{1,2m} & a_{1,2m-1} & \cdots & a_{1,m+2} & a_{1,m+1} & a_{1,m} & \cdots & a_{1,2} & a_{1,1} \end{pmatrix}.$$

Let J_n be the exchange matrix of size n. This is an $n \times n$ $\{0,1\}$-matrix in which an entry is unit if and only if it lies on counterdiagonal of J_n. It is clear that the matrix A is centrosymmetric if and only if $AJ = JA$. The set of all centrosymmetric matrices is denoted by **Cen**.

Theorem 1 (See [1] for details)**.** *If $A_{n\times n} \in$ **Cen** and $n = 2m$, then*

$$\mathbf{A} = \begin{pmatrix} B & J_mCJ_m \\ C & J_mBJ_m \end{pmatrix}$$

in which B, C are $m \times m$ matrices. If $n = 2m + 1$, then

$$\mathbf{A} = \begin{pmatrix} B & J_mb & J_mCJ_m \\ a^T & \alpha & a^TJ_m \\ C & b & J_mBJ_m \end{pmatrix}$$

in which $B, C \in R^{m\times m}$, $a, b \in R^{m\times 1}$ and α is a real number. Moreover, for $n = 2m$, we have

$$\mathbf{Q^TAQ} = \begin{pmatrix} B - J_mC & 0 \\ 0 & B + J_mC \end{pmatrix},$$

where

$$\mathbf{Q} = \frac{\sqrt{2}}{2}\begin{pmatrix} I_m & I_m \\ -J_m & J_m \end{pmatrix}.$$

If $n = 2m + 1$, then

$$\mathbf{Q^TAQ} = \begin{pmatrix} B - J_mC & 0 & 0 \\ 0 & \alpha & \sqrt{2}a^T \\ 0 & \sqrt{2}J_mb & B + J_mC \end{pmatrix},$$

where

$$\mathbf{Q} = \frac{\sqrt{2}}{2}\begin{pmatrix} I_m & 0 & I_m \\ 0 & \sqrt{2} & 0 \\ -J_m & 0 & J_m \end{pmatrix}.$$

A graph G is called centrosymmetric, if its vertices has a labeling such that its adjacent matrix is centrosymmetric. We now introduce two classes of matrices, named block centrosymmetric and centrosymmetric block. Suppose

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ . & . & \dots & . \\ . & . & \dots & . \\ . & . & \dots & . \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix},$$

where its blocks are $s \times s$, $s \geq 2$, matrices. $\mathbf{A}$ is called a *block centrosymmetric* if for $1 \leq i, j \leq m$, $A_{ij} = A_{m-i+1,m-j+1}$. It is called *centrosymmetric block* if all blocks are centrosymmetric. The set of all block centrosymmetric matrices is denoted by **BCen** and the set of all centrosymmetric block matrices is denoted by **CenB**.

For example the matrix

$$\mathbf{A} = \begin{pmatrix} \begin{pmatrix} 5 & 6 \\ 6 & 5 \end{pmatrix} & \begin{pmatrix} 7 & 9 \\ 9 & 7 \end{pmatrix} \\ \begin{pmatrix} 0 & 3 \\ 3 & 0 \end{pmatrix} & \begin{pmatrix} 6 & 2 \\ 6 & 2 \end{pmatrix} \end{pmatrix}$$

belongs to **CenB**, but it is not a member of **Cen** or **BCen**. Also, the matrix

$$\mathbf{B} = \begin{pmatrix} \begin{pmatrix} 3 & 2 \\ 5 & 7 \end{pmatrix} & \begin{pmatrix} 0 & 8 \\ 1 & 5 \end{pmatrix} \\ \begin{pmatrix} 0 & 8 \\ 1 & 5 \end{pmatrix} & \begin{pmatrix} 3 & 2 \\ 5 & 7 \end{pmatrix} \end{pmatrix}$$

is in **BCen**, but not in **Cen** or **CenB**. Finally, the matrix

$$\mathbf{C} = \begin{pmatrix} \begin{pmatrix} 1 & 2 \\ 9 & 7 \end{pmatrix} & \begin{pmatrix} 3 & 4 \\ 0 & 8 \end{pmatrix} \\ \begin{pmatrix} 8 & 0 \\ 4 & 3 \end{pmatrix} & \begin{pmatrix} 7 & 9 \\ 2 & 1 \end{pmatrix} \end{pmatrix}$$

is a member of **Cen**, but not a member of **BCen** or **CenB**.

Let

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ . & . & \dots & . \\ . & . & \dots & . \\ . & . & \dots & . \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix}$$

be the block form of $\mathbf{A} = [a_{i,j}]$, $1 \le i,j \le n$, and all blocks are $s \times s$ matrices. The relationship between these matrices is shown in the following theorem.

Theorem 2. *The following are equivalent.*

(a) $\mathbf{A} \times \mathbf{\Psi} = \mathbf{\Psi} \times \mathbf{A}$ *in which* $\mathbf{\Psi} = J_m \otimes J_s$ *the tensor product of matrices* J_m *and* J_s.

(b) $A_{ij} \times J_s = J_s \times A_{m-i+1,m-j+1}$.

(c) $\mathbf{A} \in \mathbf{Cen}$.

Proof. For equivalence of (a) and (b) notice that

$$\begin{aligned}
\mathbf{\Psi} \times \mathbf{A} &= \begin{pmatrix} 0 & \dots & 0 & J_s \\ 0 & \dots & J_s & 0 \\ . & \dots & . & . \\ . & \dots & . & . \\ . & \dots & . & . \\ J_s & 0 & .. & .0 \end{pmatrix} \times \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ . & . & \dots & . \\ . & . & \dots & . \\ . & . & \dots & . \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix} \\
&= \begin{pmatrix} J_sA_{m,1} & J_sA_{m,2} & \dots & J_sA_{m,m} \\ J_sA_{m-1,1} & J_sA_{m-1,2} & \dots & J_sA_{m-1,m} \\ . & . & \dots & . \\ . & . & \dots & . \\ . & . & \dots & . \\ J_sA_{1,1} & J_sA_{1,2} & \dots & J_sA_{1,m} \end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
\mathbf{A} \times \mathbf{\Psi} &= \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ . & . & \dots & . \\ . & . & \dots & . \\ . & . & \dots & . \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix} \times \begin{pmatrix} 0 & \dots & 0 & J_s \\ 0 & \dots & J_s & 0 \\ . & \dots & . & . \\ . & \dots & . & . \\ . & \dots & . & . \\ J_s & 0 & \dots & 0 \end{pmatrix} \\
&= \begin{pmatrix} A_{1,m}J_s & A_{1,m-1}J_s & \dots & A_{1,1}J_s \\ A_{2,m}J_s & A_{2,m-1}J_s & \dots & A_{2,1}J_s \\ . & . & \dots & . \\ . & . & \dots & . \\ . & . & \dots & . \\ A_{m,m}J_s & A_{m,m-1}J_s & \dots & A_{m,1}J_s \end{pmatrix}
\end{aligned}$$

and so the equality $\mathbf{A} \times \mathbf{\Psi} = \mathbf{\Psi} \times \mathbf{A}$ holds if and only if $A_{i,j}J_s = J_sA_{m-i+1,m-j+1}$.

Since

$$A_{i,j} = \begin{pmatrix} a_{(i-1)s+1,(j-1)s+1} & a_{(i-1)s+1,(j-1)s+2} & \cdots & a_{(i-1)s+1,js} \\ a_{(i-1)s+2,(j-1)s+1} & a_{(i-1)s+2,(j-1)s+2} & \cdots & a_{(i-1)s+2,js} \\ . & . & \cdots & . \\ . & . & \cdots & . \\ . & . & \cdots & . \\ a_{is,(j-1)s+1} & a_{is,(j-1)s+2} & \cdots & a_{is,js} \end{pmatrix},$$

we have

$$A_{i,j}J_s = \begin{pmatrix} a_{(i-1)s+1,js} & a_{(i-1)s+1,js-1} & \cdots & a_{(i-1)s+1,(j-1)s+1} \\ a_{(i-1)s+2,js} & a_{(i-1)s+2,js-1} & \cdots & a_{(i-1)s+2,(j-1)s+1} \\ . & . & \cdots & . \\ . & . & \cdots & . \\ . & . & \cdots & . \\ a_{is,js} & a_{is,js-1} & \cdots & a_{is,(j-1)s+1} \end{pmatrix}.$$

On the other hand,

$$A_{m-i+1,m-j+1} = \begin{pmatrix} a_{(m-i)s+1,(m-j)s+1} & a_{(m-i)s+1,(m-j)s+2} & \cdots & a_{(m-i)s+1,(m-j+1)s} \\ a_{(m-i)s+2,(m-j)s+1} & a_{(m-i)s+2,(m-j)s+2} & \cdots & a_{(m-i)s+2,(m-j+1)s} \\ . & . & \cdots & . \\ . & . & \cdots & . \\ . & . & \cdots & . \\ a_{(m-i+1)s,(m-j)s+1} & a_{(m-i+1)s,(m-j)s+2} & \cdots & a_{(m-i+1)s,(m-j+1)s} \end{pmatrix}$$

and so

$$J_sA_{m-i+1,m-j+1}$$

$$= \begin{pmatrix} a_{(m-i+1)s+1,(m-j)s+1} & a_{(m-i+1)s+1,(m-j)s+2} & \cdots & a_{(m-i+1)s+1,(m-j+1)s} \\ a_{(m-i)s+s-1,(m-j)s+1} & a_{(m-i)s+s-1,(m-j)s+2} & \cdots & a_{(m-i)s+s-1,(m-j+1)s} \\ . & . & \cdots & . \\ . & . & \cdots & . \\ . & . & \cdots & . \\ a_{(m-i)s+1,(m-j)s+1} & a_{(m-i)s+1,(m-j)s+2} & \cdots & a_{(m-i)s+1,(m-j+1)s} \end{pmatrix}$$

$$= \begin{pmatrix} a_{n-(is-s+1)s+1,n-js+1} & a_{n-(is-s+1)s+1,n-(js-1)+1} & \cdots & a_{n-(is-s+1)s+1,n-(js-s+1)+1} \\ a_{n-(is-s+2)s+1,n-js+1} & a_{n-(is-s+2)s+1,n-(js-1)+1} & \cdots & a_{n-(is-s+2)s+1,n-(js-s+1)+1} \\ . & . & \cdots & . \\ . & . & \cdots & . \\ . & . & \cdots & . \\ a_{n-is+1,n-js+1} & a_{n-is+1,n-(js-1)+1} & \cdots & a_{n-is+1,n-(js-s+1)+1} \end{pmatrix}.$$

Now if $A_{i,j}J_s = J_sA_{m-i+1,m-j+1}$, then $a_{i,j} = a_{n-i+1,n-j+1}$ and so $\mathbf{A} \in \mathbf{Cen}$. The converse is trivial. So, b and c are equivalent. ■

In Theorem 2, if $\mathbf{A} \in \mathbf{BCen}$, then all statements are equivalent to $\mathbf{A} \in \mathbf{CenB}$. Furthermore, if $\mathbf{A} \in \mathbf{CenB}$, then they are equivalent to $\mathbf{A} \in \mathbf{BCen}$.

Theorem 3. *Let*

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & \cdots & A_{1m} \\ A_{21} & \cdots & A_{2m} \\ . & \cdots & . \\ . & \cdots & . \\ . & \cdots & . \\ A_{m1} & \cdots & A_{mm} \end{pmatrix}$$

be the block form of $\mathbf{A}$. *If* $m = 2k$ *and* $A_{i,j}J = JA_{2k-i+1,2k-j+1}$, *then* $\boldsymbol{A}$ *is orthogonally similar to the following block matrix:*

$$\begin{pmatrix} \bigsqcup+\Psi\bigcup & O \\ O & \bigsqcup-\Psi\bigcup \end{pmatrix}$$

in which

$$\bigsqcup = \begin{pmatrix} A_{1,1} & \dots & A_{1,k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{k,1} & \dots & A_{k,k} \end{pmatrix}$$

and

$$\bigcup = \begin{pmatrix} A_{k+1,1} & \dots & A_{k+1,k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{2k,1} & \dots & A_{2k,k} \end{pmatrix}.$$

Proof. Put small

$$\mathbf{B} = \begin{pmatrix} A_{1,k+1} & \dots & A_{1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{k,k+1} & \dots & A_{k,2k} \end{pmatrix}, \ \mathbf{D} = \begin{pmatrix} A_{k+1,k+1} & \dots & A_{k+1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{2k,k+1} & \dots & A_{2k,2k} \end{pmatrix}.$$

So,

$$\begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} \times \begin{pmatrix} \bigsqcup & \mathbf{B} \\ \bigcup & \mathbf{D} \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 0 & \dots & 0 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 0 & \dots & 0 \end{pmatrix} & \begin{pmatrix} 0 & \dots & 1 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 1 & \dots & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \dots. & 1 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 1 & \dots & 0 \end{pmatrix} & \begin{pmatrix} 0 & \dots & 0 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 0 & \dots & 0 \end{pmatrix} \end{pmatrix}$$

$$\times \begin{pmatrix} \begin{pmatrix} A_{1,1} & \dots & A_{1,k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{k,1} & \dots & A_{k,k} \end{pmatrix} & \begin{pmatrix} A_{1,k+1} & \dots & A_{1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{k,k+1} & \dots & A_{k,2k} \end{pmatrix} \\ \begin{pmatrix} A_{k+1,1} & \dots & A_{k+1,k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{2k,1} & \dots & A_{2k,k} \end{pmatrix} & \begin{pmatrix} A_{k+1,k+1} & \dots & A_{k+1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{2k,k+1} & \dots & A_{2k,2k} \end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} \begin{pmatrix} J_sA_{2k,1} & \dots & J_sA_{2k-1,k} \\ J_sA_{2k-1,1} & \dots & J_sA_{2k,1} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ J_sA_{k+1,1} & \dots & J_sA_{k+1,k} \end{pmatrix} & \begin{pmatrix} J_sA_{2k,k+1} & \dots & J_sA_{2k,2k} \\ J_sA_{2k-1,k+1} & \dots & J_sA_{2k-1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ J_sA_{k+1,k+1} & \dots & J_sA_{k+1,2k} \end{pmatrix} \\ \begin{pmatrix} J_sA_{k,1} & \dots & J_sA_{k,k} \\ J_sA_{k-1,1} & \dots & J_sA_{k-1,k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ J_sA_{1,1} & \dots & J_sA_{1,k} \end{pmatrix} & \begin{pmatrix} J_sA_{k,k+1} & \dots & J_sA_{k,2k} \\ J_sA_{k-1,k+1} & \dots & J_sA_{k-1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ J_sA_{1,k+1} & \dots & J_sA_{1,2k} \end{pmatrix} \end{pmatrix}.$$

On the other hand,

$$\begin{pmatrix} \bigsqcup & \mathbf{B} \\ \bigcup & \mathbf{D} \end{pmatrix} \times \begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} A_{1,1} & \dots & A_{1,k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{k,1} & \dots & A_{k,k} \end{pmatrix} & \begin{pmatrix} A_{1,k+1} & \dots & A_{1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots. & . \\ A_{k,k+1} & \dots & A_{k,2k} \end{pmatrix} \\ \begin{pmatrix} A_{k+1,1} & \dots & A_{k+1,k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{2k,1} & \dots & A_{2k,k} \end{pmatrix} & \begin{pmatrix} A_{k+1,k+1} & \dots & A_{k+1,2k} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ A_{2k,k+1} & \dots & A_{2k,2k} \end{pmatrix} \end{pmatrix}$$

$$\times \begin{pmatrix} \begin{pmatrix} 0 & \dots & 0 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 0 & \dots & 0 \end{pmatrix} & \begin{pmatrix} 0 & \dots & 1 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 1 & \dots & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \dots & 1 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 1 & \dots & 0 \end{pmatrix} & \begin{pmatrix} 0 & \dots & 0 \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ 0 & \dots & 0 \end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} \begin{pmatrix} A_{1,2k}J_s & \ldots & A_{1,k+1}J_s \\ A_{2,2k}J_s & \ldots & A_{2,k+1}J_s \\ . & \ldots & . \\ . & \ldots & . \\ . & \ldots & . \\ A_{k,2k}J_s & \ldots & A_{k,k+1}J_s \end{pmatrix} & \begin{pmatrix} A_{1,k}J_s & \ldots & A_{1,1}J_s \\ A_{2,k}J_s & \ldots & A_{2,1}J_s \\ . & \ldots & . \\ . & \ldots & . \\ . & \ldots & . \\ A_{k,k}J_s & \ldots & A_{k,1}J_s \end{pmatrix} \\ \begin{pmatrix} A_{k+1,2k}J_s & \ldots & A_{k+1,k+1}J_s \\ A_{k+2,2k}J_s & \ldots & A_{k+2,k+1}J_s \\ . & \ldots & . \\ . & \ldots & . \\ . & \ldots & . \\ A_{2k,2k}J_s & \ldots & A_{2k,k+1}J_s \end{pmatrix} & \begin{pmatrix} A_{k+1,k}J_s & \ldots & A_{k+1,1}J_s \\ A_{k+2,k}J_s & \ldots & A_{k+2,1}J_s \\ . & \ldots & . \\ . & \ldots & . \\ . & \ldots & . \\ A_{2k,k}J_s & \ldots & A_{2k,1}J_s \end{pmatrix} \end{pmatrix}.$$

Therefore,

$$\begin{pmatrix} \bigsqcup & \mathbf{B} \\ \bigcup & \mathbf{D} \end{pmatrix} \begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} = \begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} \begin{pmatrix} \bigsqcup & \mathbf{B} \\ \bigcup & \mathbf{D} \end{pmatrix},$$

$$\begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} \begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}.$$

So, $\mathbf{D} = \mathbf{\Psi} \bigsqcup$, and $\mathbf{B} = \mathbf{\Psi} \bigcup$. Hence,

$$\mathbf{A} = \begin{pmatrix} \bigsqcup & \Psi \bigcup \Psi \\ \bigcup & \Psi \bigsqcup \Psi \end{pmatrix}.$$

We now put

$$\mathbf{Q} = \frac{\sqrt{2}}{2} \begin{pmatrix} \begin{pmatrix} I_s & 0 \\ 0 & I_s \end{pmatrix} & -\begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & J_s \\ J_s & 0 \end{pmatrix} & \begin{pmatrix} I_s & 0 \\ 0 & I_s \end{pmatrix} \end{pmatrix}.$$

It is clear that $\mathbf{Q}$ is an orthonormal matrix and has the following property

$$\mathbf{Q^t A Q} = \begin{pmatrix} \bigsqcup + \Psi \bigcup & 0 \\ 0 & \Psi \bigsqcup \Psi - \bigcup \Psi \end{pmatrix}.$$

In a similar way, we have $\Psi \bigsqcup \Psi - \bigcup \Psi = \bigsqcup - \Psi \bigcup$. Hence $\mathbf{Q^t A Q}$ is similar to the following matrix:

$$\begin{pmatrix} \bigsqcup + \Psi \bigcup & 0 \\ 0 & \bigsqcup - \Psi \bigcup \end{pmatrix}.$$

■

3. A LOWER BOUND FOR THE ENERGY OF C_{10n}

In this section, we consider an infinite class of fullerene graphs C_{10n} with exactly $10n$ vertices. The fullerene graph C_{10n} is constructed by a pentagon surrounding by five pentagons. Then we continue by adding hexagons until we obtain $5n$ vertices. Two copies of this figure will construct the fullerene graph C_{10n}. We use an special labeling depicted in Figure 1 to prove that the adjacency matrix of this graph is centrosymmetric.

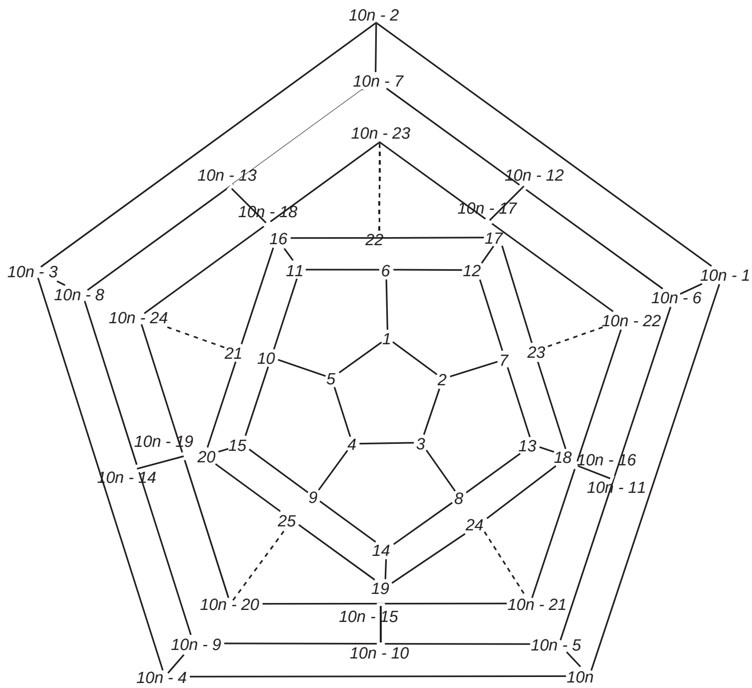

Figure 1. A Labeling of C_{10n}.

By a tedious calculation, we can compute the adjacency matrix of this graph as follows

$$\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}$$

in which $Q = P^t$ and all blocks are 5×5 matrices given by

$$I = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad P = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \end{pmatrix} X = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

By Theorem 3, the adjacency matrix is as follows

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}$$

in which

$$\mathbf{A} = \begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & 0 \end{pmatrix} \mathbf{B} = \begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ P & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & 0 \end{pmatrix}$$

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & Q \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & 0 \end{pmatrix} \mathbf{D} = \begin{pmatrix} 0 & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}.$$

So, the matrix $\mathbf{A}(C_{10n})$ is similar to the matrix

$$\begin{pmatrix} \mathbf{A} + \mathbf{\Psi C} & 0 \\ 0 & \mathbf{A} - \mathbf{\Psi C} \end{pmatrix}.$$

Furthermore,

$$\mathbf{A}+\mathbf{\Psi C}=\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & JQ \end{pmatrix}$$

and

$$\mathbf{A}-\mathbf{\Psi C}=\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & -JQ \end{pmatrix}.$$

So, $\varepsilon(\mathbf{A}(C_{10n}))=\varepsilon(\mathbf{A}+\mathbf{\Psi C})+\varepsilon(\mathbf{A}-\mathbf{\Psi C})$. Notice that

$$\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & JQ \end{pmatrix}+\begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & X-JQ \end{pmatrix}$$

$$=\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}.$$

Hence, by Key-Fan theorem,

$$\varepsilon(\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & JQ \end{pmatrix}) + \varepsilon(\begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & X - JQ \end{pmatrix})$$

$$\geq \varepsilon(\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}).$$

Using similar argument as above, we have

$$\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & -JQ \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & X + JQ \end{pmatrix}$$

$$= \begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}.$$

Again by applying Key-Fan theorem, we have

$$\varepsilon(\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & -JQ \end{pmatrix}) + \varepsilon(\begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & X+JQ \end{pmatrix})$$

$$\geq \varepsilon(\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}).$$

Notice that

$$\begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & X-JQ \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & 1 \end{pmatrix} \otimes (X-JQ).$$

Thus, the eigenvalues of

$$\begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & X-JQ \end{pmatrix}$$

are equivalent to the eigenvalues of $X - JQ$ and so $\varepsilon(X - JQ) \approx 6.4721$. By a similar argument, the energy of

$$\begin{pmatrix} 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & X+JQ \end{pmatrix}$$

is equal to the energy of $\varepsilon(X + JQ) \approx 10.4721$. Therefore,

$$\varepsilon((A(C_{10n}))) \geq 2\varepsilon(\begin{pmatrix} X & I & 0 & 0 & . & . & . & 0 & 0 \\ I & 0 & P & 0 & . & . & . & 0 & 0 \\ 0 & Q & 0 & I & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ . & . & . & . & . & . & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}) - 16.9442.$$

The right hand side matrix is again centrosymmetric and its size is half of the size of $\mathbf{A}(C_{10n})$. So, if n is even, then by repeating the above procedure we obtain the following lower bound for the energy of $\mathbf{A}(C_{10n})$.

Theorem 4. *If $n = 2^k m$, then*

$$\varepsilon(A(C_{10n})) = \varepsilon(A(C_{10(2^k m)})) > 2^k \varepsilon(A(C_{10m})) - 16.9442(2^k - 1).$$

With the best of our knowledge there is just one result in the literature on the energy of fullerenes. In fact, Gutman *et al.* [10, Theorem 6] proved that the energy E of the molecular graph of a fullerene or a nanotube with n carbon atoms is bounded, $\frac{3}{\sqrt{5}} < E < \sqrt{3}n$. We now record in Table 1, our calculations of the graph energy and bounds of the fullerene graph C_{10n}, $n \geq 2$. From Table 1 we can see that our bound given in Theorem 4 is better than the bound presented by Gutman et al. [10], in the case of $n = 100, 140, 220, 260$. We conjecture that if $n = 2m$, m is odd, then our bound is better than the mentioned bound in [10].

In [11, Conjecture 1], the authors conjectured that the adjacency matrix of a fullerene graph is centrosymmetric. One of the referees of this paper pointed out that there is an infinite number of fullerenes that do not have any centrosymmetric labeling in the sense of the present paper. The symmetry requirements characterising the minority of fullerenes that have not a centrosymmetric adjacency matrix are discussed in paper [5].

n	Energy	Our Bound	1.34n
40	61.6085	41.8886	53.60
60	93.1815	74.4630	80.40
80	124.6957	66.8330	107.20
100	156.2026	137.8784	134.00
120	187.7085	131.9818	160.80
140	219.2143	200.9370	187.60
160	250.7201	116.7218	214.40
180	282.2259	263.9546	241.20
200	313.7317	258.8126	268.00
220	345.2374	326.9670	294.80
260	408.2490	389.9786	348.40

Table 1. Calculations of the energy and two bounds for C_{10n}.

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