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ATOM BOND-CONNECTIVITY ENERGY OF A GRAPH

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ABSTRACT. The purpose of this paper is to introduce and investigate the atom bond-connectivity energy $ABCE(G)$ of a graph G. We present some upper and lower bounds for $ABCE(G)$ and calculate it for several graph classes and also for some graphs with one edge deleted which enables us to calculate this index for larger graphs by means of smaller graphs. Also $ABCE(G)$ is calculated for some complements of several graphs..

Keywords: Atom bond-connectivity matrix, atom bond-connectivity energy, atom bond-connectivity characteristic polynomial, k-complement, $k(i)$-complement.

AMS Subject Classification: 05C50

1. INTRODUCTION

Let G be a simple graph and let $\{v_1, v_2, \cdots, v_n\}$ be its vertices. Let $i = 1, 2, \cdots, n$. If two vertices v_i and v_j of G are adjacent, then we use the notation $v_i \sim v_j$. For $v_i \in V(G)$, the degree of the vertex v_i, denoted by d_i, is the number of the vertices adjacent to v_i (the number of first neighbours).

In the last seven decades, topological graph indices increasingly attracted the researchers by their countless applications, especially in Chemistry. One of the example is Prediction of Corrosion Inhibition Effectiveness by Molecular Descriptors of Weighted Chemical Graphs which has been studied by Niko Tratnik et al.,[6]. The graph energy, Estrada index, resolvent energy, and the Laplacian energy were tested accurately as parameters by Izudin Redžepović et al., [5] in the prediction of boiling points, heats of formation,

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and octanol/water partition coefficients of alkanes. Estrada et al., [1], introduced a new topological index, called atom bond-connectivity (ABC) index which is defined as

$$ABC(G) = \sum_{v_i \sim v_j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

The concept of the atom bond-connectivity index suggests that it is purposeful to associate a symmetric square matrix $ABC(G)$ to the graph G. The atom bond-connectivity matrix $ABC(G) = (S_{ij})_{n\times n}$ is defined as

$$S_{ij} = \begin{cases} \sqrt{\frac{d_i+d_j-2}{d_i d_j}} & \text{if } v_i \sim v_j, \\ 0 & otherwise. \end{cases}$$

Throughout this paper, $ABC(G)$ will denote the atom bond-connectivity matrix of a graph G and should not be confused with the atom bond-connectivity index.

2. The atom bond-connectivity energy of a graph

Let G be a simple, finite, undirected graph. The energy $E(G)$ of G is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. For more details on energy of a graph, see [2, 3]. Several authors defined several types of energy by taking a variety of matrices obtained from the given graph instead of the classical adjacency matrix. In this paper, we particularly study the atom-bond conectivity energy of a graph.

Let $ABC(G)$ be the atom bond-connectivity matrix of the graph G. The characteristic polynomial of $ABC(G)$ is denoted by $\phi_{ABC}(G, \lambda)$ and defined by

$$\phi_{ABC}(G, \lambda) = det(\lambda I - ABC(G)).$$

Since the atom bond-connectivity matrix is real and symmetric, its eigenvalues are all real numbers. Let us label them in non-increasing order as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The atom bond-connectivity energy is denoted by $ABCE(G)$ and is defined by

$$ABCE(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{1}$$

This paper is organized as follows: In Section 3, we give some basic properties of atom bond-connectivity energy of a graph. In Section 4, the atom bond-connectivity energy of some standard graphs are obtained. In Section 5, we calculate the atom bond-connectivity energy of some specific graphs with one edge deleted. In Section 6, we find the atom bond-connectivity energy of the complements of some specific graphs.

3. Some basic properties of the atom bond-connectivity energy of a graph

Let us consider the number

$$P = \sum_{i<j} \frac{d_i + d_j - 2}{d_i d_j}.$$

Then we have

Proposition 3.1. *The first three coefficients of the polynomial $\phi_{ABC}(G, \lambda)$ are given as follows:*

(i) $a_0 = 1$,

(ii) $a_1 = 0$,
(iii) $a_2 = -P$.

Proof. **(i)** From the definition, $\Phi_{ABC}(G, \lambda) = det[\lambda I - ABC(G)]$ and then we get $a_0 = 1$ after easy calculations.

(ii) The sum of the determinants of all 1×1 principal submatrices of $ABC(G)$ is equal to the trace of $ABC(G)$. Therefore

$$a_1 = (-1)^1 \cdot \text{trace of } [ABC(G)] = 0.$$

(iii) Similarly we have

$$\begin{aligned}
(-1)^2 a_2 &= \sum_{1 \le i < j \le n} \begin{vmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{vmatrix} \\
&= \sum_{1 \le i < j \le n} a_{ii}a_{jj} - a_{ji}a_{ij} \\
&= \sum_{1 \le i < j \le n} a_{ii}a_{jj} - \sum_{1 \le i < j \le n} a_{ji}a_{ij} \\
&= -P.
\end{aligned}$$

□

We now have an interesting and useful result for the sum of the squares of the atom bond-connectivity eigenvalues:

Proposition 3.2. *If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the atom bond-connectivity eigenvalues of $ABC(G)$, then*

$$\sum_{i=1}^{n} {\lambda_i}^2 = 2P.$$

Proof. We know that

$$\begin{aligned}
\sum_{i=1}^{n} \lambda_i^2 &= \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}a_{ji} \\
&= 2\sum_{i<j} a_{ij}^2 + \sum_{i=1}^{n} a_{ii}^2 \\
&= 2\sum_{i<j} a_{ij}^2 \\
&= 2P.
\end{aligned}$$

□

The next result gives an upper bound for the atom bond-connectivity energy of a graph G in terms of the number of vertices and the number P:

Theorem 3.1. *Let G be a graph with n vertices. Then*

$$ABCE(G) \le \sqrt{2nP}$$

.

Proof. Let $\lambda_1,\ \lambda_2,\ \ldots,\ \lambda_n$ be the eigenvalues of $ABC(G)$. Now by the Cauchy-Schwartz inequality we have

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

We let $a_i = 1$ and $b_i = \lambda_i$. Then

$$\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \leq \left(\sum_{i=1}^{n} 1\right)\left(\sum_{i=1}^{n} |\lambda_i|^2\right)$$

which implies that

$$[ABCE(G)]^2 \leq n(2P)$$

and finally

$$ABCE(G) \leq \sqrt{2nP}$$

which is an upper bound. □

The next result gives a lower bound for the atom bond-connectivity energy of a graph G in terms of the number of vertices, the number P and the determinant of the atom bond-connectivity matrix of G:

Theorem 3.2. *Let G be a graph with n vertices. If R= det $ABC(G)$, then*

$$ABCE(G) \geq \sqrt{2P + n(n-1)R^{\frac{2}{n}}}.$$

Proof. By definition,

$$\begin{aligned}
(ABCE(G))^2 &= \left(\sum_{i=1}^{n} \mid \lambda_i \mid\right)^2 \\
&= \sum_{i=1}^{n} \mid \lambda_i \mid \sum_{j=1}^{n} \mid \lambda_j \mid \\
&= \left(\sum_{i=1}^{n} \mid \lambda_i \mid^2\right) + \sum_{i \neq j} \mid \lambda_i \mid\mid \lambda_j \mid .
\end{aligned}$$

Using arithmetic mean and geometric mean inequality, we have

$$\frac{1}{n(n-1)} \sum_{i \neq j} \mid \lambda_i \mid\mid \lambda_j \mid \quad \geq \quad \left(\prod_{i \neq j} \mid \lambda_i \mid\mid \lambda_j \mid\right)^{\frac{1}{n(n-1)}}.$$

Therefore,

$$
\begin{aligned}
(ABCE(G))^2 &\geq \sum_{i=1}^{n} |\lambda_i|^2 + n(n-1)\left(\prod_{i\neq j} |\lambda_i||\lambda_j|\right)^{\frac{1}{n(n-1)}} \\
&\geq \sum_{i=1}^{n} |\lambda_i|^2 + n(n-1)\left(\prod_{i=1}^{n} |\lambda_i|^{2(n-1)}\right)^{\frac{1}{n(n-1)}} \\
&= \sum_{i=1}^{n} |\lambda_i|^2 + n(n-1)R^{\frac{2}{n}} \\
&= 2P + n(n-1)R^{\frac{2}{n}}.
\end{aligned}
$$

Thus,

$$ABCE(G) \geq \sqrt{2P + n(n-1)R^{\frac{2}{n}}}.$$

□

4. Atom bond-connectivity energy of some standard graphs

Theorem 4.1. *The atom bond-connectivity energy of a complete graph K_n is*

$$ABCE(K_n) = 2\sqrt{2n-4}.$$

Proof. Let K_n be the complete graph with vertex set $V = \{v_1, v_2, ..., v_n\}$. The atom bond-connectivity matrix is

$$ABC(K_n) = \begin{bmatrix} 0 & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} \\ \frac{\sqrt{2n-4}}{n-1} & 0 & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} \\ \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & 0 & \cdots & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & 0 & \frac{\sqrt{2n-4}}{n-1} \\ \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & 0 \end{bmatrix}.$$

Hence the characteristic equation will be

$$\left(\lambda - \frac{\sqrt{2n-4}}{n-1}\right)^{n-1} \left(\lambda - \sqrt{2n-4}\right) = 0$$

and therefore the spectrum becomes

$$Spec_{ABC}(K_n) = \begin{pmatrix} \frac{\sqrt{2n-4}}{n-1} & \sqrt{2n-4} \\ n-1 & 1 \end{pmatrix}.$$

Therefore,

$$ABC(K_n) = 2\sqrt{2n-4}.$$

□

Theorem 4.2. *The atom bond-connectivity energy of the cycle graph C_{2n} is*

$$ABCE(C_{2n}) = \sqrt{2}\left(2 + \sum_{m=1, m\neq n}^{2n-1} |\cos\frac{\pi m}{n}|\right).$$

Proof. The atom bond-connectivity matrix corresponding to the cycle graph C_{2n} is

$$ABC(C_{2n}) = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \dots & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \dots & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & \dots & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}.$$

This is a circullant matrix of order $2n$. Its eigenvalues are

$$\lambda_m = \begin{cases} \sqrt{2}, & \text{for } m = 0 \\ -\sqrt{2}, & \text{for } m = n \\ \sqrt{2}\cos\frac{\pi m}{n}, & \text{for } 0 < m < n \text{ or } n < m \le 2n-1. \end{cases}$$

Therefore the atom bond-connectivity energy is

$$SDD(C_{2n}) \quad = |-\sqrt{2}| + |\sqrt{2}| + \sum_{m=1, m\neq n}^{2n-1} |\sqrt{2}\cos\frac{\pi m}{n}|$$

and finally we get

$$ABCE(C_{2n}) = \sqrt{2}\left(2 + \sum_{m=1, m\neq n}^{2n-1} |\cos\frac{\pi m}{n}|\right).$$

□

Theorem 4.3. *The atom bond-connectivity energy of the star graph $K_{1,n-1}$ is*

$$ABCE(K_{1,n-1}) = 2\sqrt{n-2}.$$

Proof. Let $K_{1,n-1}$ be the star graph with vertex set $V = \{v_0, v_1 ... v_{n-1}\}$. The atom bond-connectivity matrix is

$$ABC(K_{1,n-1}) = \begin{bmatrix} 0 & \sqrt{\frac{n-2}{n-1}} & \sqrt{\frac{n-2}{n-1}} & \dots & \sqrt{\frac{n-2}{n-1}} & \sqrt{\frac{n-2}{n-1}} \\ \sqrt{\frac{n-2}{n-1}} & 0 & 0 & \dots & 0 & 0 \\ \sqrt{\frac{n-2}{n-1}} & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \sqrt{\frac{n-2}{n-1}} & 0 & 0 & \dots & 0 & 0 \\ \sqrt{\frac{n-2}{n-1}} & 0 & 0 & \dots & 0 & 0 \end{bmatrix}.$$

Then the characteristic equation would be

$$\lambda^{n-2}(\lambda - \sqrt{n-2})(\lambda + \sqrt{n-2}) = 0$$

and therefore the spectrum is

$$Spec_{ABC}(K_{1,n-1}) = \begin{pmatrix} \sqrt{n-2} & 0 & -\sqrt{n-2} \\ 1 & n-2 & 1 \end{pmatrix}.$$

Therefore,

$$ABCE(K_{1,n-1}) = 2\sqrt{n-2}.$$

□

Theorem 4.4. *The atom bond-connectivity energy of the crown graph S_n^0 is*

$$ABCE(S_n^0) = 4\sqrt{2n-4}$$

Proof. Let S_n^0 be the crown graph of order $2n$ with vertex set $\{u_1,\ u_2,\ \cdots,\ u_n,\ v_1,\ v_2,\ \cdots,\ v_n\}$. The atom bond-connectivity matrix is

$$ABC(S_n^0) = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} \\ 0 & 0 & 0 & \cdots & 0 & \frac{\sqrt{2n-4}}{n-1} & 0 & \cdots & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} \\ 0 & 0 & 0 & \cdots & 0 & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \cdots & 0 & \frac{\sqrt{2n-4}}{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & 0 \\ 0 & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & 0 & 0 & \cdots & 0 & 0 \\ \frac{\sqrt{2n-4}}{n-1} & 0 & \frac{\sqrt{2n-4}}{n-1} & \cdots & \frac{\sqrt{2n-4}}{n-1} & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & 0 & \cdots & \frac{\sqrt{2n-4}}{n-1} & 0 & 0 & \cdots & 0 & 0 \\ \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}.$$

In that case the characteristic equation is

$$\left(\lambda - \frac{\sqrt{2n-4}}{n-1}\right)^{n-1} \left(\lambda + \frac{\sqrt{2n-4}}{n-1}\right)^{n-1} \left(\lambda + \sqrt{2n-4}\right) \left(\lambda - \sqrt{2n-4}\right) = 0$$

implying that the spectrum is

$$Spec_{ABC}(S_n^0) = \begin{pmatrix} -\sqrt{2n-4} & \sqrt{2n-4} & \frac{\sqrt{2n-4}}{n-1} & \frac{\sqrt{2n-4}}{n-1} \\ 1 & 1 & n-1 & n-1 \end{pmatrix}.$$

Therefore,

$$ABCE(S_n^0) = 4\sqrt{2n-4}.$$

□

Theorem 4.5. *The atom bond-connectivity energy of the cocktail party graph $K_{n\times 2}$ is*

$$ABCE(K_{n\times 2}) = 2\sqrt{4n-6}.$$

Proof. Let $K_{n\times 2}$ be the cocktail party graph of order $2n$ with vertex set $\{u_1,\ u_2,\ \cdots,\ u_n,\ v_1,\ v_2,\ \cdots,\ v_n\}$. The atom bond-connectivity matrix is

$$ABC(K_{n\times 2}) = \begin{bmatrix} 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \cdots & 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} \\ \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \cdots & \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} \\ \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} & \cdots & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} \\ \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 & \cdots & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \cdots & 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} \\ \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \cdots & \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} \\ \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} & \cdots & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 & \frac{\sqrt{4n-6}}{2n-2} \\ \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 & \cdots & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & \frac{\sqrt{4n-6}}{2n-2} & 0 \end{bmatrix}.$$

This implies that the characteristic equation becomes

$$\lambda^n \left(\lambda + \frac{\sqrt{4n-6}}{n-1}\right)^{n-1} (\lambda - \frac{(2n-1)\sqrt{4n-6}}{n-1}) = 0.$$

Hence, the spectrum is

$$Spec_{ABC}(K_{n\times 2}) = \begin{pmatrix} -\frac{\sqrt{4n-6}}{n-1} & 0 & \sqrt{4n-6} \\ n-1 & n & 1 \end{pmatrix}.$$

Therefore,

$$ABCE(K_{n\times 2}) = 2\sqrt{4n-6}.$$

□

Theorem 4.6. *The atom bond-connectivity energy of the complete bipartite graph $K_{m,n}$ is*

$$ABCE(K_{m,n}) = 2\sqrt{m+n-2}.$$

Proof. Let $K_{m,n}$ be the complete bipartite graph of order $2n$ with vertex set $\{u_1,\ u_2,\ \cdots,\ u_m,\ v_1,\ v_2,\ \cdots,\ v_n\}$. The atom bond-connectivity matrix is

$$ABC(K_{m,n}) = \begin{bmatrix} 0 & 0 & 0 & \cdots & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} \\ 0 & 0 & 0 & \cdots & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} \\ 0 & 0 & 0 & \cdots & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \cdots & 0 & 0 & 0 \\ \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \cdots & 0 & 0 & 0 \\ \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \frac{\sqrt{m+n-2}}{mn} & \cdots & 0 & 0 & 0 \end{bmatrix}.$$

So the characteristic equation is

$$\lambda^{m+n-2}(\lambda - \sqrt{m+n-2})(\lambda + \sqrt{m+n-2}) = 0$$

and hence, the spectrum will be

$$Spec_{ABC}(K_{m,n}) = \begin{pmatrix} \sqrt{m+n-2} & 0 & -\sqrt{m+n-2} \\ 1 & m+n-2 & 1 \end{pmatrix}.$$

Therefore,

$$ABCE(K_{m,n}) = 2\sqrt{m+n-2}.$$

□

Definition 4.1. *The friendship graph, denoted by F_3^n, is the graph obtained by taking n copies of the cycle graph C_3 with a vertex in common.*

It is easy to see that $|V(F_3^n)| = 2n+1$.

Theorem 4.7. *The atom bond-connectivity energy of the friendship graph F_3^n is*

$$ABCE(F_3^n) = \left(\frac{2n-1+\sqrt{8n+1}}{\sqrt{2}}\right)$$

Proof. Let F_3^n be the friendship graph with $2n+1$ vertices. The atom bond-connectivity matrix is

$$\begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \dots & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \dots & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \dots & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \dots & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{2} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & \dots & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & \dots & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}.$$

Therefore the characteristic equation will be

$$\left(\lambda^2 - \frac{1}{\sqrt{2}}\lambda - n\right)\left(\lambda - \frac{1}{\sqrt{2}}\right)^{n-1}\left(\lambda + \frac{1}{\sqrt{2}}\right)^{n} = 0.$$

Hence, the spectrum is

$$Spec_{ABC}(F_3^n) = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1+\sqrt{8n+1}}{2\sqrt{2}} & \frac{1-\sqrt{8n+1}}{2\sqrt{2}} \\ n & n-1 & 1 & 1 \end{pmatrix}.$$

Therefore,

$$ABCE(F_3^n) = \left(\frac{2n-1+\sqrt{8n+1}}{\sqrt{2}}\right).$$

□

Definition 4.2. *The double star graph $S_{n,m}$ is the graph constructed from the star graphs $K_{1,n-1}$ and $K_{1,m-1}$ by joining their centers v_0 and u_0.*

It is clear that

$$V(S_{n,m}) = V(K_{1,n-1}) \,\cup\, V(K_{1,m-1})$$

and

$$E(S_{n,m}) = \{v_0u_0, v_0v_i, u_0u_j \;:\; 1 \,\le\, i \,\le\, n-1,\; 1 \,\le\, i \,\le\, n-1\}.$$

Therefore, the double star graph is a bipartite graph.

Theorem 4.8. *The atom bond-connectivity energy of the double star graph $S_{n,n}$ is*

$$ABCE(S_{n,n}) = 2\frac{\sqrt{4n^3-8n^2+6n-2}}{n}.$$

Proof. The atom bond-connectivity matrix is

$$ABC(S_{n,n}) = \begin{bmatrix} 0 & \sqrt{\frac{n-1}{n}} & \sqrt{\frac{n-1}{n}} & \dots & \sqrt{\frac{n-1}{n}} & \frac{\sqrt{2n-2}}{n} & 0 & 0 & \dots & 0 \\ \sqrt{\frac{n-1}{n}} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \sqrt{\frac{n-1}{n}} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \sqrt{\frac{n-1}{n}} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \frac{\sqrt{2n-2}}{n} & 0 & 0 & \dots & 0 & 0 & \frac{\sqrt{n-1}}{n} & \frac{\sqrt{n-1}}{n} & \dots & \frac{\sqrt{n-1}}{n} \\ 0 & 0 & 0 & \dots & 0 & \sqrt{\frac{n-1}{n}} & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & \sqrt{\frac{n-1}{n}}0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 & \sqrt{\frac{n-1}{n}} & 0 & 0 & \dots & 0 \end{bmatrix}.$$

The characteristic equation is

$$\lambda^{2n-4}\left(\lambda^2 + \frac{\sqrt{2n-2}}{n}\lambda - \frac{(n-1)^2}{n}\right)\left(\lambda^2 - \frac{\sqrt{2n-2}}{n}\lambda - \frac{(n-1)^2}{n}\right) = 0$$

and hence, the spectrum becomes

$$Spec_{ABC}(S_{n,n}) = \begin{pmatrix} 0 & \frac{\sqrt{2n-2}}{2n} + \frac{K}{2n} & \frac{\sqrt{2n-2}}{2n} + \frac{K}{2n} & \frac{-\sqrt{2n-2}}{2n} - \frac{K}{2n} & \frac{-\sqrt{2n-2}}{2n} + \frac{K}{2n} \\ 2n-4 & 1 & 1 & 1 & 1 \end{pmatrix}$$

where $K = \sqrt{4n^3 - 8n^2 + 6n - 2}$. Therefore,

$$ABCE(S_{n,n}) = 2\frac{\sqrt{4n^3 - 8n^2 + 6n - 2}}{n}.$$

□

Definition 4.3. *A graph that can be constructed by coalescencing n copies of the cycle graph C_4 of length 4 with a common vertex is called the Dutch windmill graph and it is denoted by D_4^n.*

It is clear that the Dutch windmill graph D_4^n has $3n + 1$ vertices and $4n$ edges.

Theorem 4.9. *The atom bond-connectivity energy of the Dutch windmill graph D_4^n is $ABCE(D_4^n) = 2[n - 1 + \sqrt{n+1}]$.*

Proof. Let D_4^n be the Dutch windmill graph with $3n + 1$ vertices. The atom bond-connectivity matrix is

$$ABC(D_4^n) = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \dots & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \dots & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \dots & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \dots & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & \dots & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}.$$

Then the characteristic equation is

$$(\lambda^2 - (n+1))(\lambda^2 - 1)^{n-1}\lambda^{n+1} = 0.$$

Hence, the spectrum will be

$$Spec_{ABC}(D_4^n) = \begin{pmatrix} 1 & -1 & 0 & \sqrt{n+1} & -\sqrt{n+1} \\ n-1 & n-1 & n+1 & 1 & 1 \end{pmatrix}.$$

Therefore,

$$ABCE(D_4^n) = 2[n - 1 + \sqrt{n+1}].$$

□

5. Atom bond-connectivity energy of graphs with one edge deleted

Edge deletion is a method used in Graph Theory very often to calculate a property of a given graph in terms of the same property of a smaller (edge deleted) graph. Using this successively, we can obtain the required property in terms of the property of much smaller graphs with known values. In this section we obtain the atom bond-connectivity energy for certain graphs with one edge deleted. First we have

Theorem 5.1. *Let e be an edge of the complete graph K_n. The atom bond-connectivity energy of $K_n - e$ is*

$$ABCE(K_n - e) = \frac{(n-3)\sqrt{2n-4} + \sqrt{2n^3 - 14n + 4}}{n-1}.$$

Proof. First

$$ABC(K_n - e) = \begin{pmatrix} 0_{2\times 2} & \sqrt{\frac{2n-5}{n^2-3n+2}} J_{2\times(n-2)} \\ \sqrt{\frac{2n-5}{n^2-3n+2}} J_{(n-2)\times 2} & \frac{\sqrt{2n-4}}{n-1}(J-I)_{(n-2)} \end{pmatrix}.$$

The characteristic equation is

$$\lambda\left(\lambda - \frac{\sqrt{2n-4}}{n-1}\right)^{n-3}\left(\lambda^2 - \frac{n-3}{n-1}\sqrt{2n-4}\,\lambda - \frac{4n-10}{n-1}\right) = 0.$$

Hence the spectrum would be

$$Spec_{ABC}(K_n - e) = \begin{pmatrix} \frac{\sqrt{2n-4}}{n-1} & \frac{(n-3)\sqrt{2n-4}+\sqrt{2n^3-14n+4}}{2n-2} & \frac{(n-3)\sqrt{2n-4}-\sqrt{2n^3-14n+4}}{2n-2} & 0 \\ n-3 & 1 & 1 & 1 \end{pmatrix}.$$

Therefore,

$$ABCE(K_n - e) = \frac{(n-3)\sqrt{2n-4} + \sqrt{2n^3 - 14n + 4}}{n-1}.$$

□

Theorem 5.2. *Let e be an edge of the complete bipartite graph $K_{n,n}$. The atom bond-connectivity energy of $K_{n,n} - e$ is*

$$ABCE(K_{n,n} - e) = 2\sqrt{\frac{2n^3 + 3n^2 - 4n - 1}{2n(2n-1)}}.$$

Proof. The atom bond-connectivity matrix is

$$SC(K_{n,n}-e)=\begin{bmatrix} 0 & 0 & 0 & \dots & 0 & \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} \\ 0 & 0 & 0 & \dots & \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \frac{\sqrt{2n-2}}{n} & \frac{\sqrt{2n-2}}{n} \\ 0 & 0 & 0 & \dots & \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \frac{\sqrt{2n-2}}{n} & \frac{\sqrt{2n-2}}{n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \dots & 0 & 0 & 0 \\ \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \frac{\sqrt{2n-2}}{n} & \dots & 0 & 0 & 0 & \\ \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \frac{\sqrt{2n-2}}{n} & \dots & 0 & 0 & 0 & \\ \frac{\sqrt{2n-3}}{\sqrt{n(n-1)}} & \frac{\sqrt{2n-2}}{n} & \frac{\sqrt{2n-2}}{n} & \dots & 0 & 0 & 0 \end{bmatrix}.$$

Then the characteristic equation is

$$\lambda^{2n-4}\lambda^2+\left(\frac{n-1}{\sqrt{2n}}\lambda-\frac{n-1}{2n-1}\right)\left(\lambda^2-\frac{n-1}{\sqrt{2n}}\lambda-\frac{n-1}{2n-1}\right)=0$$

and therefore the spectrum becomes

$$Spec_{ABC}(K_{n,n}-e)=\begin{pmatrix} \frac{-n+1}{2\sqrt{2\sqrt{2n}}}+T & \frac{-n+1}{2\sqrt{2\sqrt{2n}}}+T & \frac{n-1}{2\sqrt{2\sqrt{2n}}}+T & \frac{n-1}{2\sqrt{2\sqrt{2n}}}-T & 0 \\ 1 & 1 & 1 & 1 & 2n-4 \end{pmatrix}$$

where $T=\sqrt{\frac{2n^3+3n^2-4n-1}{2n(2n-1)}}$. Therefore,

$$ABCE(K_{n,n}-e)=2\sqrt{\frac{2n^3+3n^2-4n-1}{(2n-2)2n}}.$$

□

6. Atom bond-connectivity energy of complements

Theorem 6.1. *The atom bond-connectivity energy of the complement $\overline{K_n}$ of the complete graph is*

$$ABCE\overline{(K_n)}=0.$$

Proof. Let K_n be the complete graph with vertex set $V=\{v_1,\ v_2,\ \cdots,\ v_n\}$. The atom bond-connectivity matrix is

$$ABC(\overline{K_n})=\begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{bmatrix}.$$

Then the characteristic equation is $\lambda^n=0$. Therefore,

$$ABCE(\overline{K_n})=0.$$

□

Theorem 6.2. *The atom bond-connectivity energy of the complement $\overline{K_{1,n-1}}$ of the star graph is*
$$ABCE(\overline{K_{1,n-1}}) = 2\sqrt{2n-6}.$$

Proof. Let $\overline{(K_{1,n-1})}$ be the complement of star graph with vertex set $V = \{v_0, v_1...v_{n-1}\}$. The Atom bond-connectivity matrix is

$$ABC(\overline{K_{1,n-1}}) = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2n-6}}{n-2} & \dots & \frac{\sqrt{2n-6}}{n-2} & \frac{\sqrt{2n-6}}{n-2} \\ 0 & \frac{\sqrt{2n-6}}{n-2} & 0 & \dots & \frac{\sqrt{2n-6}}{n-2} & \frac{\sqrt{2n-6}}{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \frac{\sqrt{2n-6}}{n-2} & \frac{\sqrt{2n-6}}{n-2} & \dots & 0 & \frac{\sqrt{2n-6}}{n-2} \\ 0 & \frac{\sqrt{2n-6}}{n-2} & \frac{\sqrt{2n-6}}{n-2} & \dots & \frac{\sqrt{2n-6}}{n-2} & 0 \end{bmatrix}.$$

Then the characteristic equation is
$$\lambda^1 \left(\lambda - \frac{\sqrt{2n-6}}{n-2}\right)^{n-2} \left(\lambda - \sqrt{2n-6}\right) = 0$$
and therefore the spectrum is
$$Spec_{ABC}\overline{K_{1,n-1}} = \begin{pmatrix} \frac{\sqrt{2n-6}}{n-2} & 0 & \sqrt{2n-6} \\ n-2 & 1 & 1 \end{pmatrix}.$$

Therefore,
$$ABCE(\overline{K_{1,n-1}}) = 2\sqrt{2n-6}.$$

□

Theorem 6.3. *The atom bond-connectivity energy of the complement $\overline{K_{n\times 2}}$ of the cocktail party graph of order $2n$ is*
$$ABCE(\overline{K_{n\times 2}}) = 0.$$

Proof. Let $\overline{K_{n\times 2}}$ be the complement of the cocktail party graph with vertex set $\{u_1,\ u_2,\ \cdots,\ u_n,\ v_1,\ v_2,\ \cdots,\ v_n\}$. The atom bond-connectivity matrix is

$$ABC(\overline{K_{n\times 2}}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Then the characteristic equation becomes $\lambda^n = 0$. Hence, the spectrum is obtained as
$$Spec_{ABC}(K_{n\times 2}) = \begin{pmatrix} 0 \\ n \end{pmatrix}.$$

Therefore,
$$ABCE(\overline{K_{n\times 2}}) = 0.$$

□

Theorem 6.4. *The atom bond-connectivity energy of the $2(i)$-complement of the double star graph $S_{n,n}$ is*

$$ABCE(\overline{(S_{n,n})_{2(i)}}) = \frac{(2n-4)\sqrt{4n-6}}{2n-2} + \frac{\sqrt{24n^2-60n+34}}{2n-2} + \frac{\sqrt{16n^3-48n^2+44n-14}}{2n-2}.$$

Proof. The atom bond-connectivity matrix for the 2(i)-complement of the double star graph is

$$ABC(\overline{(S_{n,n})_{2(i)}}) = \begin{bmatrix} 0 & A & A & \dots & A & 0 & 0 & 0 & \dots & 0 \\ A & 0 & B & \dots & B & 0 & B & B & \dots & B \\ A & B & 0 & \dots & B & 0 & B & B & \dots & B \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ B & B & B & \dots & 0 & 0 & B & B & \dots & B \\ 0 & 0 & 0 & \dots & 0 & 0 & A & A & \dots & A \\ 0 & B & B & \dots & B & A & 0 & B & \dots & B \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & B & B & \dots & B & A & B & B & \dots & B \\ 0 & B & B & \dots & B & A & B & B & \dots & 0 \end{bmatrix}$$

where $A = \frac{\sqrt{3n-5}}{2n^2-4n+2}$ and $B = \frac{\sqrt{4n-6}}{2n-2}$. Then the characteristic equation becomes

$$\left(\lambda + \frac{\sqrt{4n-6}}{2n-2}\right)^{2n-4} \left(\lambda^2 + \frac{\sqrt{4n-6}}{2n-2}\lambda - \frac{3n-5}{2n-2}\right) \left(\lambda^2 - \frac{(2n-3)\sqrt{4n-6}}{2n-2}\lambda - \frac{3n-5}{2n-2}\right) = 0$$

and hence, the spectrum is

$$Spec_{ABC}(\overline{(S_{n,n})_{2(i)}}) = \begin{pmatrix} -\frac{\sqrt{4n-6}}{2n-2} & \frac{-\sqrt{4n-6}+C}{4n-4} & \frac{-\sqrt{4n-6}-C}{4n-4} & \frac{(2n-3)\sqrt{4n-6}+D}{4n-4} & \frac{(2n-3)\sqrt{4n-6}+D}{4n-4} \\ 2n-4 & 1 & 1 & 1 & 1 \end{pmatrix}$$

where $C = \sqrt{24n^2-60n+34}$ and $D = \sqrt{16n^3-48n^2+44n-14}$. Therefore,

$$ABCE(\overline{(S_{n,n})_{2(i)}}) = \frac{(2n-4)\sqrt{4n-6}}{2n-2} + \frac{\sqrt{24n^2-60n+34}}{2n-2} + \frac{\sqrt{16n^3-48n^2+44n-14}}{2n-2}.$$

□

Theorem 6.5. *The atom bond-connectivity energy of the 2-complement of the cocktail party graph $K_{n\times 2}$ is*

$$ABCE(\overline{K_{n\times 2(2)}}) = \frac{2}{n}(2n-2)^{\frac{3}{2}}.$$

Proof. Consider the 2-complement $\overline{K_{n\times 2(2)}}$ of the cocktail party graph. The atom bond-connectivity matrix is

$$ABC(\overline{K_{n\times 2(2)}}) = \begin{bmatrix} 0 & D & D & \dots & D & D & 0 & \dots & 0 & 0 \\ D & 0 & D & \dots & D & 0 & D & \dots & 0 & 0 \\ D & D & 0 & \dots & D & 0 & 0 & \dots & D & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ D & D & D & \dots & 0 & 0 & 0 & \dots & 0 & D \\ D & 0 & 0 & \dots & 0 & 0 & D & \dots & D & D \\ 0 & D & 0 & \dots & 0 & D & 0 & \dots & D & D \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & D & \dots & 0 & D & D & \dots & 0 & D \\ 0 & 0 & 0 & \dots & D & D & D & \dots & D & 0 \end{bmatrix}$$

where $D = \frac{\sqrt{2n-2}}{n}$. Then the characteristic polynomial would be

$$\lambda^{n-1}\left(\lambda + \frac{2\sqrt{2n-2}}{n}\right)^{n-1}\left(\lambda - \frac{(n-2)\sqrt{2n-2}}{n}\right)\left(\lambda - \sqrt{2n-2}\right) = 0$$

and the atom bond-connectivity spectrum is

$$Spec_{ABC}(\overline{K_{n\times 2(2)}}) = \begin{pmatrix} 0 & -\frac{2\sqrt{2n-2}}{n} & \frac{(n-2)\sqrt{2n-2}}{n} & \sqrt{2n-2} \\ n-1 & n-1 & 1 & 1 \end{pmatrix}.$$

Finally, the atom bond-connectivity energy will be

$$ABCE(\overline{K_{n\times 2(2)}}) = \frac{2}{n}(2n-2)^{\frac{3}{2}}.$$

□

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