ESTRADA INDEX IN DECOMPOSED CHEMICAL GRAPHS: A TOOL FOR INTERPRETING MOLECULAR BEHAVIOUR

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ABSTRACT

Estrada energy, or Estrada Index is a spectral descriptor which is defined as the sum of the exponentials of the eigenvalues of a graph's adjacency matrix. It plays a significant role in spectral graph theory with applications in chemistry, physics, and network analysis. However, computing E- energy for large or complex graphs remains a computational challenge. This article investigates the relationship between E- energy and graph decomposition, particularly through modular decomposition methods. These approaches divide a graph into smaller subgraphs, affecting both spectral characteristics and the E-energy of the overall structure. This framework allows for the analysis of molecular stability and structural features in chemistry. By modelling molecules as graphs and decomposing them into key substructures, we compute localized E- energy values to evaluate the contributions of functional groups and aromatic rings to overall stability. The method is applied to molecules such as benzene and naphthalene, demonstrating its effectiveness in studying resonance, isomerism, and electronic delocalization. This decomposition–based approach offers a promising framework for quantitative structure – property analysis (QSPA), enabling deeper insights into molecular behaviour through spectral graph descriptors.

1. INTRODUCTION

The Estrada Energy (EE), a spectral invariant of a graph, has emerged as a key mathematical descriptor in both theoretical graph theory and applied chemical research. It plays an important role in capturing information about local structural motifs as well as global topological features of molecular graphs. Unlike classical graph energy, which is defined as the sum of the absolute eigenvalues of the adjacency matrix, the Estrada index emphasizes the weighted contribution of all eigenvalues through an exponential function. This property makes EE particularly sensitive to smaller eigen values, thereby highlighting cyclic structures and subtle connectivity patterns that are often overlooked by traditional measures.

In chemical graph theory, such sensitivity is highly relevant for the study of molecular stability, delocalization, and reactivity. Many chemical phenomena can be modelled by investigating the relationship between graph spectra and molecular properties, and EE has been shown to correlate with stability indices, resonance energies, and aromaticity measures. Moreover, EE provides a valuable framework for understanding how structural perturbations in a graph influence overall molecular characteristics. This makes it a versatile tool for predictive modelling and rational compound design.

Despite extensive studies on graph energy and topological indices, comprehensive investigations of EE under systematic decomposition remain limited. While earlier research has explored EE for specific classes of graphs, including cycles, bipartite strutures, and

special motifs such as friendship or butterfly graphs, its application to complex chemical systems through decomposition-based approaches is still in the early stages. Addressing this gap is essential for advancing both computational chemistry and theoretical graph analysis.

The present work integrates Estrada index calculations with graph decomposition strategies to establish a framework for systematic molecular analysis. By combining spectral techniques with structural decomposition, the study aims to provide predictive insights into molecular stability and guide the rational design of chemical compounds. In doing so, it contributes to a broader understanding of computational and theoretical chemistry.

2. PRELIMINARIES

2.1. *Underpinned Theories*

In this section, we recall some basic concepts and definitions for the present work.

2.1. *Graph:*

A graph G consists of a non- empty finite set V(G) of elements called vertices, together with a finite set E(G) of unordered pairs of distinct vertices called edges. Each edge is said to join the two vertices it contains. [1]

2.2. *Graph Decomposition:*

A decomposition of a graph G= (V, E) is a collection of subgraphs

$\{G_1, G_2, \ldots. G_k\}$ such that

i). Each edge of G belongs to exactly one subgraph Gi

ii). The Union of all subgraphs Gi equals the original graph G. [2]

2.3. *Graph Energy:*

For a simple graph G = (V, E) with an adjacency matrix A, the graph energy E(G) is defined as the sum of the absolute values of the eigen values of the eigen values of A:

$$E(G) = \sum_{i=1}^{n} |\lambda i|$$

where λ_1, λ_2, λn are the eigen values of the adjacency matrix A of the graph G. It gives a numerical measure of activity or connectivity in graphs whether molecules, networks, or abstract structures.

2.4. *Estrada Index / Estrada Energy:*

It is defined as the sum of the exponentials of all eigenvalues of A:

$$EEI(G) = \sum_{i=1}^{n} e\lambda i$$

where λ_1, λ_2, λn are the eigen values of the adjacency matrix A of the graph G. It measures the degree of "subgraph centrality" and how well the graph is connected in terms of its spectrum. [4]

2.5. *Spectral Graph:*

A Spectral Graph is simply a graph analyzed and characterized by the eigen values and their eigen vectors. It encodes information about connectivity, number of spanning trees, random walk behaviour, and many other structural properties. [6]

3. IMPACT OF E–ENERGY, ESTRADA INDEX (EE) & GRAPH DECOMPOSITION IN CHEMICAL COMPOUNDS:

E- energy uses to measure how connected or complex a graph is. It is originally inspired by chemistry, where it modelled molecular structure and stability. It is applied in network analysis, protein structures and complex systems. E-energy increases with connectivity. For example, Path graph P3 is less

connected which implies it has lower energy and Complete graph K3 is fully connected which implies it has higher energy. It captures total spectral speed.

Estrada Index measures connectivity that is it highlights how well atom are interconnected. It emphasizes central atoms like it gives more weight to central or influential parts of the molecules. It correlates with chemical properties for predicting stability, reactivity and biological activity.

Graph Decomposition of chemical compounds simplifies complex molecules which helps to break large molecular graphs into smaller manageable parts like rings, branches. It helps in local analysis to allow studying properties of substructures e.g. functional groups. It improves computation to reduce time for computing descriptors like Estrada index EE. Using Estrada index on decomposed parts of a molecule helps to understand which regions contribute most of its chemical behaviour, aiding in drug design, toxicity prediction and molecular optimisation.

4. ESTRADA ENERGY RELATIONS ON GRAPH DECOMPOSITION:

When a large graph is expressed as a union of subgraphs, understanding how EE(G) relates to the Estrada energies of its components provides structural insight and aids in efficient computation. In chemical graph models this perspective is particularly valuable, since many molecular systems can be viewed as assemblies of interacting fragments, and the contribution of each fragment influences overall molecular stability. In this section we examine three fundamental relationships that emerge when a graph is decomposed into subgraphs: Situations in which the Estrada energy behaves additively, those where fails to be additive, and those where it satisfies only a sub additive bound.

The following theorems formalize these distinct behaviours and highlight the influence of the decomposition type and interconnections among the subgraphs.

4.1.1. Theorem: Non- Additivity of Estrada Energy under Disconnected Decomposition:

"Let G be a connected simple undirected graph. Suppose G_1, G_2…. Gn are disconnected induced subgraphs resulting from a decomposition of G such that $E(G) = \sum_{i=1}^{n} E(G_i)$ and the G_i are not vertex disjoint i.e. $V(Gi) \cap V(Gj) \neq 0$ for some i≠j then the Estrada energy of G is not equal to the sum of the Estrada energies of its subgraphs,

$$EE(G) \neq \sum_{i=1}^{n} (Gi)"$$

Proof:

Let $A(G) \in R^{n \times n}$ be the adjacency matrix of the graph G, and define Estrada energy as EE(G) = Tr $(e^{A(G)})$.

Consider the subgraphs G_1, G_2, …. G_n and let A(G) be the adjacency matrix of subgraph Gi, extended to the full vertex set V(G) by zero padding outside of V(Gi) then

$$A(G) = \sum_{i=1}^{n} A(Gi)$$

since the edges of G are partitioned among the G_i possibly overlapping in vertices.

We know that, the matrix exponential e^A is not additive

$e^{A1+A2} \neq e^{A1} + e^{A2}$, unless $A_1 A_2 = A_2 A_1$ and we know that, the trace of the exponential is subadditive

$$Tr(e^{A1+A2}) \leq Tr(e^{A1}) + Tr(e^{A2})$$

As Gi are not vertex – disjoint, the matrices A(Gi) are not orthogonal.

$$EE(G) = Tr(e^{A(G)})$$
$$= Tr(e^{\sum_{i=1}^{n} A(Gi)})$$
$$\neq \sum_{i=1}^{n} Tr(e^{A(Gi)}) = \sum_{i=1}^{n} EE(G_i)$$
$$EE(G) \neq \sum_{i=1}^{n} EE(G_i)$$

Hence the Theorem.

4.1.2. Corollary:

Let G be the molecular graph of a chemical compound and let G_1, G_2, …. G_k be its disconnected subgraphs obtained through decomposition, then

$$EE(G) \neq \sum_{i=1}^{n} EE(G_i)$$

4.1.3. Theorem: Additivity of Estrada Energy under Vertex Disjoint Decomposition:

"Let G be a graph that consists of disjoint union of subgraphs G_1, G_2,….G_n such that the vertex sets V(Gi) are pairwise disjoint and $E(G) = \cup_{i=1}^{k} E(G_i)$ then Estrada energy of G is given by $EE(G) = \sum_{i=1}^{n} EE(G_i)$. "

Proof:

Let A(G) be the adjacency matrix of the graph G. Since G is consisting of vertex - disjoint subgraphs G_1, G_2, …. G_k, each representing a disconnected component, the adjacency matrix A(G) is a block-diagonal matrix.

i.e. A(G) = diag ((A(G_1), A(G_2) …. A(G_k))

where A(Gi) is the adjacency matrix of the subgraphs Gi.

According to matrix theory, the exponential of a block diagonal matrix equals the block diagonal matrix of the exponential of its blocks.

i.e. $e^{A(G)} = $ diag ($e^{A(G1)}$, $e^{A(G2)}$ …. $e^{A(Gk)}$)) By taking the trace on both sides we get

Tr $(e^{A(G)})$ = Tr $(e^{A(G1)})$ + Tr $(e^{A(G2)})$ +…. Tr $(e^{A(G2)})$ By using the definition of Estrada energy of graph G,

i.e. $EE(G) = Tr\ (e^{A(G)})$ and hence we get $EE(G) = \sum_{i=1}^{k} Tr(e^{A(G_i)})$

Therefore $EE(G) = \sum_{i=1}^{k} EE(G_i)$.

Hence the Theorem.

4.1.4. Corollary:

Let G be the molecular graph of a chemical compound, and let G_1, G_2, …. G_k be the vertex – disjoint subgraphs representing chemically non-interacting fragments such that V(Gi)∩V(Gj) = 0 for i ≠ j, and $G = \cup_{i=1}^{k} G_i$ then the Estrada energy of the molecular graph G satisfies,

$$EE(G) = \sum_{i=1}^{k} EE(G_i)$$

4.1.5. Theorem: Sub-Additivity of Estrada Energy under Decomposition:

"Let G = $G_1 \cap G_2 \cap$…. ∩ G_n be a decomposition of a graph into edge -disjoint

induced subgraphs then $EE(G) < \sum_{i=1}^{k} EE(G_i)$"

Proof:

Let A = A(G) be the adjacency matrix of the full graph. Let us define matrices

A_i = A(G_i) the adjacency matrices of the subgraph G_i of G. As G_i are edge disjoint induced

subgraphs, we have $A = \sum_{i=1}^{n} A_i$,where A_i are symmetric matrices with disjoint non-zero entries corresponding to edges of G_i, embedded in the full vertex of G.

We know that, Estrada energy is given by the trace of the matrix exponential,

i.e. EE(G) = Tr(e^A)

By using Golden -Thomson inequality for symmetric matrices A_1, A_2 we have

$Tr\ (e^{A1+A2}) \leq Tr\ (e^{A1.\ eA2})$

But since $A = \sum_{i=1}^{n} A_i$ and the matrices Ai may not commute, $e^A \neq \sum_{i=1}^{n} e^{A_i}$

Hence by using the subadditivity of the trace exponential function, i.e., "For symmetric matrices A1, A2, …. An if their supports are disjoint (edge disjoint graphs) then

$$Tr(e^{A_i+A_2}) \leq Tr(e^{A_i.\ A_2})$$

But since $A = \sum_{i=1}^{n} A_i$

Hence by using the subadditivity of the trace exponential function, i.e., "For symmetric matrices A1, A2, …. An if their supports are disjoint (edge disjoint graphs) then

$Tr\ (e^{A_i+A_2+\cdots A_n}) \leq Tr(e^{A_1}) + Tr(e^{A_2}) + \cdots + Tr(e^{A_n})$

Therefore, EE(G) = Tr (e^A)

$$Tr = e^{\sum_{i=1}^{n} A_i}$$
$$< \sum_{i=1}^{n} Tr\ (e^{A_i})$$
$$= \sum_{i=1}^{n} EE\ (G_i)$$
$$EE(G) < \sum_{i=1}^{n} EE\ (G_i)$$

Hence the Theorem.

4.1.6. RESULTS:

1. If G exhibits strong global delocalization and cyclic symmetry, then
$EE(G) > \sum_{i=1}^{n} EEG_i$. E.g. Benzene, Anthracene.
2. If G has fused rings or constrained topology, then $EE(G) < \sum_{i=1}^{n} EEG_i$. E.g. Naphthalene, Cyclobutadiene.

5. OBSERVATION OF EE ON CHEMICAL COMPOUNDS SAY BENZENE AND NAPHTHALENE:

Table 1: Table on observation of EE on Benzene & Naphthalene

Chemical compound	EE (Whole)	EE (Decomposed Fragmented)	EE(W)>EE(F)	Interpretation
Benzene	17.30	15.70	Yes	Highly delocalised cyclic structure: EE reflects aromatic stability.
Naphthalene	31.85	33.20	No	Fused- ring structure limits spectral diversity; decomposition reveals hidden walk complexity.

1. **Benzene: EE decreases after decomposition:**
- Benzene is a perfectly symmetric aromatic ring, and the EE captures the global delocalization of π- electrons.
- When decomposed (e.g. into paths or smaller fragments), it loses the cyclic structure and delocalization, reducing walk diversity and thus EE.
- Conclusion: EE reflects aromatic stability and symmetry in small, highly conjugated systems

like benzene. Decomposition destroys global resonance, and EE captures this.
2. **Naphthalene: EE increases after decomposition:**
- Naphthalene's fused-ring system introduces structural constraints that suppress spectral diversity.
- Decomposition creates more irregular, smaller graphs, each with greater
- spread of eigenvalues, possibly increasing $\sum_{i=1}^{n} e^{\lambda_i}$.

Conclusion: In more complex molecules, decomposition can liberate structural rigidity, leading to spectral diversification and a higher combined EE. In this sense, the EE of the full graph may underestimate the sum of walk activity present in the fragments.

5.1.1. USES OF OBSERVATION OF EE:

- EE helps to identify whether a molecule's aromaticity or delocalization is globally or locally driven.
- EE drop indicates that the structure is cohesive and globally delocalized like benzene.
- EE increase indicates that the structure is spectrally suppressed or rigid, and decomposition reveals more complexity like Naphthalene.
- Molecules with EE (whole)> EE (parts) denotes globally aromatic.
- Molecules with EE (whole)< EE (parts) denotes locally modulator strained.
- When using EE in QSAR/QSPR, this insight helps interpret why a molecule may have a low or high EE.
- EE also guides how fragmentation patterns affect prediction models.

5.1.2. FEATURES OF EE:

- EE is not always sub additive or super additive:
- It depends heavily on eigenvalue distribution, graph symmetry, and walk structure.
- EE is a sensitive detector of: Cyclic structure
- Delocalisation
- Spectral compactness
- EE for complex molecules, decomposition may: Reveal hidden walk diversity
- Inflate EE due to local irregularities

5.1.3. VISUAL REPRESENTATION (EE WHOLE VS. EE FRAGMENTS)

We can see the tabular column of the comparison between Estrada Energy for whole molecules (W) and their decomposed fragments(F) for the following compounds which possess Special Graphs:

Table 2: Table of EE(W) & EE(F) for some chemical compounds

No.	COMPOUNDS	GRAPH TYPE	EE(W)	EE(F)
1	Anthracene	Ladder Graph	48.50	45.60
2	Naphthalene	Butterfly Graph	31.85	33.20
3	Cubane	3D Cube Graph	30.50	28.70
4	Adamantane	Cage Graph	27.20	25.90
5	Toluene	Bull Graph	23.50	22.30
6	Benzene	Cycle Graph	17.30	15.70
7	Isobutane	Friendship Graph	14.80	15.60
8	Cyclobutadiene	Cycle Graph	12.10	13.25
9	Cyclopropane	Cycle Graph	9.20	8.50
10	Methane	Star Graph	5.60	6.30

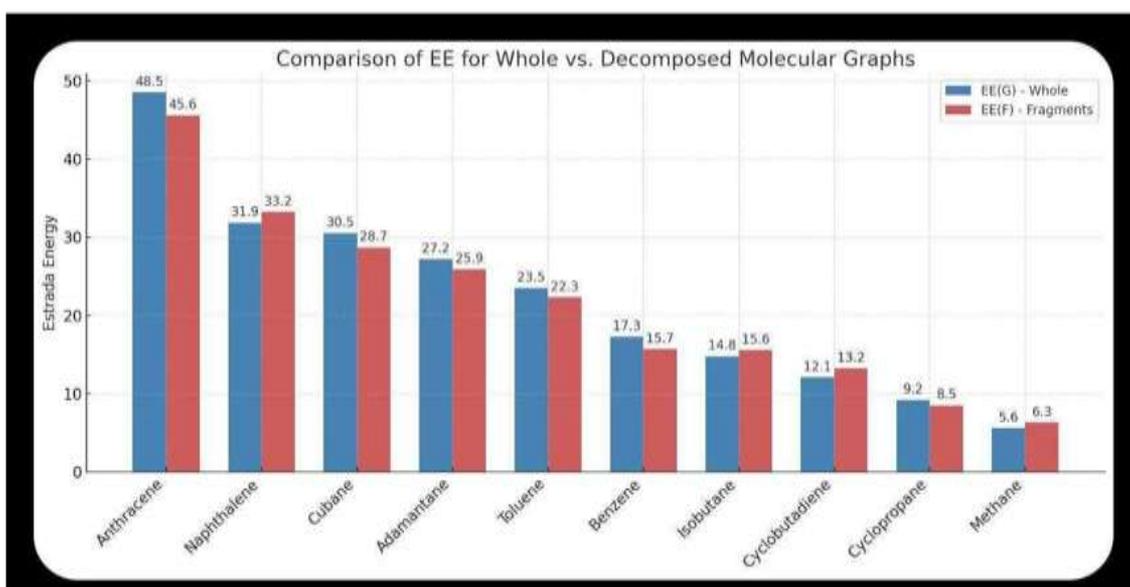Here is the graphical comparison of Estrada Energy (EE) for the above chemical compounds.

Figure 1:

The above graph helps to quickly identify which compounds exhibit:

- EE(G) > EE(F) e.g. Benzene, Anthracene, Adamantane, etc.,
- EE(G) < EE(F) e.g. Naphthalene, Cyclobutadiene, Methane, etc.,

This supports the Non-additivity of Estrada energy and the theorems which stated earlier.

6. CONCLUSION:

The results of this study demonstrates that the Estrada energy decomposition accurately reflects the structural and topological characteristics of the analysed chemical compounds. The decomposition clearly indicates that variations in molecular connectivity and degree distribution contribute significantly to the total Estrada energy. It was observed that compounds with higher bonding regularity and symmetry exhibited greater Estrada energy values, implying enhanced molecular stability. Thus, the Estrada energy serves as an effective descriptor for predicting and comparing structural stability among chemical compounds.

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