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Spectral Analysis of Edge Mass Graph Energy with Applications to Benzenoid Compounds

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Abstract: ***This paper presents a spectral analysis of edge mass graph energy, highlighting its theoretical properties and chemical applications. The spectral radius and energy parameters of the edge mass adjacency matrix are derived and applied to benzenoid compounds. Analytical results reveal strong correlations between graph-based spectral descriptors and physicochemical properties, demonstrating the potential of edge mass energy in molecular modeling.***

Keywords: Graph energy, spectral analysis, edge mass adjacency matrix, benzenoid compounds, molecular descriptors.

1. Introduction

Graph energy, rooted in chemical graph theory, measures molecular stability via eigenvalues of adjacency matrices [8], [9]. Building on Zagreb indices [1], [3], this work introduces the **edge mass adjacency matrix** (A_w(G)), defined such that entries reflect edge degrees. The spectral radius (\lambda_w) and corresponding energy (E_w(G)) are investigated. Our contributions include theoretical bounds for these parameters and their applications to chemical compounds, specifically benzenoid hydrocarbons.

2. Preliminaries

- **Vertex and edge weights**: (w(v) = d_G(v)); (w(e=uv) = d_G(u)+d_G(v)-2).
- **Edge mass adjacency matrix**:
  [
  (A_w(G))_{ij} =
  \begin{cases}
  d_G(v_i)+d_G(v_j)-2, & v_i \sim v_j \
  0, & \text{otherwise}
  \end{cases}
  ]
- **Edge mass energy:**
  [
  E_w(G) = \sum_{i=1}^n |\lambda^w_i|
  ]
  where (\lambda^w_i) are eigenvalues of (A_w(G)).

Properties link (E_w(G)) with the reformulated Zagreb index (EM_1(G)).

3. Theoretical Results

Key bounds established:

- **Spectral radius:**
  [
  4(\Delta-1) \leq \lambda_w(G) \leq 2(\Delta-1)\sqrt{2m-n+1}
  ]
  with equality for regular and complete graphs.
- **Energy bounds:**
  [
  \sqrt{2EM_1(G)} \leq E_w(G) \leq \sqrt{2n , EM_1(G)}
  ]
  Additional refinements incorporate eigenvalue extremes.

Examples:

- (E_w(K_n) = 4(n-1)(n-2))
- (E_w(K_{m,n}) = 2(m+n-2)\sqrt{mn})

4. Applications to Benzenoid Hydrocarbons

Molecular graphs of 22 benzenoid hydrocarbons were analyzed. Energies (E(G)) and (E_w(G)) were computed programmatically. Experimental data for boiling point, entropy, acentric factor, octanol-water partition coefficient (log P), Kovats retention index, and enthalpy were compared with graph energies [17].

Correlation results:

- (E_w(G)) showed stronger correlations with physicochemical properties than classical (E(G)), with coefficients (r > 0.93).
- High correlations also observed between (E_w(G)) and 11 molecular descriptors (Zagreb indices, Randic index, ABC index, etc.), with (r > 0.97).

5. Regression Models

Quadratic regressions demonstrated predictive potential:

- With **(E(G))**: best fit for acentric factor ((r = 0.9823)), moderate for boiling point and log P ((r \approx 0.92)), weaker for entropy and enthalpy.

- With **(E_w(G))**: excellent fits for boiling point ((r = 0.9705)) and retention index ((r = 0.9741)), with consistent improvements across properties.

6. Discussion

The results validate **edge mass energy** as a robust molecular descriptor. It improves upon classical graph energy in correlating structural parameters with measurable physicochemical properties, offering enhanced predictive ability in cheminformatics and QSAR modeling.

7. Conclusion

This work introduced and analyzed the edge mass adjacency matrix, derived spectral bounds, and established its energy as a valuable invariant. Applications to benzenoid hydrocarbons demonstrated strong correlations with experimental properties, highlighting the utility of (E_w(G)) in molecular property prediction. Future work may extend this framework to larger polycyclic systems and machine-learning-based descriptor integration.

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