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Graph energy and its applications in chemistry: A review

Abstract

Graph energy is derived from Hückel molecular orbital theory. It is determined as the sum of the absolute values of eigenvalues of a graph. This is now a significant concept in mathematical chemistry. Scientists can model molecules using graphs, with atoms being vertices and bonds being edges. This enables them to approximate π-electron energy, molecular stability, and chemical reactivity. This approach is widely applied in the prediction of resonance energy, QSAR/QSPR model building, and examination of chemical properties without much experimental effort. Its recent modifications, including Laplacian, Randić, and Sombor energies, make it even more prominent in drug discovery, nanotechnology, and materials science. Therefore, graph energy is a critical bridge between mathematics and chemistry.

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Introduction

Definition 1.1.

The idea of graph energy was first introduced by Ivan Gutman in 1978, although its roots go back to earlier work in theoretical and mathematical chemistry (Gutman, 1978). Specifically, Hückel molecular orbital (HMO) theory, developed in the 1930s, established one of the first links between molecular structure and linear algebra. Hückel's method estimated the total π-electron energy of conjugated hydrocarbons by connecting it to the eigenvalues of the adjacency matrix of the related molecular graph. In this context, each carbon atom in the molecule is treated as a vertex, and each carbon-carbon bond serves as an edge. This creates a purely mathematical object that captures key chemical information (Coulson, 1940 and McClelland, 1971 and Gutman, 1977). This strong abstraction led Gutman to expand the idea beyond chemistry, resulting in the modern definition of graph energy.

Let G be a simple graph G of order n with adjacency matrix A(G) having eigenvalues $\lambda_1, \lambda_2, \lambda_3 \ldots \ldots \lambda_n$, form the spectrum of G. The graph energy is defined as

$$E(G) = \sum_{i=0}^{n} |\lambda_i|$$

This seemingly simple definition has far-reaching implications. From a mathematical perspective, it introduces a spectral parameter of graphs that connects combinatorial structure with linear algebraic properties. From a

chemical perspective, it provides a way to approximate molecular stability, reactivity, and electron distribution without requiring extensive quantum-mechanical computations.

Over the years, graph energy has become a central concept not only in chemical graph theory but also in pure graph theory and applied mathematics. Researchers discovered that graph energy exhibits interesting mathematical properties: it is invariant under graph isomorphism, closely related to the degree distribution of a graph, and sensitive to structural modifications such as edge deletion or addition. These traits make it valuable for both theory and practical use. For instance, in chemistry, two molecules that differ by a slight structural change, known as isomers, can have different graph energies. This often relates to differences in stability or reactivity. In mathematics, graph energy serves as a standard for extreme problems. This includes finding graphs with the lowest or highest energy under specific conditions (Estrada & Benzi 2017).

In chemistry, graph energy is particularly valuable in the investigation of conjugated systems such as benzene, polycyclic aromatic hydrocarbons, and fullerenes. Such molecules find significant use in organic chemistry and material science. Direct estimation of their π-electron energy from graph spectra provides both theoretical information and tangible application. Graph energy finds other applications in quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR). It is used as a descriptor for linking molecular structure with biological activity or physical property.

The concept has developed into a broader family of energy-like parameters. Its variants such as Laplacian energy, signless Laplacian energy, Randić energy, and Sombor energy generalize the original idea. They do this either by replacing other graph matrices or by giving different weights to the eigenvalues (Veeragoudar et al. 2022). These extensions have refined the mathematics and added predictive capability in chemical and biological modeling. For example, Laplacian energy is related to the network structure and stability, while Sombor energy is degree-based information relevant to molecular branching.

In short, graph energy began as a mathematical understanding of molecular orbital theory. Through the passage of time, however, it has developed into a flexible concept linking mathematics, chemistry, and applied sciences. It continues to play its original role in theoretical chemistry, shedding light on molecular stability and electronic structure while motivating novel studies on spectral graph measures. Graph energy's marriage of mathematical beauty and chemical relevance thus renders it a useful tool and an intriguing field of current study.

2. Graph energy and its variants:

Let G be a graph of order n, as previously mentioned, and let $\lambda_1, \lambda_2, \lambda_3 \ldots \ldots \lambda_n$ be the eigenvalues of its adjacency matrix. Presume that the labels on them are not in ascending order. According to the Hu¨ckel molecular orbital theory, the total energy of an unsaturated conjugated hydrocarbon's π-electrons is then determined by (Graovac et al. 1977)

$$E_{\pi}=\begin{cases} 2\sum_{i=1}^{n/2}\lambda_i & if\ n\ is\ even, \\ 2\sum_{i=1}^{(n-1)/2}\lambda_i + \lambda_{(n+1)/2} & if\ n\ is\ odd, \end{cases} \qquad (2.1)$$

It should be emphasized that the graph G, to which Eq. (2.1) applies, represents a “molecular graph” that must adhere to certain structural constraints. In particular, G must be connected, and no vertex can have a degree greater than three. Therefore, it is understandable that mathematicians were not especially inclined to explore such a peculiar graph-spectral expression as the right-hand side of Eq. (2.1), since its relevance is confined to only a limited class of graphs.

On the other hand, it could be easily shown that if the conditions

$$\lambda_{\frac{n}{2}} \geq 0 \geq \lambda_{n/2+1} \qquad if\ n\ is\ even, \qquad (2.2)$$

$$\lambda_{(n+1)/2} = 0 \qquad if\ n\ is\ odd.$$

are satisfied, then Eq. (2.1) reduces to

$$E_\pi = \sum_{i=0}^{n} |\lambda_i|$$

The observation naturally led to the formulation of graph energy as defined in Eq. (1.1).

Details on the validity of conditions (2.2), as well on other mathematical arguments in favor of Eq. (1.1) can be found elsewhere (Gutman et al. 2019 and Shi & Gutman, 2012 and Gutman & Furtula, 2017).

A quarter of a century later, a thorough investigation into graph energy began and is currently ongoing. The book presents the primary outcomes attained in this domain (Shi & Gutman, 2012).

Inspired by the graph energy theory's success, variations based on matrices other than the adjacency matrix were put out. Here, we define the initial set of these graph energies.

The degree of the graph (G) i-th vertex is shown by deg(i).

Let (G) be the vertex degrees diagonal matrix. Then Laplacian matrix (G) is

$$L(G) = (G) - A(G).$$

The extended adjacency matrix is the square matrix of order n, whose (i, j)-element is equal to

$$\frac{1}{2}\left(\frac{\deg(i)}{\deg(j)} + \frac{\deg(j)}{\deg(i)}\right)$$

if the vertices i and j are adjacent, and is zero otherwise.[15]

The Randić matrix of a graph G is an $n \times n$ square matrix. whose (i, j)-element is equal to

$$\frac{1}{\sqrt{\deg(i)\,\deg(j)}}$$

if i and j are adjacent vertices, and is zero otherwise [16].

The distance matrix of a connected graph G is defined as a square matrix of order n, in which the (i,j)-element denotes the distance between vertices i and j.

Definition 2.1.

a) The extended energy is the sum of absolute values of the eigenvalues of the extended adjacency matrix (Yang et al. 1994).

b) The total of the absolute values of the eigenvalues of $L(G) - \frac{2m}{n} I_n$, is the Laplacian energy of a graph of order n and size m. where $I_n$is the unit matrix od order n (Gutman & Zhou, 2010).

c) The distance energy of a connected graph is the sum of absolute values of the eigenvalues of the distance matrix (Indulal et al. 2008).

d) The Randi´c energy is the sum of absolute values of the eigenvalues of the Randi´c matrix (Bozkur et al. 2010).

Assume that M is a $p \times q$ matrix, and that $M^t$is its inverse. The positive square roots of the eigenvalue MM^t are then the singular values of M.

A significant step forward in the theory of graph energy was made by Vladimir Nikiforov (Nikiforov, 2007).

Definition 2.2. (Nikiforov, 2007) Let $\sigma_1, \sigma_2, \sigma_3, \ldots\ldots\ldots \sigma_n$be the singular values

of the matrix M. Then the energy of M is

$$E(M) = \sum_{i=0}^{n} \sigma_i$$

Needless to say, that in the case of square symmetric matrices, the energies defined in Definitions 1.1, 2.1, and 2.2 coincide.

3. literature review:

Reja & Nayeem (2024) The Sombor index of a graph $G = (V(G), E(G))$ is defined as the sum $\sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}$,where d_x denotes the degree of a vertex $x \in V(G)$. Meanwhile, the energy of a graph is calculated as the sum of the absolute values of the eigenvalues of its adjacency matrix. In this study, we enhance the understanding of the relationship between the Sombor index and graph energy, establishing explicit connections for various graph classes including trees, unicyclic, bicyclic, and tricyclic graphs, as well as fortriangular chains, square cactus chains, and hexagonal cactus chains. Furthermore, we determine sharp bounds for the graph energy of zigzag and linear hexagonal chain structures, offering deeper insights into their structural and spectral properties. This work provides a comprehensive framework linking topological indices with spectral characteristics of complex graph systems.

Zhang et al. (2024) Molecular topology has become an essential tool in drug discovery because it helps identify molecules with similar topological structures, which often share similar biological properties. In this study, a strength-weighted graph approach was applied to calculate distance-based topological indices for the 2D lattice geometry of BCZ benzene molecules. These indices were then used to construct a linear regression model to predict the graph energy of the molecules, showing strong correlation. Additionally, their 13C NMR signals and intensity patterns were compared using distance matrices and HOMO-LUMO energy gaps, offering insights into both electronic characteristics and structural behavior. This integrated approach highlights how graph theory and molecular topology can work together to advance the understanding and design of pharmacologically significant molecules.

Zemljič & Žigert Pleteršek (2023) provides meaningful information regarding the connection between cyclic and acyclic molecular graph energies, which include linear equations allowing for accurate prediction of said topological index based solely on knowledge of the order of the molecular graph. The article also suggests some measures to characterize the smoothness of graph energy and studies their behavior systematically for different chemical graphs. In the future, one potential direction is to benchmark these findings against other molecular descriptors to determine how accurately graph energy predicts molecular properties relative to other topological indices. Comparisons such as these would further solidify the validity of graph energy in computational chemistry and further apply its usefulness to quantitative structure–activity and structure–property relationship studies. Through such associations, researchers are able to determine the predictive power and merit of graph energy as a molecular descriptor.

Jahanbani et al. (2023) sets a number of lower and upper bounds for graph energy in terms of known topological indices, including the first general multiplicative Zagreb index, the general Randić index, the general zeroth-order Randić index, redefined Zagreb indices, and the atom-bond connectivity (ABC) index. In addition to these, the research also obtains new estimates for graph energy by relating it to some basic graph invariants such as diameter, girth, algebraic connectivity, and radius. These findings not only add to the theoretical discipline of spectral graph theory but also find applications in the practical fields of chemistry and network science, where energy and topological indices are potent predictors of molecular and structural characteristics.

Veeragoudar et al. (2022) The correlation coefficient (r) is commonly used to quantify the ability of a topological index in forecasting the physico-chemical characteristics of chemical compounds in QSPR studies. A larger value

of r indicates a stronger relationship between the chosen index and the property under investigation, thereby confirming its effectiveness as a predictive measure. QSPR research has shown that regression models developed using such indices often yield the most reliable and statistically significant predictions of physico-chemical properties. This highlights the importance of topological descriptors, such as graph energy, in explaining chemical behavior and in guiding the synthesis of new compounds with predetermined characteristics. By incorporating these models, researchers can achieve more accurate predictions and improve molecular design strategies.

Iram, (2021) For a graph G, its eigenvalues are computed from the adjacency matrix, and graph energy, denoted by E(G), is the sum of the absolute values of these eigenvalues. Graph energy is of practical relevance in chemistry since it gives a good estimate for the total π-electron energy in molecular structures. Based on this relationship, researchers have also considered the energy of certain classes of graphs, such as the triangular book graph $B(3,n)$,the quadrilateral book graph B_n^4, and the restricted square of the $B_{(n,n)}$ graph, emphasizing the more general applications of graph energy in mathematics and chemistry.

Vaidya & Popat (2017) A graph $G's$ eigenvalue is equal to the adjacency matrix's eigenvalue. Summing the absolute values of these eigenvalues provides the energy of G, or $E(G)$. This introduces an obvious question: What is the best way to relate the energy of a given graph G to a graph that is generated from G using a particular graph operation? Author have looked at two specific graphs to answer this question: the splitting graph, which is represented by the symbol $S'(G)$, and the shadow graph, which is designated as $D_2(G)$. The conclusive results of the study show that $E(D_2(G)) = 2E(G)$ and $E(S'(G)) = \sqrt{5}\,E(G)$.

Thomas et al. (2017) The authors highlight that graph theory, as a branch of mathematics, forms the basis for structural studies in chemistry. Since any molecule or compound can be modeled as a graph with vertices representing atoms and edges representing bonds, this perspective naturally raised questions about whether such representations could predict physical and chemical properties. Using graph-theoretical methods, properties such as the molecular spectrum, π-electron energy, and spectral radius can indeed be analyzed and estimated. This work serves as an introduction to the study of spectrum and graph energy in molecular graphs, emphasizing their usefulness in mathematical chemistry.

4. Applications of Graph Energy in Chemistry

Graph energy, initially conceived as a mathematical abstraction within spectral graph theory, has proven to be a remarkably effective tool in theoretical and computational chemistry. The concept of graph energy was originally motivated by the aim of calculating the sum of the π-electron energy in conjugated hydrocarbons within the framework of Hückel molecular orbital (HMO) theory. By representing molecules as graphs, where vertices denote atoms and edges represent covalent bonds, the eigenvalues of the adjacency matrix can be utilized to determine the "energy" of the graph. This graph-theoretical energy closely corresponds to the total π-electron energy of conjugated systems, allowing approximate assessments of molecular stability, reactivity, and related electronic properties without requiring complete quantum chemical calculations. This approach provides a computationally efficient means of analyzing complex molecules while maintaining a strong link to chemical theory.

One of the principal applications of graph energy in chemistry is the study of conjugated hydrocarbons such as benzene, naphthalene, anthracene, and polyenes. In these systems, delocalized π-electrons are distributed across conjugated bonds, imparting characteristic stability and reactivity. Graph representations enable the calculation of the energy spectrum of the molecular graph, which serves as an analogue of the π-electron distribution. Comparing the graph energies of different conjugated molecules makes it possible to estimate relative stability, identify resonance structures, and gain insight into electron delocalization. For instance, the stability of benzene

is effectively captured by the graph energy of its cyclic structure compared with acyclic analogues, offering a theoretical estimate of resonance energy. This methodology has also been extended to polycyclic aromatic hydrocarbons (PAHs), where graph energy has been shown to account for trends in stability, reactivity, and electronic properties across different isomers (Gutman, 1977).

Graph energy is also a useful tool for the estimation of aromaticity and resonance stabilization. Aromatic compounds by definition have higher stability resulting from electron delocalization in cyclic conjugated systems. Older ways of determining aromaticity, for example, resonance energy computation or Nucleus-Independent Chemical Shifts (NICS), usually involve complicated quantum chemical calculations. Graph energy provides a less complicated but very informative alternative. Through the computation of the energy of the graph of a molecule and comparison with an imaginary acyclic isomer with the same number of vertices, the difference gives an approximation of resonance stabilization.

Pharmaceutical chemistry and drug design have also seen the applications of graph energy, especially in Quantitative Structure–Activity Relationship (QSAR) research (Veeragoudar et al. 2022). Here, molecules are represented as graphs, and resultant graph energies are used as molecular descriptors that are related to biological activity, toxicity, or pharmacokinetics. In combining graph energy with statistical and machine learning methods, scientists are able to filter through large collections of drug candidates effectively, forecast likely toxicity, and rank compounds for experimental testing. As an illustration, graph energy has been used to anticipate antiviral, anticancer, and antibacterial compounds' binding affinity, stability, or cellular interaction. This method decreases drug discovery cost and time considerably by shortlisting lead candidates prior to experimental screening.

Graph energy also finds uses in polymer science and macromolecular chemistry. Polymers and macromolecules, such as proteins and artificial polymers, can be modeled as linear or dendritic graphs with monomer units or amino acids as the vertices and covalent or non-covalent interactions as the edges. Computation of graph energy yields details about chain conformations, stability, solubility, and intermolecular interactions. In proteins, graph representation of amino acid sequences or secondary structure elements enables spectral comparison between low sequence identity proteins so that structural motifs or functional similarities can be identified. This has application in bioinformatics, protein engineering, and materials science, where the stability and functionality of macromolecular assemblies are issues of prime importance.

Overall, graph energy in chemistry acts as a link between chemical intuition and mathematics. It offers computationally effective methods for calculating molecular stability, evaluating aromaticity, separating isomers, examining nanostructures, drug discovery, and macromolecular interaction comprehension. Its versatility over small molecules, polymers, nanomaterials, and hierarchical clusters demonstrates its increasing relevance to contemporary chemical research. As computational capabilities improve and integration with machine learning and quantum chemistry becomes more common, applications of graph energy in chemistry should further increase, revealing more profound insights into molecular design, reactivity, and function.

Conclusion

Graph energy has become an important concept in mathematical chemistry because it links molecular structure with chemical properties. Originating from Hückel molecular orbital theory, it is used to estimate molecular stability, π-electron energy, and chemical reactivity. With the development of new forms such as Sombor, Randić, and Laplacian energies, its applications have expanded into fields like drug discovery, nanotechnology, and materials science. Ongoing studies show that graph energy is not limited to theoretical work but also serves as a practical tool connecting mathematics with real chemical research.

References

1. Graovac, I. Gutman, N. Trinajsti´c, Topological Approach to the Chemistry of Con- jugated Molecules, Springer, Berlin, 1977.
2. J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, J. Chem. Phys. 54 (1971), 640–643.
3. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, Proc. Cambridge Phil. Soc. 36 (1940), 201–203.Estrada, E., & Benzi, M. (2017). What is the meaning of the graph energy after all?. Discrete Applied Mathematics, 230, 71-77.
4. G. Indulal, I. Gutman, A. Vijayakumar, On distance energy of graphs, MATCH Com-mun. Math. Comput. Chem. 60 (2008), 461–472. Gutman, The energy of a graph, Ber. Math–Statist. Sekt. Forschungsz. Graz 103 (1978), 1–22.
5. Gutman, Acyclic systems with extremal H¨uckel π-electron energy, Theor. Chim. Acta 45 (1977) 79–87.
6. Gutman, B. Furtula, Energy of Graphs – Survey, Census, Bibliography, Serb. Acad. Sci. & Arts, and Univ. Kragujevac, Kragujevac, 2019.
7. Gutman, B. Furtula, The total π-electron energy saga Croat. Chem. Acta 90 (2017), 359–368.
8. Gutman, B. Zhou, Laplacian energy of a graph, Linear Algebra Appl. 414 (2006), 29–37.
9. Jadav, I. (2021). Energy of Some New Graph. Advances in Mathematics: Scientific Journal. https://doi.org/10.37418/AMSJ.10.3.48
10. Jahanbani, A., Sheikholeslami, S. M., & Filipovski, S. (2023). Relations between the energy and topological indices of a graph. *Mediterranean Journal of Mathematics*, *20*(5), 264.
11. Reja, M. S., & Nayeem, S. M. A. (2024). On Sombor index and graph energy of some chemically important graphs. *Examples and Counterexamples*, *6*, 100158.
12. S¸ . B. Bozkurt, A. D. G¨ung¨or, I. Gutman, A. S C¸ evik, Randi´ c matrix and Randi´c energy,MATCH Commun. Math. Comput. Chem. 64 (2010), 239–250.
13. Thomas, A. S., Kalayathankal, S. J., & Kureethara, J. V. (2017). An introductory note on the spectrum and energy of molecular graphs. *Mapana Journal of Sciences*, *16*(2), 17.
14. V. Nikiforov, The energy of graphs and matrices, J. Math. Anal. Appl. 326 (2007), 1472–1475.
15. Vaidya, S. K., & Popat, K. M. (2017). Some new results on energy of graphs. MATCH commun. Math. Comput. chem, 77, 589-594. MATH, A. ENERGY OF SOME NEW GRAPH.
16. Veeragoudar, J. B., Patil, S. V., & Bhadre, B. S. (2022). QSPR analysis on graph energies of chemical graphs. *Eurasian Chemical Communications*, *5*, 246-263.
17. X. Li Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.
18. Y. Q. Yang, L. Xu, C. Y. Hu, Extended adjacency matrices and their applications, J.Chem. Inf. Comput. Sci. 34 (1994), 1140–1145.
19. Zemljič, K., & Žigert Pleteršek, P. (2023). Smoothness of graph energy in chemical graphs. *Mathematics*, *11*(3), 552.
20. Zhang, X., Prabhu, S., Arulperumjothi, M., Prabhu, S. M., Arockiaraj, M., & Manimozhi, V. (2024). Distance based topological characterization, graph energy prediction, and NMR patterns of benzene ring embedded in P-type surface in 2D network. *Scientific Reports*, *14*(1), 23766.