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Survey of Graph Energies

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Abstract

The graph energy is a graph–spectrum–based quantity, introduced in the 1970s. After a latent period of 20–30 years, it became a popular topic of research both in mathematical chemistry and in "pure" spectral graph theory, resulting in over 600 published papers. Eventually, scores of different graph energies have been conceived. In this article we provide the basic facts on graph energies, in particular historical and bibliographic data.

Keywords: Energy, spectrum, graph.

2010 Mathematics Subject Classification: 05C50.

1. Introduction

The number of papers concerned with various graph energies, published since 2001 (i.e., in the 21st century), increased well over 600, showing no sign of attenuation. To be more precise: these > 600 are the publications known to the authors of this survey (at the moment of writing it in March 2016). There certainly exists a non-negligible number of additional publications, in particular in the nowadays mushrooming obscure electronic journals. Anyway, in good fate that all hitherto published, scientifically significant, contributions to the theory of graph energy have been noticed and recorded, it may be purposeful to offer a few statistical data on their bibliography.

Throughout this article, the number of vertices and edges of the graph G will be denoted by n and m, respectively. For the definitions of other graph–theoretical notions and the meaning of the symbols used, the readers should consult the references quoted or the books [105, 115, 116].

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2. History

The first paper in which graph energy was defined as the sum of absolute values of the eigenvalues of the $(0,1)$-adjacency matrix, namely as

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

appeared in 1978 [3]. The paper [3] is based on a series of lectures held by the author on a graph–theoretical conference in Stift Rein, Austria, in 1978. It is published (in English language) in a difficult-to-find journal whose full title is "*Berichte der Mathematisch–Statistischen Sektion im Forschungszentrum Graz*". A scanned copy of [3] is appended at the end of this article.

The idea to define $E(G)$ as in Eq. (1) and to name it "*energy*" comes from quantum chemistry.

If the eigenvalues of a molecular graph (of a conjugated π-electron system) are labeled as

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \tag{2}$$

then the total π-electron energy E_π (of the underlying molecule in its ground electronic state), as calculated within the Hückel molecular orbital (HMO) approximation, is equal to

$$E_\pi = n\alpha + \beta\left[2\sum_{i=1}^{n/2}\lambda_i\right]$$

if n is even, and

$$E_\pi = n\alpha + \beta\left[\lambda_{(i+1)/2} + 2\sum_{i=1}^{(n-1)/2}\lambda_i\right]$$

if n is odd, with α and β being constants.

For many molecular graphs, the conditions

$$\lambda_{n/2} > 0 > \lambda_{n/2+1} \tag{3}$$

in the case of even n, and

$$\lambda_{(n+1)/2} = 0 \tag{4}$$

in the case of odd n, hold, which in the 1970s was a well known fact. For such graphs, it is elementary to show that

$$E_\pi = n\alpha + \beta\left[\sum_{i=1}^{n}|\lambda_i|\right].$$

Studying HMO theory, one of the authors of the present survey noticed that two important earlier discovered results, namely Coulson's integral formula [1]

$$E_\pi = n\alpha + \beta\frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\left[n - \frac{ix\,\phi'(G,ix)}{\phi(G,ix)}\right]dx$$

and McClelland's inequality [7]

$$\left[2\sum_{i=1}^{n/2}\lambda_i\right] \leq \sqrt{2mn} \qquad \text{or} \qquad \left[\lambda_{(i+1)/2} + 2\sum_{i=1}^{(n-1)/2}\lambda_i\right] \leq \sqrt{2mn}$$

hold if and only if the conditions (3) or (4) are satisfied. In other words, the actual results of Coulson and McClelland were

$$\sum_{i=1}^{n}|\lambda_i| = \frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\left[n - \frac{ix\,\phi'(G,ix)}{\phi(G,ix)}\right]dx$$

and

$$\sum_{i=1}^{n}|\lambda_i| \leq \sqrt{2mn}\,.$$

This observation was the prime motivation to move from the mathematically repelling expressions for HMO total π-electron energy, equal to

$$2\sum_{i=1}^{n/2}\lambda_i \qquad \text{or} \qquad \lambda_{(i+1)/2} + 2\sum_{i=1}^{(n-1)/2}\lambda_i$$

to the much simpler expression $\sum\limits_{i=1}^{n}|\lambda_i|$. By means of this change, the previous HMO results would anyway remain valid for the majority (but not all!) chemically interesting cases.

The other motivation was that the right–hand side of Eq. (1) is independent of the labeling of graph eigenvalues, i.e., it does not require the validity of (2), i.e., the graph energy is a *symmetric function* of graph eigenvalues. By this, graph energy belongs among the algebraically much studied symmetric functions.

By introducing the concept of graph energy, Eq. (1), the author of [3] hoped that it will attract the attention of "pure" mathematicians, and that the Coulson and McClleland formulas are just the first in a long series of exact and non-trivial mathematical results for $E(G)$ to be discovered.

This indeed happened, but more than a quarter-of-century later.

Already before the publication of [7], a few results that pertain to the energy of trees were obtained [2]. Paper [3] was followed by several attempts to popularize the graph–energy concept (e.g., [4–6]), but the mathematical and mathematico–chemical community remained uninterested until the beginning of the 21-st century. The only exception was the Chinese mathematician Fuji Zhang (e.g. [8, 9]). Then, however, a dramatic change happened, and almost suddenly a large number of colleagues, from unrelated and geographically very distant places, started to study graph energy. It may be that a conference lecture, later published as [5], has triggered this turn.

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3. Statistics

Somewhere around the year 2007, the number of publications on graph energy started to significantly increase. This trend is illustrated by the Table 1 and Figure 1 where the distribution of graph–energy–papers by years in the last two decades are shown.

Table 1: Number of papers on graph energies published in the last twenty years, a total of over 630 papers. In the last few years, such papers were produced faster than one per week (= o.p.w.). Based on these data, an attenuation of this speed is not to be expected in the foreseen future. The authors of this table are aware of the fact that there must be numerous additional papers published in China (especially those in Chinese language) that are not accounted for.

year	no.	comment	year	no.	comment
1996	2		2007	34	
1997	0		2008	54	> o.p.w.
1998	2		2009	68	> o.p.w.
1999	6		2010	62	> o.p.w.
2000	4		2011	56	> o.p.w.
2001	12		2012	57	> o.p.w.
2002	3		2013	57	> o.p.w.
2003	5		2014	59	> o.p.w.
2004	9		2015	77	> o.p.w.
2005	15		2016	35	as in March
2006	11				

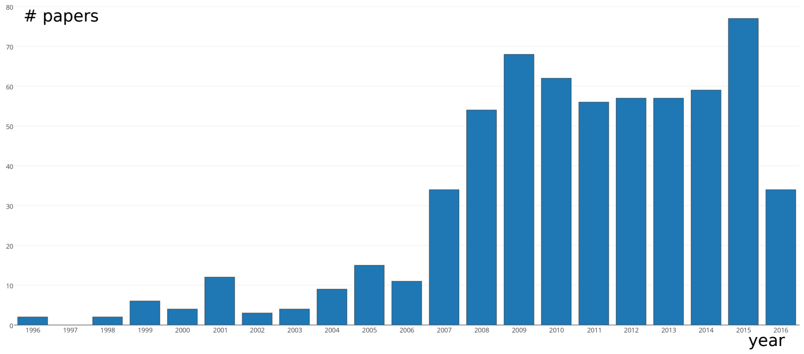

Figure 1: Distribution of the published graph energy papers by years.

Table 2 and Figures 2 and 3 show the distribution of authors of graph–energy–papers by the country of affiliations. In Figure 2 is shown a world map indicating the countries in which these authors were employed, when creating their graph–energy articles. Figure 3 indicates the relative number of authors who were publishing graph–energy–papers by their affiliation's countries.

country	no.	country	no.	country	no.	country	no.
Australia	5	Georgia	1	Mexico	1	Slovenia	1
Austria	1	Germany	9	Norway	1	South Africa	2
Belgium	1	Greece	2	Netherlands	4	South Korea	7
Brazil	14	Hungary	2	Pakistan	7	Spain	2
Canada	9	India	91	Portugal	2	Sweden	1
Chile	11	Indonesia	1	Romania	2	Thailand	2
China	203	Iran	35	Russia	1	Turkey	11
Colombia	8	Ireland	1	Saudi Arabia	1	UK	6
Croatia	4	Italy	6	Serbia	32	USA	38
France	3	Japan	2	Slovakia	2	Venezuela	8

Table 2: Number of scholars from various countries who authored or coauthored at least one article on graph energy in the period 1996–2016 (as on March 31, 2016). Their true count is somewhat greater because we did not distinguish between scholars with the same surname and different names beginning with the same letter. Thus, Xia Li, Xuechao Li, and Xueliang Li were counted as one. Note that all continents, with the regretful exception of Antarctica, are represented in this field of research.

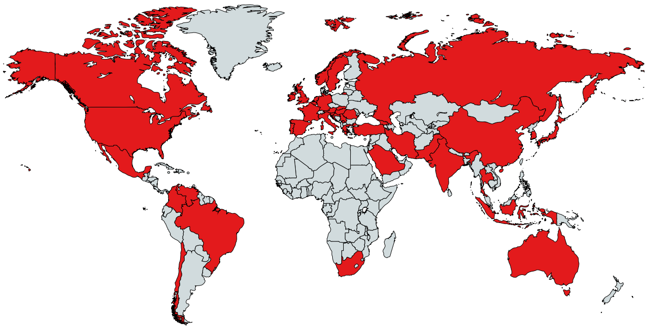

Figure 2: Countries where researches on graph energy were conducted.

The bibliography on which the data in Tables 1 and 2 are based, is the one compiled by the authors of this survey. They made it as complete as they could, but it certainly is not 100% complete. This implies that in reality, the count of

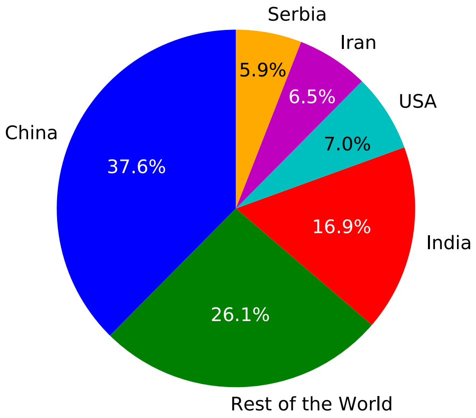

Figure 3: Relative number of authors by countries where they have been working in the time when their graph–energy articles were produced. This pie-chart emphasize countries where the percentage of authors is greater than 5% .

articles and authors, stated in Tables 1 and 2, is still greater. It also may be that some more countries would need to be added to Table 2.

It should be noted that the mentioned bibliography does not include papers that are not directly related to graph energies. Thus, among others, not included are the papers concerned with the following topics:

- Excluded are the countless approximate formulas for total π-electron energy (in terms of n, m, and other graph parameters), in particular such formulas for E_π of benzenoid hydrocarbons.

- Excluded are empirical correlations between E_π and various structural parameters, in particular the "Hall rule" relating $E(G)$ and the number of perfect matchings.

- Excluded are researches on the Türker angle Θ, defined as $\cos\Theta = E(G)/\sqrt{2mn}$, and on similar "angles".

- Excluded are resonance energies, defined as the difference between E_π and an appropriately designed "reference energy". This, in particular, applies to the "topological resonance energy" equal to the difference between $E(G)$ and what nowadays is called "matching energy".

- Excluded are studies of the energy effect of individual cycles in polycyclic conjugated molecules, defined as the difference between $E(G)$ and an appropriately designed cycle–dependent reference.

4. The Multitude of Graph Energies

Graph energy, Eq. (1), is based on the eigenvalues of the ordinary $(0,1)$-adjacency matrix. Its mathematical examination resulted in scores of newly established properties and, consequently, in scores of published papers. In view of this success, a natural idea was to look for some variant of graph energy that would also provide a basis for prolific mathematical researches.

The most obvious step in this direction was to employ eigenvalues of another graph matrix. The most obvious candidate for this was the Laplacian matrix. Let its eigenvalues be denoted by $\mu_1, \mu_2, \ldots, \mu_n$. Then, in analogy with Eq. (1) one could conceive the Laplacian energy of the graph G as

$$LE!(G) = \sum_{i=1}^{n} |\mu_i| \, .$$

However, because all Laplacian eigenvalues are non-negative, and because their sum is equal to $2m$, we would arrive at the trivial result $LE!(G) = 2m$. The way out of this difficulty was found by defining the Laplacian energy as [39]

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| \, .$$

Alas, as a consequence of this definition, $LE(G_1 \cup G_2) = LE(G_1) + LE(G_2)$ is not satisfied in the general case.

The Laplacian energy was the first in a long series of energies based on other graph matrices. It was followed by the distance energy (based on the eigenvalues of the distance matrix) [41], signless Laplacian energy (based on the eigenvalues of the signless Laplacian matrix) [10], normalized Laplacian energy (based on the eigenvalues of the normalized Laplacian matrix) [24], resistance–distance or Kirchhoff energy (based on the eigenvalues of the resistance–distance matrix) [28, 50], skew energy (based on the eigenvalues of the skew adjacency matrix) [13], Seidel energy (based on the eigenvalues of the Seidel matrix) [40], etc. Consonni and Todeschini [26] defined the energy of any real symmetric matrix with eigenvalues $\xi_1, \xi_2, \ldots, \xi_n$ as

$$E_{CT} = \sum_{i=1}^{n} \left| \xi_i - \frac{S}{n} \right|$$

where $S = \xi_1 + \xi_2 + \cdots + \xi_n$. The definition of the Hermitian energy [48] is analogous.

An often used method for designing a new graph energy is to start from a topological index of the form

$$TI(G) = \sum_{v_i, v_j} f(v_i, v_j)$$

where $v_1, v_2, \ldots, v_n$ are the vertices of the graph G and the summation goes over all pairs of its adjacent vertices. Based on the above formula, one defines the matrix $\mathbf{M}_{TI} = (m_{ij})$ as

$$m_{ij} = \begin{cases} f(v_i, v_j) & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$$

The respective energy is then the sum of absolute values of the eigenvalues of M_{TI}. Such are the Randić [23], Szeged [30], geometric–arithmetic [64], and common–neighbourhood energy [20], based on the Randić, Szeged, geometric–arithmetic, and common–neighbourhood indices, respectively.

Nikiforov extended the energy–concept to any matrix [58]. If $\mathbf{M}$ is a $p \times q$ matrix (where p and q need not be equal), then the positive square roots of the eigenvalues of $\mathbf{M}\mathbf{M}^t$ are the singular values of $\mathbf{M}$. Their sum if defined as the energy of the matrix $\mathbf{M}$. In the case of real and symmetric (square) matrices, the new and the old energy–concepts coincide.

The first non-square matrix to which Nikiforov's concept was applied was the incidence matrix, resulting in the incidence energy $IE(G)$ [44]. Short time earlier, Liu and Liu [49] introduced the so-called *Laplacian–energy–like invariant*, defined as

$$LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i}\,.$$

From a formal point of view, LEL is not a graph energy. However, it was soon discovered that for bipartite graphs, $LEL(G) = IE(G)$, whereas in the general case (including non-bipartite graphs),

$$IE(G) = \sum_{i=1}^{n} \sqrt{\mu_i^+}$$

where $\mu_1^+, \mu_2^+, \ldots, \mu_n^+$ are the eigenvalues of the signless Laplacian matrix.

Followed the oriented incidence energy [66], normalized incidence energy [25], Laplacian incidence energy [65], Randić incidence energy [31], etc.

A subset $\mathcal{D}$ of the vertex set V of the graph G is said to be a dominating set of G if every vertex of $V \setminus \mathcal{D}$ is adjacent to some vertex in $\mathcal{D}$. Any dominating set with minimum cardinality is said to be a minimum dominating set. The minimum dominating adjacency matrix of G, denoted by $\mathbf{A}_{\mathcal{D}} = (a_{ij}^{\mathcal{D}})$, is the $n \times n$ matrix defined as

$$a_{ij}^{\mathcal{D}} = \begin{cases} 1 & \text{if } v_i \sim v_j \\ 1 & \text{if } i = j\,,\ v_i \in \mathcal{D} \\ 0 & \text{otherwise.} \end{cases}$$

The minimum dominating energy is defined as [61]

$$E_{\mathcal{D}}(G) = \sum_{i=1}^{n} |\lambda_i^{\mathcal{D}}|$$

where $\lambda_i^{\mathcal{D}}$, $i = 1, 2, \ldots, n$, are the eigenvalues of $\mathbf{A}_{\mathcal{D}}$.

A subset $\mathcal{C}$ of V is said to be a covering set of G if every edge of G is incident to at least one vertex of $\mathcal{C}$. Any covering set with minimum cardinality is called a minimum covering set. The minimum covering matrix of G, denoted by $\mathbf{A}_{\mathcal{C}} = (a_{ij}^{\mathcal{C}})$, is the $n \times n$ matrix defined as

$$a_{ij}^{\mathcal{C}} = \begin{cases} 1 & v_i \sim v_j \\ 1 & i = j, v_i \in \mathcal{C} \\ 0 & \text{otherwise.} \end{cases}$$

The minimum-covering energy is defined as [14]

$$E_{\mathcal{C}}(G) = \sum_{i=1}^{n} |\lambda_i^{\mathcal{C}}|$$

where $\lambda_i^{\mathcal{C}}$, $i = 1, 2, \ldots, n$, are the eigenvalues of $\mathbf{A}_{\mathcal{C}}$.

If T is a tree of order n, then its ordinary energy satisfies the Coulson integral formula

$$E(T) = \frac{1}{\pi} \int\limits_{-\infty}^{+\infty} \left[n - \frac{ix\, \alpha'(T, ix)}{\alpha(T, ix)} \right] dx \tag{5}$$

where $\alpha(G, \lambda)$ denotes the matching polynomial of the graph G. Extending the validity of the right–hand side of (5) to all graphs, one arrived at the concept of matching energy [38]:

$$ME(G) = \frac{1}{\pi} \int\limits_{-\infty}^{+\infty} \left[n - \frac{ix\, \alpha'(G, ix)}{\alpha(G, ix)} \right] dx\,.$$

A coloring of a graph G is a coloring of its vertices such that adjacent vertices have different colors. The minimum number of colors needed for coloring of a graph is the its chromatic number. For such a coloring, the color matrix is defined so that its (i, j)-entry is equal to $+1$ (resp. -1) if the vertices v_i and v_j are adjacent and thus differently colored (resp. non-adjacent and equally colored), and is zero otherwise. The sum of the absolute values of the eigenvalues of the color matrix is referred to as the color energy [15].

The "ultimate" generalization of the energy–concept is achieved by considering an n-tuple $\mathcal{X}$ of real numbers, $x_1, x_2, \ldots, x_n$ which need not have a graph–theoretical or any other interpretation. If the arithmetic average of these numbers is $\overline{x}$, then the ultimate energy of $\mathcal{X}$ is [36]

$$UE(\mathcal{X}) = \sum_{i=1}^{n} \left| x_i - \overline{x} \right| .$$

It is remarkable that already such a poorly defined energy is bounded as

$$\sqrt{n\,Var(x) + n(n-1)|P(\overline{x})|^{2/n}} \leq UE(\mathcal{X}) \leq n\sqrt{Var(x)} \tag{6}$$

where $Var(x)$ is the variance of the numbers $x_1, x_2, \ldots, x_n$, whereas $P(x) = \prod_{i=1}^{n} (x - x_i)$. The bounds (6) were first established in 1971 by McClelland (for the ordinary graph energy), and were then repeatedly "discovered" for dozens of other graph energies.

* * * * *

In our records, we have data on more than 60 different graph energies. In what follows, we give a list thereof, ordered according to the time of their first occurrence in the literature, with reference to the place where these have been considered for the first time. In reality, the number of existing graph energies may be still greater, and more such will for sure appear in the future.

no	graph energy	reference
1	(ordinary) graph energy	[35]
2	Laplacian energy	[39]
3	energy of matrix	[58]
4	robust domination energy	[11]
5	energy of set of vertices	[12]
6	distance energy	[41]
7	Laplacian–energy–like invariant	[49]
8	Consonni–Todeschini energies	[26]
9	energy of $(0,1)$-matrix	[45]
10	incidence energy	[44]
11	maximum-degree energy	[16]
12	skew Laplacian energy	[17]
13	oriented incidence energy	[66]
14	skew energy	[13]
15	Randić energy	[23]
16	normalized Laplacian energy	[24]

no	graph energy	reference
17	energy of matroid	[19]
18	energy of polynomial	[52]
19	Harary energy	[34]
20	sum-connectivity energy	[69]
21	second–stage energy	[21]
22	signless Laplacian energy	[10]
23	PI energy	[55]
24	Szeged energy	[30]
25	He energy	[27]
26	energy of orthogonal matrix	[22]
27	common-neighbourhood energy	[20]
28	matching energy	[38]
29	ultimate energy	[36]
30	minimum-covering energy	[14]
31	resistance-distance energy	[28]
32	Kirchhoff energy	[50]
33	color energy	[15]
34	normalized incidence energy	[25]
35	Laplacian distance energy	[68]
36	Laplacian incidence energy	[65]
37	Laplacian minimum dominating energy	[60]
38	minimum-domination energy	[61]
39	minimum-covering distance energy	[59]
40	Seidel energy	[40]
41	domination energy	[46]
42	general Randić energy	[32]
43	Randić incidence energy	[31]
44	Laplacian minimum-covering energy	[62]
45	e-energy	[54]
46	n-energy	[54]
47	Hermitian energy	[48]
48	minimum hub distance energy	[51]
49	minimum monopoly energy	[56]
50	minimum monopoly distance energy	[57]

no	graph energy	reference
51	complementary dominating energy	[53]
52	minimum-maximal-domination energy	[29]
53	minimum-covering color energy	[63]
54	α-distance energy	[47]
55	α-incidence energy	[47]
56	*so*-energy	[42]
57	Nikiforov energy	[18]
58	resolvent energy	[37]
59	Laplacian resolvent energy	[67]
60	signless Laplacian resolvent energy	[67]
61	skew Randić energy	[33]
62	geometric–arithmetic energy	[64]
63	*o*-energy	[43]

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5. Applications of Graph Energies

In addition to its standard chemical application (in view of its close relations with the HMO total π-electron energy), the ordinary graph energy, Eq. (1), and some other graph energies found unexpected applications in other areas of science.

Use of $E(G)$ in QSPR/QSAR studies was attempted in [74, 76]. In particular, graph energies are related to entropy [72, 75]. Properties of proteins (especially those of biological relevance) were modeled in [73, 78, 80]. Graph energy was used in the search for the genetic causes of Alzheimer disease [71] and for modeling of the spread of epidemics [79].

The Laplacian energy found applications in image analysis [77, 81], which, in addition, is attempted to be used in medical investigations of brain activity [70].

More details along these lines can be found in the references quoted.

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6. Monographs and Reviews on Graph Energy

In this section we first provide a list of review articles on various graph energies.

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At the present moment there are only two monographs entirely devoted to graph energies [114, 116]. However, graph–energy–related topics can be found in numerous other books and textbooks, sometimes in the form of entire chapters, sometimes mentioned only in a few lines. The list that follows is believed to be complete or, at least, nearly complete.

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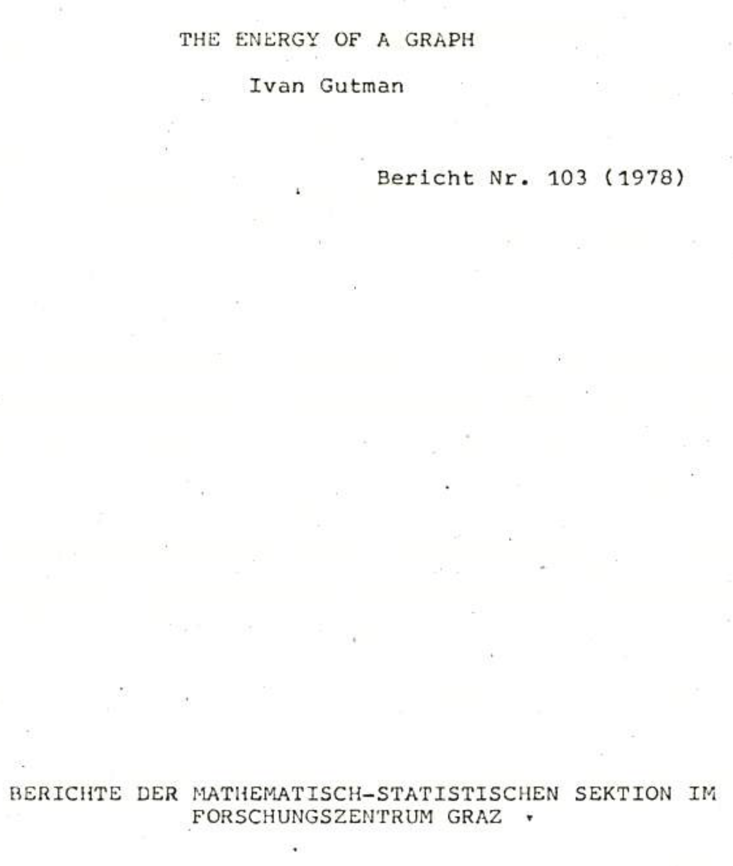
7. Appendix

The seminal paper on graph energy [I. Gutman, The energy of a graph, *Ber. Math–Statist. Sekt. Forschungsz. Graz* **103** (1978) 1–22.] is frequently cited even though it is quite hard to acquire its copy. In order to help authors in the future, the scanned copy of this article is given below.



THE ENERGY OF A GRAPH

Ivan Gutman

Bericht Nr. 103 (1978)

BERICHTE DER MATHEMATISCH-STATISTISCHEN SEKTION IM
FORSCHUNGSZENTRUM GRAZ

THE ENERGY OF A GRAPH

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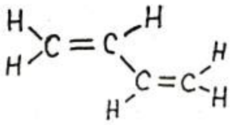
Summary. The energy E(G) of a graph G is the sum of the absolute values of all the graph eigenvalues, eq. (1). Results concerning E(G) are exposed, with an emphasis on the dependence of E(G) on the structure of G.

In the present work we shall consider a quantity called in theoretical chemistry "the total π-electron energy of a conjugated hydrocarbon, as calculated with the Hückel molecular orbital method", but we will call it simply "energy" and denote it by E. For details of Hückel theory and how it is related to graph spectral theory see[7,21]. The reader should also consult the books[7,21] and the references cited therein for all chemical aspects of our considerations.

Conjugated hydrocarbons are of great importance for both science and technology. A conjugated hydrocarbon can be characterized as a molecule composed entirely of carbon and hydrogen atoms, every carbon atom having exactly three neighbours (which may be either carbon or hydrogen atoms). Butadiene (I), benzyl (II) and azulene (III) are examples of conjugated hydrocarbons.



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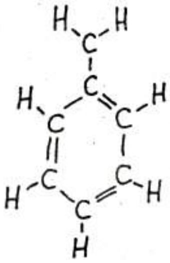

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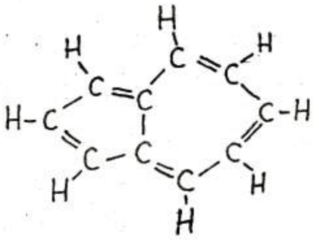
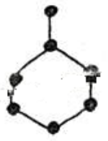


III

There are theoretical reasons[7,21] to associate a graph with a conjugated hydrocarbon according to the following rule: every carbon atom is represented by a vertex and every carbon-carbon bond by an edge. Hydrogen atoms are ignored. Thus the graphs G_a, G_b and G_c are "the molecular graphs" of the compounds I, II and III, respectively. It is worth mentioning

G_a



G_b

G_c

that for chemical reasons these "molecular graphs" are necessarily connected and their vertex degrees must not exceed three. However, both these restrictions are important only for the chemical interpretation of the obtained results and they need not be taken into account in mathematical considerations. Thus in the following we shall deal with arbitrary graphs.

It is assumed that the reader is familiar with elements of graph theory, but no special knowledge of graph spectral theory[4] is required. We introduce now our notation and terminology.

Let G be a simple graph (i.e. a graph without loops and multiple edges) with n = n(G) vertices and m edges. Let the vertices of G be labeled by $v_1, v_2, \ldots, v_n$. The adjacency matrix $\underset{\sim}{A}$ of a (labeled) graph G is a square matrix of order n defined via $A_{pq} = 1$ if the vertices v_p and v_q are adjacent, and $A_{pq} = 0$ if the vertices v_p and v_q are not adjacent and if p = q. The characteristic polynomial of this matrix, $P(G, x) = \det(x\underset{\sim}{I} - \underset{\sim}{A})$, is called the characteristic polynomial of the graph G. The eigenvalues $x_1, x_2, \ldots, x_n$ of $\underset{\sim}{A}$ are called the eigenvalues of G. They form the spectrum of G. The characteristic polynomial and the spectrum are, of course, independent of the labeling of the vertices of the graph.

The energy E = E(G) of a graph G is then defined as the sum of the absolute values of all the elements of the spectrum of G:

$$(1) \qquad E = \sum_{j=1}^{n} |x_j|$$

When G is a molecular graph, then E is rather important for theoretical chemistry. One of the problems which arise there is how E depends on the molecular structure. From a mathematician´s point of view this question reads: how E(G), as defined by eq. (1), depends on the structure of the graph G? What can be said about E(G) if the structure of G is known, but without the actual calculation of the spectrum of G? Such kind of problems will be considered in our paper.

Research in this direction started some fourty years ago[2] and has a continuation up to the present days. A recent bibliography[15] of the work in this field contains 65 titles.

THE SACHS THEOREM

The characteristic polynomial of a graph G will be written in the form

$$(2) \qquad P(G, x) = \sum_{k=0}^{n} a_k \, x^{n-k}$$

where, of course, $a_0 = 1$ for all G. The dependence of the coefficients $a_k = a_k(G)$ on the structure of the graph is summarized in a remarkable theorem of Sachs.[4,22]

$$(3) \qquad a_k = \sum_{s \in S_k} (-1)^{p(s)} \, 2^{c(s)}$$

Here s denotes a so called "basic figure". Basic figures* are graphs, the only components of which are complete graphs with two vertices and/or cycles. The summation in (3) goes over the

---

* In chemical literature basic figures are usually called "Sachs graphs".

set $S_k = S_k(G)$ of all basic figures with exactly k vertices which are, as subgraphs, contained in G. There are p(s) components and among them c(s) cyclic components in the basic figure s.

Substituting (3) back into (2) we obtain

$$P(G, x) = \sum_{s \in S} (-1)^{p(s)} 2^{c(s)} x^{n(G)-n(s)} \tag{4}$$

where $S = S(G)$ is the set of all basic figures contained in G, and n(s) is the number of vertices of s.

Elementary consequences of the Sachs theorem (3) are $a_1 = 0$ and $a_2 = -m$, since there are no basic figures with one vertex, and every edge represents a basic figure with two vertices. Therefrom,

$$\sum_{j=1}^{n} x_j^2 = 2m \tag{5}$$

From the Sachs theorem we can deduce important spectral properties of bipartite graphs and forests. In the following we denote bipartite graphs by B, forests by F and trees by T. If not stated otherwise, it is assumed that these graphs possess n vertices.

A graph is bipartite if, and only if it contains no odd-membered cycles. Now, basic figures with odd number of vertices must possess at least one odd-membered cycle. Therefore, bipartite graphs contain no basic figures with odd number of vertices, $S_{2k+1}(B) = \emptyset$ for all k and all B. Consequently,

$$(6) \qquad a_{2k+1}(B) = 0 \quad \text{for all } k; \qquad P(B, x) = \sum_k a_{2k} \, x^{n-2k}$$

If G is not bipartite, then at least one $a_{2k+1}(G)$ differs from zero.

The even coefficients of P(B, x) alternate in sign, i.e. $(-1)^k \, a_{2k}(B) \geqslant 0$ for all k.

Bipartite graphs are particularly important in chemical applications. Namely, the great majority of molecular graphs which are of chemical interest are bipartite. (Instead of "bipartite" chemists use to say "alternant".) Therefore formulas and theorems for E, valid only for bipartite graphs might be rather useful in practice. It is a fortunate fact that the spectral properties of graphs are often considerably simplified if one restricts to bipartite graphs.

A graph F is called a forest if it contains no cycles. A connected forest T is called a tree. Since a forest contains no cycles, it must be $c(s) = 0$ for all $s \in S(F)$. In other words, basic figures of forests represent selections of independent edges (of this forest). Let p(G, k) be the number of ways in which one can select k independent edges in G and let p(G, 0) = 1. Then we have

$$(7) \qquad P(F, x) = \sum_{k=0}^{[n/2]} (-1)^k \, p(F, k) \, x^{n-2k}$$

If G is not a forest, at least one $a_{2k}(G)$ differs from $(-1)^k \, p(G, k)$.

We give now without proof two properties of the numbers p(G, k), which we shall need later.[11,12] First, p(G, 1) = m. Second, if v_p is a terminal vertex of G (i.e. v_p is adjacent to a unique vertex, say v_q), then

$$(8) \qquad p(G, k) = p(G-v_p, k) + p(G-v_p-v_q, k-1)$$

The Sachs theorem solved the problem of the dependence of P(G, x) on the structure of G. The importance of this result for the study of E becomes evident if we know that it is possible to express the energy of a graph as a function of its characteristic polynomial. This is exposed in the subsequent section.

INTEGRAL FORMULAS FOR ENERGY

In the following we shall use the abbreviate notation

$$\frac{1}{\pi} \int_{-\infty}^{+\infty} F(x) \, dx \equiv \langle F(x) \rangle \equiv \langle F \rangle$$

for a frequently occuring type of integrals.

Theorem 1.[2] Let $P'(G, x)$ be the first derivative (with respect to x) of the characteristic polynomial and i the square root of -1. Then

$$(9) \qquad E = \left\langle n - \frac{ix\, P'(G, ix)}{P(G, ix)} \right\rangle = \left\langle n - x \frac{d}{dx} \log P(G, ix) \right\rangle$$

Proof. The above identity is easily obtained by means of contour integration.[2] We offer here another elementary and straightforward derivation of (9), based on the observation that

$$\frac{P'(G, x)}{P(G, x)} = \sum_{j=1}^{n} \frac{1}{x-x_j}$$

Let us consider the simple integrals $I_1 = \langle t^2/(t^2+x^2) \rangle = |t|$; $I_2 = \langle xt/(t^2+x^2) \rangle = 0$. Since $|t| = I_1 + iI_2$, we obtain $|t| = \langle (t^2+ixt)/(t^2+x^2) \rangle = \langle 1 - ix/(ix-t) \rangle$. Therefrom,

$$\sum_{j=1}^{n} |x_j| = \sum_{j=1}^{n} \left\langle 1 - \frac{ix}{ix - x_j} \right\rangle = \left\langle n - \sum_{j=1}^{n} \frac{ix}{ix - x_j} \right\rangle =$$

$$= \left\langle n - \frac{ix\, P'(G, ix)}{P(G, ix)} \right\rangle \text{ Q.E.D.}$$

Corollary 1.1.[3,19] Let G and H be graphs with equal number of vertices. Then,

$$E(G) - E(H) = \left\langle \log \frac{P(G,\ ix)}{P(H,\ ix)} \right\rangle = \left\langle \log \left| \frac{P(G,\ ix)}{P(H,\ ix)} \right| \right\rangle \tag{10}$$

Proof. From eq. (9),

$$E(G) - E(H) = -\left\langle x \frac{d}{dx} \log \frac{P(G,\ ix)}{P(H,\ ix)} \right\rangle = -x \log \frac{P(G,\ ix)}{P(H,\ ix)} \Bigg|_{-\infty}^{+\infty} + \left\langle \log \frac{P(G,\ ix)}{P(H,\ ix)} \right\rangle$$

Eq. (10) follows now from $x \log \frac{P(G,\ ix)}{P(H,\ ix)} \to c$ for $x \to \pm\infty$ and from the fact that energy is a real number. Q.E.D.

In[18] is proved another

Corollary 1.2.

$$E = \langle x^{-2} \log Q(G,\ x) \rangle = \langle x^{-2} \log |Q(G,\ x)| \rangle \tag{11}$$

where $Q(G,\ x) = (-ix)^n\ P(G,\ i/x)$. Note that

$$Q(G,\ x) = \sum_{k=0}^{n} a_k\ (-ix)^k =$$

$$= \sum_k (-1)^k\ a_{2k}\ x^{2k} - i \sum_k (-1)^k\ a_{2k+1}\ x^{2k+1}$$

Substitution of this latter equation back into (11) gives

$$E = \frac{1}{2} \left\langle x^{-2} \log \left[\left(\sum_k (-1)^k a_{2k} x^{2k} \right)^2 + \left(\sum_k (-1)^k a_{2k+1} x^{2k+1} \right)^2 \right] \right\rangle$$

Using (6) we gain a considerable simplification for bipartite graphs: $Q(B, x) = \sum_k (-1)^k a_{2k} x^{2k}$ is real and

(12) $$E(B) = \left\langle x^{-2} \log \sum_k (-1)^k a_{2k} x^{2k} \right\rangle$$

Further integral formulas for energy are collected elsewhere.[6,9] All such results enable one to calculate E(G) from the knowledge of P(G, x). We can symbolize this fact by an operator $\hat{f}$.

(13) $$E(G) = \hat{f} P(G, x)$$

On the other hand, using eq. (4) one can calculate P(G,x) from the knowledge of all basic figures of G. We can symbolize this operation by

(14) $$P(G, x) = \hat{g} S(G)$$

Then, of course, $E(G) = \hat{f}\hat{g} S(G)$.

BOUNDS FOR ENERGY

Several lower and upper bounds for E are known. Some of them will be presented in this section.

Theorem 2.[20] Let D be the absolute value of the determinant of the adjacency matrix $\underset{\sim}{A}$. Then,

$$2m + n(n-1)\, D^{2/n} \leqslant E^2 \leqslant 2nm$$

Proof of the left inequality. We start with an identity for E, based on eq. (5).

$$E^2 = \left(\sum_{j=1}^{n} |x_j|\right)^2 = \sum_{j=1}^{n} x_j^{\,2} + \sum_{j \neq k} |x_j|\,|x_k| = 2m + \sum_{j \neq k} |x_j|\,|x_k|$$

Since for non-negative numbers the arithmetic mean is not smaller than the geometric mean,

$$\frac{1}{n(n-1)} \sum_{j \neq k}^{n} |x_j|\,|x_k| \geqslant \left(\prod_{j \neq k}^{n} |x_j|\,|x_k|\right)^{1/n(n-1)} =$$

$$= \left(\prod_{j=1}^{n} |x_j|^{2(n-1)}\right)^{1/n(n-1)} = \left(\prod_{j=1}^{n} |x_j|\right)^{2/n} = D^{2/n}$$

Combination of the above two relations gives the lower bound for energy. Q.E.D.

Proof of the right inequality. From

$$n \sum_{j=1}^{n} x_j^{\,2} - \left(\sum_{j=1}^{n} |x_j|\right)^2 = \sum_{j<k}^{n} (|x_j| - |x_k|)^2$$

which is a special case of the Lagrange identity, one gets

$$2nm - E^2 = \sum_{j<k}^{n} (|x_j| - |x_k|)^2 \geqslant 0. \quad \text{Q.E.D.}$$

<u>Corollary 2.1</u>. If $D \neq 0$, then $E^2 \geqslant 2m + n(n-1)$.

<u>Corollary 2.2</u>. If $D \neq 0$, then $E \geqslant n$.

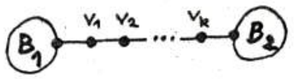
<u>Proof</u>. If $D \neq 0$ then also $a_n \neq 0$ and consequently G possesses a basic figure with n vertices. Such a basic figure contains at least n/2 edges. Therefore $m \geqslant n/2$ and corollary 2.2 follows from corollary 2.1. Q.E.D.

Theorem 2 was later improved.

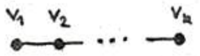
<u>Theorem 3</u>.[8] For all graphs, $U \leqslant 2nm - E^2 \leqslant (n-1)U$, while for bipartite graphs, $2U \leqslant 2nm - E^2 \leqslant (n-2)U$, where $U = 2m - n\,D^{2/n} \geqslant 0$.

Freely spoken, theorems 2 and 3 imply that the gross part (some 95%) of E is determined by only three invariants of the graph: n, m and D. In addition, E is roughly proportional to $(nm)^{1/2}$. These conclusions are of some value for chemical applications.

Let G_k be a graph of the form



G_k



P_k

where B_1 and B_2 are arbitrary bipartite subgraphs. Thus G_k is obtained by attaching two fragments B_1 and B_2 to the terminal vertices of the path P_k with k vertices. Without proof we state

Theorem 4.[10] $2(\sqrt{5} - 1) \leq E(G_{k+2}) - E(G_k) \leq 2(\sqrt{3} + 1 - \sqrt{2})$.

These bounds are the best possible. (There is a pair of graphs P_4 and P_2, such that $E(P_4) = 2\sqrt{5}$ and $E(P_2) = 2$ and another pair of graphs P_5 and P_3, such that $E(P_5) = 2(\sqrt{3} + 1)$ and $E(P_3) = 2\sqrt{2}$.) In addition, $E(G_{k+2}) - E(G_k) \longrightarrow 8/\pi$, when $k \longrightarrow \infty$.

FORESTS AND TREES WITH EXTREMAL ENERGY

Combination of eqs. (7) and (12) yields for a forest F

$$E(F) = \left\langle x^{-2} \log \sum_k p(F, k)\, x^{2k} \right\rangle \qquad (15)$$

Hence E(F) is a monotonously increasing function of the numbers p(F, k).

Let O_n be the graph composed of n isolated vertices. Let P_n be the path and S_n the star with n vertices. (The path is the tree with minimal number (=2) of terminal vertices, the star is the tree with maximal number (=n-1) of terminal vertices.)

Theorem 5.[11] For all forests F with n vertices, $E(O_n) \leq E(F) \leq E(P_n)$.

Proof. According to (15) it is sufficient to show that for all $k=1,2,\dots,[n/2]$

$$p(O_n, k) \leq p(F, k) \leq p(P_n, k)$$

The left inequalities are, of course, trivial since $p(O_n, k) = 0$ for all k. The validity of the right inequalities is easily checked for n = 1,2,3 and 4. Suppose now that they hold for all forests with less than n vertices. Let F_n be the forest with n vertices, such that $p(F_n, k) \geqslant p(F, k)$ for all k. We show that $F_n = P_n$.

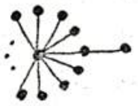
First, F_n must possess at least one edge and therefore also a terminal vertex. Let v_p be such a terminal vertex adjacent to the vertex v_q. From eq. (8), $p(F_n, k) = p(F_n-v_p, k) + p(F_n-v_p-v_q, k-1)$. But $p(F_n, k)$ is maximal if both $p(F_n-v_p, k)$ and $p(F_n-v_p-v_q, k-1)$ are maximal. According to our assumption, it must be (a) $F_n-v_p = P_{n-1}$ and (b) $F_n-v_p-v_q = P_{n-2}$. Now from (a) it follows that F_n is obtained by joining a vertex v_p to some vertex v_q of the path P_{n-1}. Because of (b), v_q must be a terminal vertex of P_{n-1}. Therefore $F_n = P_n$. Q.E.D.

Theorem 6.[11] For all trees T with n vertices, $E(S_n) \leqslant E(T) \leqslant E(P_n)$.

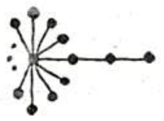
Proof. The right inequality holds because of theorem 5. In order to prove the left inequality, note that for all trees $p(T, 1) = n-1$, because all trees with n vertices have n-1 edges. In addition, $p(S_n, 2) = p(S_n, 3) = \dots = 0$. But the star is the unique tree containing no pairs of independent edges. Hence $p(T, 2) > 0$ for all other trees. Therefore, $p(S_n, k) \leqslant p(T, k)$ for all k. Q.E.D.

It should be mentioned that $E(O_n) = 0$, $E(S_n) = 2\sqrt{n-1}$ and $E(P_n) = 2 \operatorname{cosec} \frac{\pi}{2n+2} - 2$ if n is even and $E(P_n) = 2 \operatorname{cotg} \frac{\pi}{2n+2} - 2$ if n is odd.

In[11] are found further extremal trees. We present here without proof the following result. Let T_1 be obtained by joining a vertex to a terminal vertex of S_{n-1}. Let T_2 be obtained by joining two vertices to a terminal vertex of S_{n-2}. Let T_3 be obtained by joining a vertex of P_2 to a terminal vertex of S_{n-2}. Let T_4 be obtained by joining a vertex of P_2 to the vertex v_3 of P_{n-2}.


T_1


T_2


T_3


T_4

Theorem 7.[11] If T is a tree with n vertices, different than S_n, T_1, T_2, T_3, T_4 and P_n, then $E(S_n) < E(T_1) < E(T_2) < E(T_3) < E(T) < E(T_4) < E(P_n)$.

Theorems 5 - 7 identify the forests and trees with maximal and minimal energy. It is natural to pose the same question for other classes of graphs. However, this seems to be a much more difficult task and even the unicyclic graphs with extremal energy are not known.

Conjecture. Among graphs with n vertices, the complete graph has maximal energy (which is equal to $2n-2$).

THE HÜCKEL RULE

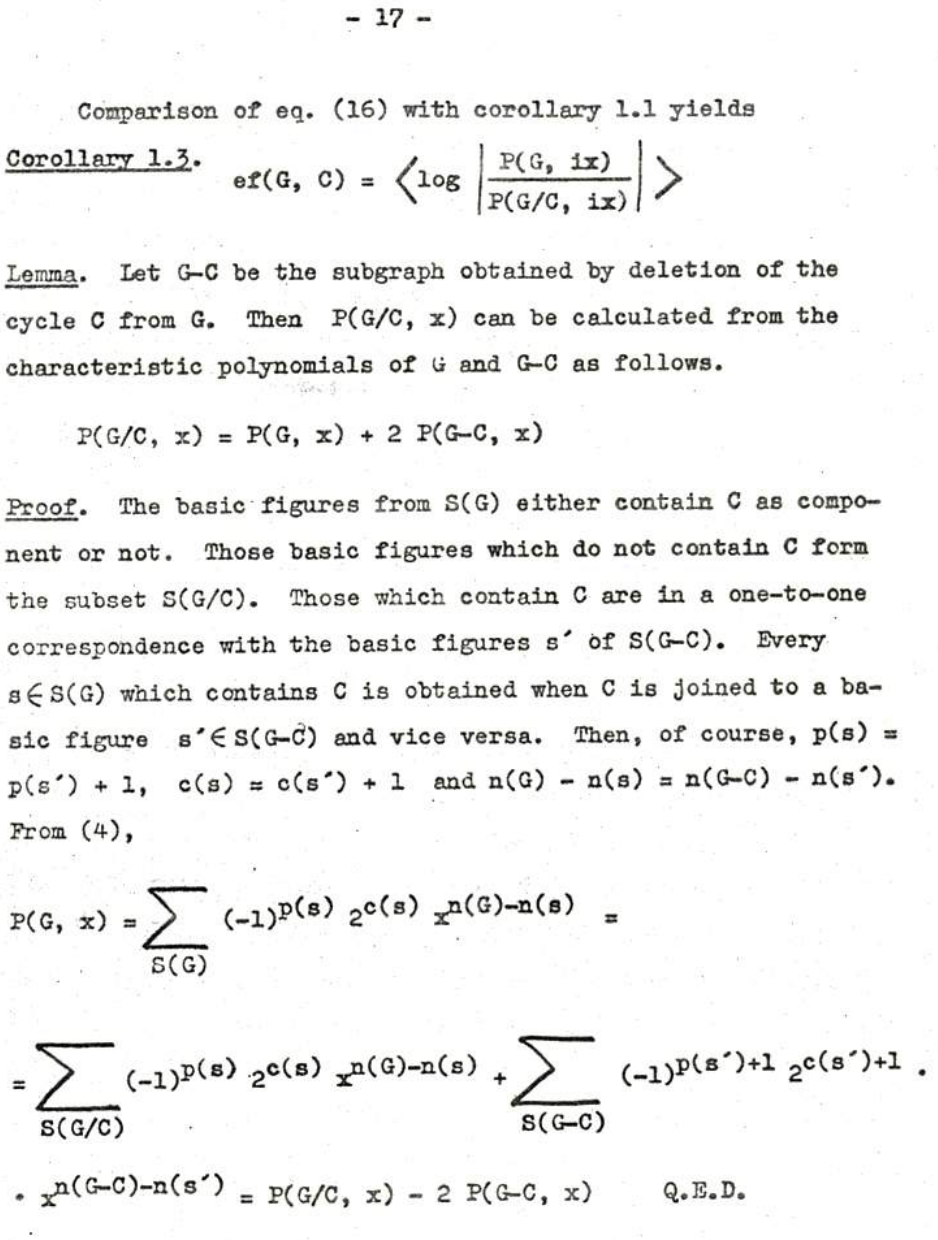
The dependence of E on the type and size of cycles which are present in the graph is a popular problem in the chemistry of conjugated hydrocarbons. An observation made long ago is known in chemistry as the Hückel 4m+2 rule: cycles of length 4m+2 (m=1,2,...) contained in G have a positive (increasing) effect on the value of E(G); cycles of length 4m (m=1,2,...) contained in G have a negative (decreasing) effect on E(G). It was recently established that this rule is not generally valid.[16] Nevertheless, its mathematical content is worth further discussion.

First one has to determine the exact meaning of "the effect of a cycle on E". Let C be a cycle of the length $|C|$ contained as subgraph in G. According to (13) and (14), E(G) is a function of all basic figures contained in G. Some of these basic figures contain C as a component.

Let S(G/C) denote the set of all basic figures of G which do not contain C as component. Then using (13) and (14) we can calculate the polynomial $P(G/C, x) = \hat{g}\, S(G/C)$ and the number $E(G/C, x) = \hat{f}\, P(G/C, x) = \hat{f}\hat{g}\, S(G/C)$. Note, however, that neither is P(G/C, x) the characteristic polynomial, nor is E(G/C) the energy of some graph.

Now, the effect ef(G, C) of the cycle C on the energy of the graph G is defined as

$$\text{ef}(G, C) = E(G) - E(G/C) \tag{16}$$



Comparison of eq. (16) with corollary 1.1 yields

Corollary 1.3.
$$ef(G, C) = \left\langle \log \left| \frac{P(G, ix)}{P(G/C, ix)} \right| \right\rangle$$

Lemma. Let G-C be the subgraph obtained by deletion of the cycle C from G. Then $P(G/C, x)$ can be calculated from the characteristic polynomials of G and G-C as follows.

$$P(G/C, x) = P(G, x) + 2\,P(G-C, x)$$

Proof. The basic figures from $S(G)$ either contain C as component or not. Those basic figures which do not contain C form the subset $S(G/C)$. Those which contain C are in a one-to-one correspondence with the basic figures s' of $S(G-C)$. Every $s \in S(G)$ which contains C is obtained when C is joined to a basic figure $s' \in S(G-C)$ and vice versa. Then, of course, $p(s) = p(s') + 1$, $c(s) = c(s') + 1$ and $n(G) - n(s) = n(G-C) - n(s')$. From (4),

$$P(G, x) = \sum_{S(G)} (-1)^{p(s)}\, 2^{c(s)}\, x^{n(G)-n(s)} =$$

$$= \sum_{S(G/C)} (-1)^{p(s)}\, 2^{c(s)}\, x^{n(G)-n(s)} + \sum_{S(G-C)} (-1)^{p(s')+1}\, 2^{c(s')+1} \cdot$$

$$\cdot\, x^{n(G-C)-n(s')} = P(G/C, x) - 2\,P(G-C, x) \qquad \text{Q.E.D.}$$

Theorem 8.[13,16] $ef(B, C) \leqslant 0$ when $|C| = 4m$ $(m=1,2,\ldots)$.

Proof.
$$ef(B, C) = - \left\langle \log \left| \frac{P(B/C, ix)}{P(B, ix)} \right| \right\rangle =$$
$$= - \left\langle \log \left| \frac{P(B, ix) + 2\, P(B-C, ix)}{P(B, ix)} \right| \right\rangle = - \left\langle \log \left| 1 + 2\, W(x) \right| \right\rangle$$

where $W(x) = P(B-C, ix)/P(B, ix)$. Using (6) we can calculate

$$W(x) = (-1)^{|C|/2} \frac{\sum_k (-1)^k a_{2k}(B-C)\, x^{n-|C|-2k}}{\sum_k (-1)^k a_{2k}(B)\, x^{n-2k}}$$

Since for bipartite graphs $(-1)^k a_{2k} \geqslant 0$, $W(x)$ is positive when $|C| = 4m$ and negative when $|C| = 4m+2$ $(m=1,2,\ldots)$. Therefore, if $|C| = 4m$, then $|1 + 2\, W(x)| \geqslant 1$ and $\log |1 + 2\, W(x)| \geqslant 0$ for all real values of x. Q.E.D.

If $|C| = 4m+2$, then $W(x) \leqslant 0$ and $\log |1 + 2\, W(x)|$ can have both positive and negative values. Therefore no simple and generally valid regularity for the sign of $ef(G, C)$ can be expected when $|C| = 4m+2$. (In many of the studied cases $ef(B, C)$ was positive when $|C| = 4m+2$, but examples are known where also $ef(B, C) < 0$.)

The extension of theorem 8 to non-bipartite graphs is missing. The factors governing the sign of $ef(G, C)$ when $|C|$ is odd are at the present moment obscure.

The quantity $ef(G, C)$ measures the effect which a particular cycle C has on $E(G)$. A related problem was also extensively studied in literature, namely the effect of all cycles.

Let S(G/c) be the set of all basic figures contained in G which have the property c(s) = 0. We introduce now the polynomial $P(G/c,\ x) = \hat{g}\ S(G/c)$ and the number $E(G/c) = \hat{f}\hat{g}\ S(G/c)$. The polynomial P(G/c, x) is called *the matching polynomial of G*.[5] Its mathematical properties are rather interesting[**] and were recently reviewed.[14] It can be shown that[1,17]

$$P(G/c,\ x) = \sum_{k=0}^{[n/2]} (-1)^k\ p(G,\ k)\ x^{n-2k}$$

where the quantities p(G, k) have been defined in connection with eq. (7). In the case of forests the matching and the characteristic polynomials coincide.

E(G) - E(G/c) is called *the topological resonance energy* and is of certain importance in chemistry.[1,17] We cannot discuss these concepts in more detail here.

* - - - * - - - * - - - * - - - *

In the present work a few properties of the energy of a graph were exposed. In fact, this should be an almost complete collection of statements about energy, which can be rigorously proved in the mathematical sense of this word. However, there are numerous known results in this field which are approximate

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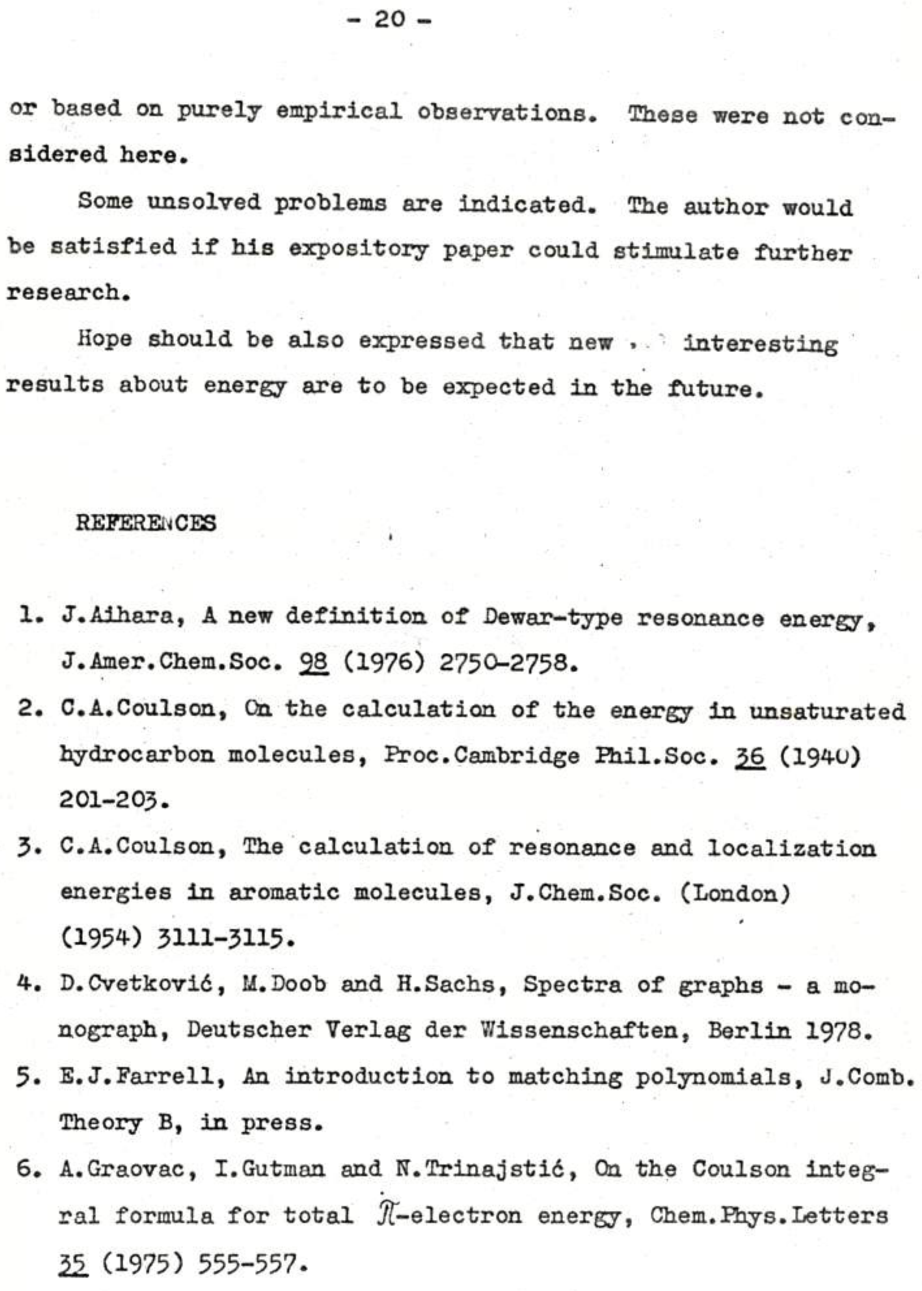
[**] In previous work by the author[12,14,17] P(G/c, x) was called "the acyclic polynomial". The term "matching polynomial" was first used by Farrell[5].



or based on purely empirical observations. These were not considered here.

Some unsolved problems are indicated. The author would be satisfied if his expository paper could stimulate further research.

Hope should be also expressed that new [illegible] interesting results about energy are to be expected in the future.

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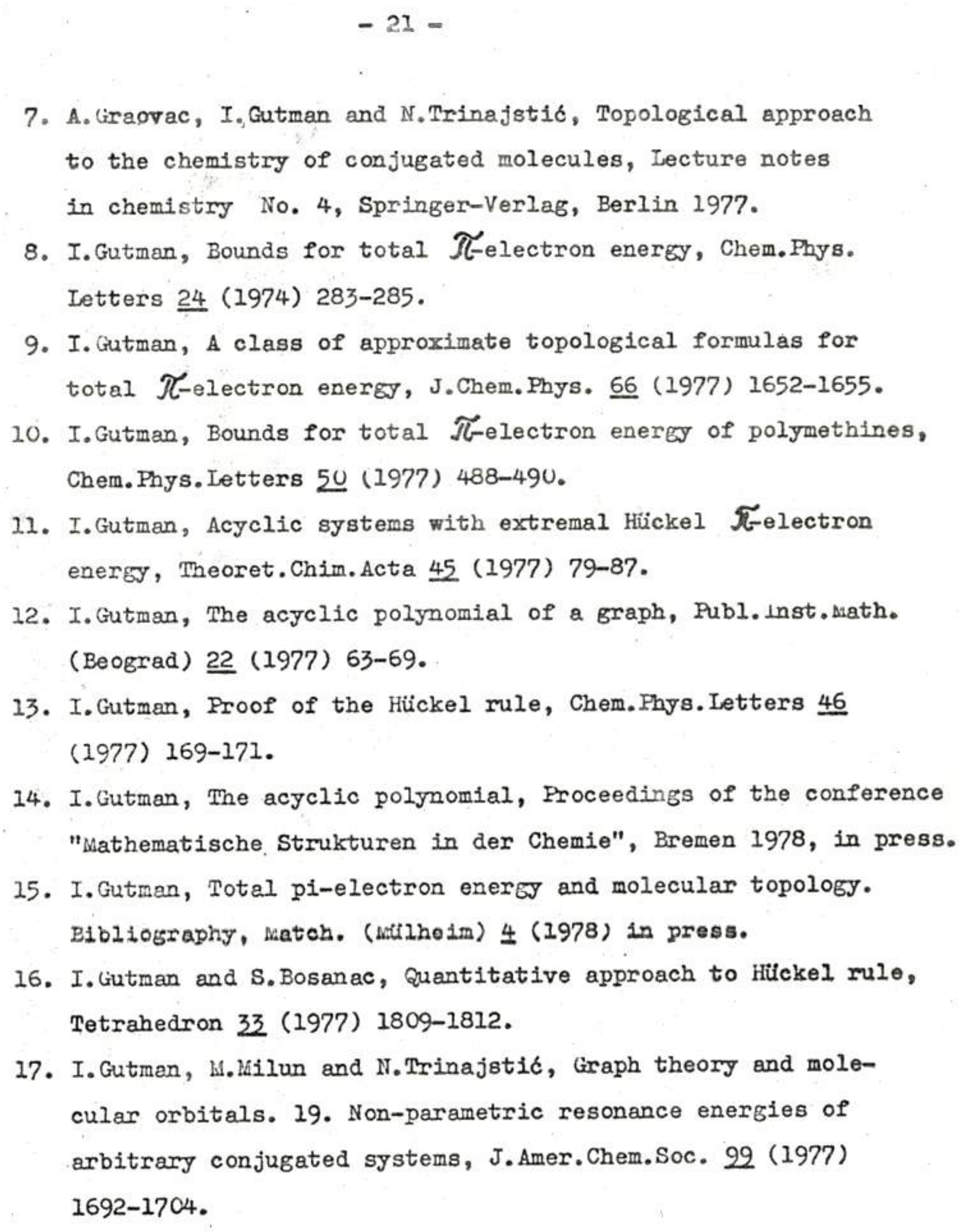

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