



What is the meaning of the graph energy after all?



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ABSTRACT

For a simple graph $G = (V, E)$ with eigenvalues of the adjacency matrix $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, the energy of the graph is defined by $E(G) = \sum_{j=1}^n |\lambda_j|$. Myriads of papers have been published in the mathematical and chemistry literature about properties of this graph invariant due to its connection with the energy of (bipartite) conjugated molecules. However, a structural interpretation of this concept in terms of the contributions of even and odd walks, and consequently on the contribution of subgraphs, is not yet known. Here, we find such an interpretation and prove that the (adjacency) energy of any graph (bipartite or not) is a weighted sum of the traces of even powers of the adjacency matrix. We then use such result to find bounds for the energy in terms of subgraphs contributing to it. The new bound are studied for some specific simple graphs, such as cycles and fullerenes. We observe that including contributions from subgraphs of sizes not bigger than 6 improves some of the best known bounds for energy, and more importantly gives insights about the contributions of specific subgraphs to the energy of these graphs.

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1. Introduction

The concept of graph energy arose in the context of the study of conjugated hydrocarbons using a tight-binding method known in chemistry as the *Hückel molecular orbital* (HMO) method (see for instance [2,3]). In this context, the total energy of a conjugated molecule M is defined by

$$E(M) = 2 \sum_{j:\lambda_j > 0} \lambda_j = \sum_{j=1}^n |\lambda_j|, \quad (1)$$

where the last equality is a consequence of the fact that such conjugated molecules can be represented by bipartite graphs, thus the spectrum of their adjacency matrices is symmetric. Here, $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ are the eigenvalues of the adjacency matrix of the (molecular) graph—typically a simple, connected, undirected graph. It should be remarked that such energy is given in units of a parameter known as β which has a negative value.

This concept was then generalized to any graph – not necessarily bipartite – by Ivan Gutman, who named it the *graph energy* [5]. Then, for simple, undirected graph $G = (V, E)$, the energy is defined as

$$E(G) = \sum_{j=1}^n |\lambda_j|. \quad (2)$$

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A myriad of papers and a couple of monographs have been written about the graph energy [6,7,10]. The monograph [10] is an excellent compilation of results, historical background and methodological approaches that may serve as a guide to the reader who wants to get deeper into this field. The concept has been generalized to other matrices apart from the adjacency one [12] (see also the corresponding Chapters of the monographs [7,10]), and many bounds and extremal properties have been reported for these graph/matrix energies. Many researchers claim in their papers that they are studying the graph energy because of the chemical implications of that quantity. As soon as this concept is extended to non-bipartite graphs, however, it completely loses all its chemical and physical meaning. Nevertheless, as a graph invariant, the graph energy can bring important structural information about the graph. But, the problem is to know what exactly the graph energy means in terms of the structure of a graph. Thus, after 30 years of research on graph energy, what is it after all?

Here we provide a structural interpretation of the graph energy using the concept of matrix function (see next section for formal definitions). In particular, we prove that the graph energy is given by the sum of the traces of the even powers of the adjacency matrix weighted in a specific way. Using this new representation we find new bounds for the energy as sums of contributions of subgraphs. Consequently, armed with this structural interpretation the graph energy can now be used in the general context of structural graph theory or even to study some real-world graphs.

2. Preliminaries

We consider here simple, undirected, connected graphs $G = (V, E)$, without multiple edges or self-loops. The adjacency matrix A of G is then square, symmetric matrix with spectral decomposition $A = V \Lambda V^T$, where

$$V = [\vec{\psi}_1 \quad \dots \quad \vec{\psi}_n]$$

is the matrix of orthonormalized eigenvectors $\vec{\psi}_j$ associated with the eigenvalues λ_j , and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$. If f is a scalar function defined on the spectrum of A we can define a function of the matrix A , $f(A)$ by means of

$$f(A) = V f(\Lambda) V^T, \quad (3)$$

where $f(\Lambda) = \text{diag}(f(\lambda_1), \dots, f(\lambda_n))$. For example, for any symmetric positive semidefinite matrix A we can define its (positive semidefinite) square root by means of $S = \sqrt{A} = V \sqrt{\Lambda} V^T$. This is the only symmetric positive semidefinite matrix with the property that $S^2 = A$.

We observe that if f is defined by a power series expansion of the form

$$f(x) = \sum_{k=0}^{\infty} a_k x^k$$

such that the series converges on an open disk containing the λ_j , then the above definition is equivalent to

$$f(A) = \sum_{k=0}^{\infty} a_k A^k. \quad (4)$$

For further information on matrix functions, the reader is referred to [8].

3. Main result

The main result of this work is the finding that the (adjacency) graph energy of any graph can be obtained as a weighted sum of even powers of the adjacency matrix. First, we observe that

$$E(G) = \text{tr} |A|, \quad (5)$$

where $|A| = V | \Lambda | V^T$ stands for the absolute value matrix function of A . Then, we have the following result.

Theorem 1. *The energy of a graph is given by*

$$E(G) = \lambda_1 \text{tr} \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} \sum_{\ell=0}^k (-1)^{k-\ell} \binom{k}{\ell} \left(\frac{A}{\lambda_1} \right)^{2\ell}. \quad (6)$$

Proof. We start by recalling that every symmetric positive semidefinite matrix has a unique positive semidefinite square root. Then, we have that

$$|A| = \sqrt{A^2}. \quad (7)$$

We now expand the square root in a power series in A^2 . Let $\lambda_1 > 0$ be the largest eigenvalue of A . We note in passing that since G is connected, λ_1 is simple. Then, $\frac{A}{\lambda_1}$ has spectral radius 1, and the matrix $B = (\lambda_1^{-1}A)^2 - I$ has all eigenvalues in the interval $[-1, 0]$. Hence, B is negative semidefinite and has spectral radius at most 1. Let us write

$$|A| = \sqrt{A^2} = \lambda_1 \sqrt{\left(\frac{A}{\lambda_1}\right)^2} = \lambda_1 \sqrt{I + \left(\left(\frac{A}{\lambda_1}\right)^2 - I\right)} = \lambda_1 (I + B)^{\frac{1}{2}}. \quad (8)$$

Recall now the following special case of the binomial theorem:

$$\sqrt{1+x} = (1+x)^{\frac{1}{2}} = \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} x^k, \quad (9)$$

where the series converges for all $x \in [-1, 1]$, and

$$\binom{\alpha}{k} := \frac{\alpha(\alpha-1)\cdots(\alpha-k+1)}{k!} \quad (10)$$

for any real α (here $\alpha = \frac{1}{2}$). Therefore we can write

$$|A| = \lambda_1 \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} B^k = \lambda_1 \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} \left(\left(\frac{A}{\lambda_1}\right)^2 - I\right)^k, \quad (11)$$

which readily gives the desired result. \square

If we consider the first few terms of the expansion for $E(G)$ we have

$$E(G) = \text{tr } |A| = \lambda_1 \text{tr} \left[I + \frac{1}{2} \left(\frac{A^2}{\lambda_1^2} - I\right) - \frac{1}{2 \cdot 4} \left(\frac{A^2}{\lambda_1^2} - I\right)^2 + \frac{1 \cdot 3}{2 \cdot 4 \cdot 6} \left(\frac{A^2}{\lambda_1^2} - I\right)^3 - \cdots \right], \quad (12)$$

which clearly indicates that the energy of a graph only depends on even powers of the adjacency matrix of the corresponding graph. That is,

$$E(G) = \text{tr } |A| = \lambda_1 \left[\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \text{tr} \left(\frac{A^2}{\lambda_1^2} - I\right)^k \right]. \quad (13)$$

It should be observed that whenever 0 is an eigenvalue of A , the matrix B has spectral radius 1, which makes the convergence of the binomial series expansion quite slow. Conversely, when A does not have zero or small eigenvalues one can expect rapid convergence. For instance, we have observed slow convergence for C_4 (for which 0 is an eigenvalue) but not for C_3 and C_5 (for which it is not). This difference in the convergence of the systems containing 0 as an eigenvalue of A —that is when the graph nullity $\eta(G)$ is larger than zero—with those having zero nullity could have some important chemical implications. In a molecule having nullity different from zero not all the electrons can be paired in a conjugated way and typically there are pairs of lone electrons in the structure that confer some magnetic properties to the molecule. Now we have discovered that for expressing the energy of those systems in terms of the power series a larger number of terms are needed than for molecular systems with zero nullity. This difference can be understood physically as follows. Consider that every term of the expansion, a spectral moment of B , is explaining the circulation of the electrons in the molecule. For instance, the non-diagonal entries of B accounts for the hop of electrons between pairs of nearest neighbour atoms, the same term in B^2 represents the hop of electrons between atoms separated by two bonds, and for higher powers of B such terms represent the long-range hop of electrons between atoms in a molecule. The same can be said about the diagonal terms of the powers of the B matrix, where electrons are hopping between atoms and then returning to the initial one. For a molecule to be stable it is needed that the electrons are maximally delocalized. Then, it is necessary that the electrons move as much as possible to nearest, second, third,... neighbours, which leads to consider higher order terms such as B^2 , B^3 , etc. in the Taylor series expansion of the energy. According to our current results, in a conjugated stable molecule like C_6 , this is reached by including only a few terms of the expansion, indicating that the molecule is stable with relatively small delocalization of the electrons. For C_4 , which is the prototype of unstable molecule, one needs to go to very large circulations of the electrons through the whole molecule to reach a certain stability, which implies to consider a large number of terms in the Taylor series expansion of the energy. In general, the nullity of cyclic graphs is (see [1] and references therein)

$$\eta(C_n) = \begin{cases} 2, & \text{if } n \equiv 0 \pmod{4} \\ 0, & \text{otherwise.} \end{cases} \quad (14)$$

Thus, for monocyclic conjugated molecules having $4n$ atoms, such as C_4 , C_8 , etc., the number of terms in the Taylor series expansion needed to account for their energy is much larger than for the well-known stable molecules with $4n + 2$ atoms, such as C_6 , C_{10} , and so forth.

4. Further developments

Here we use the main result in the previous section to obtain some upper bounds for the energy of a graph. Our goal is not to give very sharp bounds but to derive some that allow us to interpret the structural meaning of the graph energy, with special emphasis on the molecular energy in the HMO method. Recall that we have set

$$B = \left(\frac{A^2}{\lambda_1^2} - I \right) \quad (15)$$

and that B is a negative semidefinite matrix (with spectrum in $[-1, 0]$). Furthermore,

$$B_{ii} = \left(\frac{A^2}{\lambda_1^2} - I \right)_{ii} = \frac{k_i}{\lambda_1^2} - 1, \quad (16)$$

where k_i is the degree of the corresponding vertex. Clearly, these diagonal terms are all nonpositive. We now prove the following result.

Lemma 2. *Let G be a graph with n nodes and m edges. Then,*

$$E(G) \leq \left(\frac{\lambda_1}{2} \right) n + \left(\frac{1}{\lambda_1} \right) m. \quad (17)$$

Proof. It is easy to see that

$$E(G) \leq \lambda_1 \operatorname{tr} I = \lambda_1 n, \quad (18)$$

and that

$$E(G) = \lambda_1 \left[\operatorname{tr} I + \frac{1}{2} \operatorname{tr} \left(\frac{A^2}{\lambda_1^2} - I \right) - \left(\frac{1}{8} \operatorname{tr} \left(\frac{A^2}{\lambda_1^2} - I \right)^2 - \frac{1}{16} \operatorname{tr} \left(\frac{A^2}{\lambda_1^2} - I \right)^3 + \dots \right) \right], \quad (19)$$

which implies that

$$E(G) \leq \lambda_1 \left[\operatorname{tr} I + \frac{1}{2} \operatorname{tr} \left(\frac{A^2}{\lambda_1^2} - I \right) \right] = \lambda_1 n + \left(\frac{1}{2\lambda_1} \right) \sum_{i=1}^n k_i - \left(\frac{\lambda_1}{2} \right) n. \quad (20)$$

The result is now an immediate consequence of (16). \square

It can be easily verified that

$$E(G) \leq \sqrt{2mn} \leq \left(\frac{\lambda_1}{2} \right) n + \left(\frac{1}{\lambda_1} \right) m, \quad (21)$$

where the first bound is the well-known McClelland one [11]. The McClelland bound was further improved by Koolen, Moulton and Gutman (KMG bound) [9] who obtained the following one:

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)(2m - 4m^2/n^2)}. \quad (22)$$

However, we can systematically improve the bound that we have found above by using the same approach used for its proof, as we will show in the next two results.

Lemma 3. *Let G be a graph with n nodes, m edges, P_3 paths of three vertices and C_4 cycles of length four. Then,*

$$E(G) \leq \left(\frac{3\lambda_1}{8} \right) n + \left(\frac{6\lambda_1^2 - 1}{4\lambda_1^3} \right) m - \left(\frac{1}{2\lambda_1^3} \right) P_3 - \left(\frac{1}{\lambda_1^3} \right) C_4. \quad (23)$$

Proof. It is easy to see that

$$\begin{aligned} \operatorname{tr}(B^2) &= \operatorname{tr} \left(\frac{A^2}{\lambda_1^2} - I \right)^2 \\ &= \frac{1}{\lambda_1^4} \operatorname{tr} A^4 - \frac{2}{\lambda_1^2} \operatorname{tr} A^2 + \operatorname{tr} I. \end{aligned} \quad (24)$$

We can now obtain the traces of A^4 and of A^2 in terms of the subgraphs contributing to them. It is known (see, e.g., [4, page 137]) that

$$\operatorname{tr} A^4 = 2m + 4P_3 + 8C_4, \quad (25)$$

and of course

$$\operatorname{tr}A^2 = 2m. \quad (26)$$

Then, by plugging these two formulas into the expression for $\frac{\lambda_1}{8} \operatorname{tr}(B^2)$ we get

$$\frac{\lambda_1}{8} \operatorname{tr}(B^2) = \left(\frac{\lambda_1}{8}\right)n + \left(\frac{1-2\lambda_1^2}{4\lambda_1^3}\right)m + \left(\frac{1}{2\lambda_1^3}\right)P_3 + \left(\frac{1}{\lambda_1^3}\right)C_4. \quad (27)$$

Finally, by taking

$$E(G) \leq \left(\frac{\lambda_1}{2}\right)n + \left(\frac{1}{\lambda_1}\right)m - \frac{\lambda_1}{8} \operatorname{tr}(B^2) \quad (28)$$

we obtain the result. \square

An important feature of this bound is that it clearly agrees with the chemical intuition. For instance, it is well known that conjugated C_4 cycles destabilize a molecule, due to their increase in the molecular energy. We recall that the energy $E(G)$ for a molecule is given in units of β which is negative. Thus, both terms P_3 and C_4 have contributions that increase the total energy of a molecule.

We can improve the previous bound by using a similar approach.

Lemma 4. *Let G be a graph. Then,*

$$\begin{aligned} E(G) &\leq \left(\frac{5\lambda_1}{16}\right)n + \left(\frac{15\lambda_1^4 - 5\lambda_1^2 + 1}{8\lambda_1^5}\right)m - \left(\frac{5\lambda_1^2 - 3}{4\lambda_1^5}\right)P_3 - \left(\frac{5\lambda_1^2 - 6}{2\lambda_1^5}\right)C_4 \\ &\quad + \left(\frac{3}{2\lambda_1^5}\right)C_3 + \left(\frac{3}{8\lambda_1^5}\right)P_4 + \left(\frac{3}{4\lambda_1^5}\right)S_{1,3} + \left(\frac{9}{4\lambda_1^5}\right)D_4 + \left(\frac{3}{4\lambda_1^5}\right)F \\ &\quad + \left(\frac{3}{2\lambda_1^5}\right)H + \left(\frac{3}{4\lambda_1^5}\right)C_6 \end{aligned} \quad (29)$$

where C_n and P_n represent cycles and paths with n vertices, $S_{1,3}$ is the star subgraph with one central vertex and 3 pendant ones, and D_4 is the diamond graph, i.e., a graph consisting of C_4 in which an edge is added to one pair of nonadjacent vertices, F is a subgraph consisting of one square with a pendant node and H is a subgraph consisting of two triangles sharing a common node.

Proof. It is easy to see that

$$\begin{aligned} \operatorname{tr}(B^3) &= \operatorname{tr}\left(\frac{A^2}{\lambda_1^2} - I\right)^3 \\ &= \frac{1}{\lambda_1^6} \operatorname{tr}A^6 - \frac{3}{\lambda_1^4} \operatorname{tr}A^4 + \frac{3}{\lambda_1^2} \operatorname{tr}A^2 - \operatorname{tr}I. \end{aligned} \quad (30)$$

The expression for $\operatorname{tr}A^6$ in terms of subgraphs (see [4, page 139]) is given by:

$$\operatorname{tr}A^6 = 2m + 12P_3 + 24C_3 + 48C_4 + 12S_{1,3} + 6P_4 + 36D_4 + 12F + 24H + 12C_6. \quad (31)$$

Then, by plugging these two formulas into the expression for $\frac{\lambda_1}{16} \operatorname{tr}(B^3)$ we get

$$\begin{aligned} \frac{\lambda_1}{16} \operatorname{tr}(B^3) &= \left(\frac{1-3\lambda_1^2+3\lambda_1^4}{8\lambda_1^5}\right)m + \left(\frac{3-3\lambda_1^2}{4\lambda_1^5}\right)P_3 + \left(\frac{6-3\lambda_1^2}{2\lambda_1^5}\right)C_4 \\ &\quad + \left(\frac{3}{2\lambda_1^5}\right)C_3 + \left(\frac{3}{8\lambda_1^5}\right)P_4 + \left(\frac{3}{4\lambda_1^5}\right)S_{1,3} + \left(\frac{9}{4\lambda_1^5}\right)D_4 + \left(\frac{3}{4\lambda_1^5}\right)F \\ &\quad + \left(\frac{3}{2\lambda_1^5}\right)H + \left(\frac{3}{4\lambda_1^5}\right)C_6 - \frac{\lambda_1}{16}n. \end{aligned} \quad (32)$$

Then by taking

$$E(G) \leq \left(\frac{3\lambda_1}{8}\right)n + \left(\frac{6\lambda_1^2-1}{4\lambda_1^3}\right)m - \left(\frac{1}{2\lambda_1^3}\right)P_3 - \left(\frac{1}{\lambda_1^3}\right)C_4 + \frac{\lambda_1}{16} \operatorname{tr}(B^3), \quad (33)$$

we get the final result. \square

This result clearly indicates that subgraphs like C_6 contribute to decreasing the energy of a graph. In molecular systems this is an important result due to the well-known fact that benzenoid molecules, which are constructed on the basis of fusing together C_6 fragments, are very stable. However, the result shows also other fragments which contribute to the stabilization

Table 1

Values of the energy $E(G)$ and their estimation using McClelland bound $\sqrt{2mn}$, Koolen–Moulton–Gutman (KMG) bound as well as the bound obtained in this work for the cycle graphs C_n with different number of nodes.

n	$E(G)$	$\sqrt{2mn}$	KMG	Eq. (17)	Eq. (23)	Eq. (29)
3	4.000	4.243	4.000	4.5	4.219	4.113
4	4.000	5.657	5.464	6	5.500	5.250
5	6.472	7.071	6.899	7.5	7.031	6.836
6	8.000	8.485	8.325	9	8.438	8.227
7	8.988	9.899	9.746	10.5	9.844	9.570
8	9.657	11.314	11.165	12	11.250	10.938
9	11.517	12.728	12.583	13.5	12.656	12.305
10	12.944	14.142	14.000	15	14.062	13.672

of conjugated molecular systems as the ones studied in the HMO context. This includes the fragment P_4 which obviously corresponds to the butadiene fragment and which is easily recognizable as a stabilizing fragment. Other fragments appear here in a more unexpected way, such as C_3 , D_4 , F and H .

5. Bounding individual fragment contributions

One important consequence of the findings of this paper is that we can obtain bounds for the contribution of individual subgraphs to the total graph energy. For instance, suppose that we are interested in knowing how the subgraph C_8 contributes to $E(G)$. Then, we can do the following. We first identify the first spectral moment of the matrix B in which C_8 contributes. That is, C_8 appears by the first time in the term $\frac{\text{tr}A^8}{\lambda_1^8}$ of B^4 . Thus, let $\eta_C(C_8)$ be the contribution of the cycle of 8 nodes to the total energy of a graph G and let $\eta_8(C_8)$ be the contribution of C_8 to the 8th spectral moment of $A = A(C_8)$, i.e., $\eta_8(C_8) = \text{tr}A^8 - \text{tr}A^2 - \text{tr}A^4 - \text{tr}A^6 = 256 - 16 - 48 - 160 = 32$. Then,

$$\eta_C(C_8) \leq \lambda_1 \binom{2 \cdot 4}{4} \frac{(-1)^{4+1}}{2^{2 \cdot 4} (2 \cdot 4 - 1)} \left(\frac{\eta_8(C_8)}{\lambda_1^8} \right) = - \left(\frac{5}{4\lambda_1^7} \right). \quad (34)$$

The negative sign indicates that an octacycle increases the energy of the graph. In the case of molecules treated under the HMO scheme, it is well known that cycles with $4n$ atoms destabilize the molecule, which is exactly the result obtained here. Here we have considered only the contribution of $\frac{\text{tr}A^8}{\lambda_1^8}$ to the subgraph C_8 . However, this subgraph will also contribute to the higher moments $\frac{\text{tr}A^{10}}{\lambda_1^{10}}, \frac{\text{tr}A^{12}}{\lambda_1^{12}}, \dots$. Thus, this bound can be successively improved by finding these further contributions of C_8 to the higher moments, which were not taken into account here.

6. Numerical results

In this section we give some numerical results on the different bounds obtained in this paper for simple graphs of importance in chemistry. The goal of these bounds is not obtaining good approximations of the graph energy for these graphs. Indeed, the direct calculation of the energy for these graphs is easier than the calculation of the bounds. Our goal is to show how the incorporation of certain subgraphs into the bounds improves them and provides a structural interpretation of the graph energy for such graphs. In all cases we compare our bound with the one of McClelland [11], which is simple and remarkably good in approaching the graph energy.

First we study a series of cycle graphs C_n for $3 \leq n \leq 10$. In Table 1 we give the values of the energy and the results of bounding it with the three bounds obtained here as well as by McClelland's and KMG ones. As can be seen even for such simple graphs the current approach needs to incorporate terms coming from the $\text{tr}A^6$ in order to improve McClelland's and KMG bounds. In this type of graphs, a few of the subgraphs contributing to (29) are not present, e.g., $S_{1,3}$, D_4 , F , H , and some of others only appear in specific graphs, such as C_3 , C_4 , and C_6 . Thus, the main improvement in this bound in relation to the other two comes from the better account of the contributions of n , m and P_3 and the newly introduced contribution of P_4 . It should be noticed that (29) represents a better bound than the one obtained by KMG for this type of graphs.

As a second example we study a series of fullerene graphs having from 20 to 540 nodes. The results are given in Table 2. Here again, it is necessary to go beyond the contribution of $\text{tr}A^4$ to make improvements over McClelland's bound. Here the main contributions to this improvement are made by n , m , P_3 , P_4 , $S_{1,3}$, and C_6 . Notice, that the contributions of C_5 are only captured after the consideration of $\text{tr}A^{10}$, which is not studied here. It can be then said that the energy of fullerenes is bounded by the following specific expression in which we use the fact that fullerenes are cubic graphs, i.e., $\lambda_1 = 3$:

$$E(G) \leq \left(\frac{15}{16} \right) n + \left(\frac{1171}{1944} \right) m - \left(\frac{7}{162} \right) P_3 + \left(\frac{1}{648} \right) P_4 + \left(\frac{1}{324} \right) S_{1,3} + \left(\frac{1}{324} \right) C_6. \quad (35)$$

The bound (29) is always better than McClelland's one for fullerenes, but for the KMG the situation is more complex. For small fullerenes, up to approximately $n = 76$, the KMG bound gives better estimates of the graph energy than our bound

Table 2

Values of the energy $E(G)$ and their estimation using McClelland's bound $\sqrt{2mn}$, Koolen–Moulton–Gutman (KMG) bound as well as the bound obtained in this work for the fullerene graphs with different number of nodes.

n	$E(G)$	$\sqrt{2mn}$	KMG	Eq. (17)	Eq. (23)	Eq. (29)
20	29.416	34.641	34.129	40	36.111	34.4753
24	36.022	41.569	41.066	48	43.330	41.376
26	39.742	45.0333	44.533	52	46.944	44.827
28	43.107	48.497	48.000	56	50.555	48.278
30	45.704	51.962	51.466	60	54.167	51.728
32	49.150	55.425	54.933	64	57.778	55.179
36	55.244	62.350	61.864	72	65.000	62.080
50	77.579	86.602	86.120	100	90.278	86.235
60	93.162	103.923	103.444	120	108.333	103.488
76	118.326	131.636	131.160	152	137.222	131.093
80	121.617	135.1	138.089	156	140.833	134.543
180	282.066	311.769	311.300	360	325.000	310.525
240	376.535	415.692	415.224	480	433.333	414.043
320	502.831	554.256	553.789	640	577.778	552.067
540	848.924	935.307	934.842	1080	975.000	931.636

(29). However, for mid size and large fullerenes our bound is a better estimator of $E(G)$. It is worth saying that the main advantage of the method proposed here is that we can continuously add more terms in the power series in order to improve the corresponding bounds.

7. Conclusions

The main conclusion of this work is that the graph energy is a weighted sum of the traces of even powers of the adjacency matrix. The potential advantages of this finding are that new techniques can be designed to bound the energy of graphs, in which the specific contribution of subgraphs can be obtained. This is of great importance in chemistry where the search for additive rules for molecular properties is a golden rule for understanding such properties in structural terms. Finally, we hope that the new findings reported here would allow to better understand properties of the graph energy in certain families of graphs.

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