

Estimating the Laplacian Energy-Like Molecular Structure Descriptor

Ivan Gutman

Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia

Reprint requests to I. G.; E-mail: gutman@kg.ac.rs

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Lower and upper bounds for the Laplacian energy-like (LEL) molecular structure descriptor are obtained, better than those previously known. These bounds are in terms of number of vertices and edges of the underlying molecular graph and of graph complexity (number of spanning trees).

Key words: Energy (of Graph); Laplacian Energy; Laplacian Energy-Like Invariant; LEL.

1. Introduction

The total π -electron energy is a quantum-chemical characteristic of conjugated molecules that is examined in theoretical chemistry for more than 50 years [1–3]. The mathematical re-formulation of this quantity is the graph energy $E(G)$ which also was extensively studied in the last 10–20 years [4, 5]. The *graph energy* is defined as

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

where n is the number of vertices of the graph G , and $\lambda_1, \lambda_2, \dots, \lambda_n$ are its eigenvalues [1, 4, 5]. Two elementary properties of the graph energy are $E(G_1 \cup G_2) = E(G_1) + E(G_2)$ for $G_1 \cup G_2$ being the graph consisting of two disconnected components G_1 and G_2 , and $E(G \cup K_1) = E(G)$, where K_1 is the graph with a single vertex.

Motivated by the success of the graph-energy concept, and in order to extend it to the Laplacian eigenvalues, the *Laplacian energy* $LE(G)$ was put forward, defined as [6]

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

where G is a graph with n vertices and m edges, and $\mu_1, \mu_2, \dots, \mu_n$ are its Laplacian eigenvalues. The Laplacian energy has two major drawbacks: Namely, neither $LE(G_1 \cup G_2) = LE(G_1) + LE(G_2)$ holds in the general case, nor is the condition $LE(G \cup K_1) = LE(G)$

satisfied. In order to overcome these difficulties, Liu and Liu invented the *Laplacian energy-like invariant* $LEL(G)$, defined as [7]

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

Indeed, the relations $LEL(G_1 \cup G_2) = LEL(G_1) + LEL(G_2)$ and $LEL(G \cup K_1) = LEL(G)$ are generally valid.

The theory of LEL is nowadays well developed; details and further references can be found in the review [8]. In particular, numerous correlations between LEL and physico-chemical properties of alkanes were reported [9]. It was shown that, in spite of its name, LEL resembles more the total π -electron energy than the Laplacian energy LE [10]. Also worth mentioning is the discovery that LEL is closely related with (and in the case of bipartite graphs identical to) the incidence energy (IE) of the same graph [11–13].

Several bounds for LEL and IE have been reported [6, 13–15] of which for the present work the following are important [6]:

$$\sqrt{2m} \leq LEL(G) \leq \sqrt{2m(n-1)}. \quad (1)$$

We now show how the estimates (1) can be improved.

2. Better Bounds for LEL

In what follows, we shall need the few well-known properties of the Laplacian eigenvalues [16–19]:

1. If the graph G is connected (which necessarily is the case with molecular graphs [1]), then $n - 1$ Laplacian eigenvalues are positive, and one is equal to zero. Thus, we can label the Laplacian eigenvalues so that $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > \mu_n = 0$.
2. If the graph G has m edges, then $\mu_1 + \mu_2 + \dots + \mu_n = 2m$.
3. If the graph G has n vertices and t spanning trees [20], then

$$t = \frac{1}{n} \prod_{i=1}^{n-1} \mu_i. \quad (2)$$

Recall that the count of spanning trees is sometimes referred to as the *complexity* of the graph. For its chemical applications see the works [21, 22] and the references cited therein.

Our starting point is Kober's inequality [23]. Let x_1, x_2, \dots, x_N be non-negative numbers, and let

$$\alpha = \frac{1}{N} \sum_{i=1}^N x_i \text{ and } \gamma = \left(\prod_{i=1}^N x_i \right)^{1/N}$$

be their arithmetic and geometric means. As well know, $\alpha \geq \gamma$ i. e., $\alpha - \gamma > 0$, with equality if and only if $x_1 = x_2 = \dots = x_N$. Kober [23] established the following bounds for the difference $\alpha - \gamma$:

$$\begin{aligned} & \frac{1}{N(N-1)} \sum_{i < j} (\sqrt{x_i} - \sqrt{x_j})^2 \\ & \leq \alpha - \gamma \leq \frac{1}{N} \sum_{i < j} (\sqrt{x_i} - \sqrt{x_j})^2. \end{aligned} \quad (3)$$

Now, by setting $N = n$ and $x_i = \mu_i, i = 1, 2, \dots, n$, we immediately obtain

$$\begin{aligned} \sum_{i < j} (\sqrt{\mu_i} - \sqrt{\mu_j})^2 &= \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (\mu_i + \mu_j - 2\sqrt{\mu_i \mu_j}) \\ &= \frac{1}{2} \left(n \sum_{i=1}^n \mu_i + n \sum_{j=1}^n \mu_j \right) - \left(\sum_{i=1}^n \sqrt{\mu_i} \right) \left(\sum_{j=1}^n \sqrt{\mu_j} \right) \\ &= 2nm - \text{LEL}^2. \end{aligned}$$

Since, in addition,

$$\alpha = \frac{1}{n} \sum_{i=1}^n \mu_i = \frac{2m}{n} \text{ and } \gamma = \left(\prod_{i=1}^n \mu_i \right)^{1/n} = 0,$$

inequalities (3) imply

$$\frac{2mn - \text{LEL}^2}{n(n-1)} \leq \frac{2m}{n} \leq \frac{2mn - \text{LEL}^2}{n}$$

from which the estimates (1) immediately follow. Thus, nothing new has been obtained.

If, however, we take into account the fact that $\mu_n = 0$, and therefore

$$\text{LEL} = \sum_{i=1}^{n-1} \sqrt{\mu_i}; \quad \sum_{i=1}^{n-1} \mu_i = 2m,$$

then we can set $N = n - 1$ and $x_i = \mu_i, i = 1, 2, \dots, n - 1$, which in view of (2) results in

$$\begin{aligned} \alpha &= \frac{1}{n-1} \sum_{i=1}^{n-1} \mu_i = \frac{2m}{n-1}, \\ \gamma &= \left(\prod_{i=1}^{n-1} \mu_i \right)^{1/(n-1)} = (nt)^{1/(n-1)} \end{aligned}$$

and

$$\begin{aligned} \sum_{i < j} (\sqrt{\mu_i} - \sqrt{\mu_j})^2 &= \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} (\mu_i + \mu_j - 2\sqrt{\mu_i \mu_j}) \\ &= \frac{1}{2} \left((n-1) \sum_{i=1}^n \mu_i + (n-1) \sum_{j=1}^n \mu_j \right) \\ &\quad - \left(\sum_{i=1}^{n-1} \sqrt{\mu_i} \right) \left(\sum_{j=1}^{n-1} \sqrt{\mu_j} \right) = 2(n-1)m - \text{LEL}^2. \end{aligned}$$

Kober's inequality yields now

$$\begin{aligned} \frac{2m(n-1) - \text{LEL}^2}{(n-1)(n-2)} &\leq \frac{2m}{n-1} - (nt)^{1/(n-1)} \\ &\leq \frac{2m(n-1) - \text{LEL}^2}{n-1} \end{aligned}$$

from which follows

$$\begin{aligned} \sqrt{\frac{4m(n-1)}{n} + (n-1)(n-2)(nt)^{1/(n-1)}} &\leq \text{LEL} \\ &\leq \sqrt{\frac{2m(n-1)^2}{n} + (n-1)(nt)^{1/(n-1)}}. \end{aligned} \quad (4)$$

It is not too difficult to see that the estimates (4) are narrower than those given by (1). Indeed,

$$\begin{aligned} &\sqrt{\frac{4m(n-1)}{n} + (n-1)(n-2)(nt)^{1/(n-1)}} \\ &\geq \sqrt{\frac{4m(n-1)}{n}} > \sqrt{2m}, \end{aligned}$$

where the latter inequality holds for $n \geq 3$. Therefore the lower bound in (4) is better than in (1).

For molecular graphs (and, in general, for graphs with small number of edges) [20], the number of spanning trees is either a constant (as in the case of trees) or increases as a linear function of n . In both cases the term $\beta = (nt)^{1/(n-1)}$ is practically independent of n and is not much greater than unity ($\beta \approx 1$). Bearing this in mind, we have

$$\begin{aligned} & \sqrt{\frac{2m(n-1)^2}{n} + (n-1)(nt)^{1/(n-1)}} \\ &= \sqrt{\left(2m - \frac{2m}{n} + \beta\right)(n-1)}. \end{aligned}$$

The upper bound in (4) will be better than that in (1) if $2m - (2m/n) + \beta < 2m$ i. e., if $\beta - 2m/n < 0$. Since $2m/n$ is the average vertex degree, which for molecular graphs is around two or greater than two, and since $\beta \approx 1$, we see that for molecular graphs the condition $\beta - 2m/n < 0$ is always satisfied.

For disconnected graphs, for which $t = 0$, the estimates (4) are simplified as

$$\sqrt{\frac{4m(n-1)}{n}} \leq \text{LEL} \leq (n-1)\sqrt{\frac{2m}{n}}.$$

Another simplification of (4) is obtained for trees.

3. Bounds for LEL of Trees

Trees are connected acyclic graphs [1]. A tree with n vertices has $n-1$ edges and a unique spanning tree ($t = 1$). In view of this, for trees the estimates (4) reduce to

$$\begin{aligned} & \sqrt{\frac{4m(n-1)}{n} + {}^{n-1}\sqrt{n(n-1)(n-2)}} \\ & \leq \text{LEL} \leq \sqrt{\frac{2m(n-1)^2}{n} + {}^{n-1}\sqrt{n(n-1)}}. \end{aligned} \quad (5)$$

The limit value of ${}^{n-1}\sqrt{n}$ for $n \rightarrow \infty$ is equal to unity. Therefore, for trees with large values of vertices, the term ${}^{n-1}\sqrt{n}$ could be left out from the bounds (5). However, in real chemical applications [9] we are interested in molecular graphs with relatively small values of n , say between 5 and 15. Because $\sqrt[4]{5} \approx 1.5$ and $\sqrt[14]{15} \approx 1.2$, for practical purposes one could safely use the much simpler bounds

$$\begin{aligned} & \sqrt{\frac{4m(n-1)}{n} + 1.2(n-1)(n-2)} \\ & \leq \text{LEL} \leq \sqrt{\frac{2m(n-1)^2}{n} + 1.5(n-1)}. \end{aligned}$$

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