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Original scientific paper

Hyper-Wiener index and Laplacian spectrum

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Abstract: The hyper-Wiener index *WWW* of a chemical tree *T* is defined as the sum of the product $n_1\, n_2\, n_3$, over all pairs u, v of vertices of *T*, where n_1 and n_2 are the number of vertices of *T*, lying on the two sides of the path which connects u and v, and n_3 is the number of vertices lying between u and v. An expression enabling the calculation of *WWW* from the Laplacian eigenvalues of *T* has been deduced.

Keywords: hyper-Wiener index, Wiener index, Laplacian spectrum, chemical trees, alkanes.

In the preceding paper[1] a new modification of the hyper-Wiener index, denoted as *WWW*, was put forward. It was demonstrated[1] that the *WWW* has certain advantages over the original hyper-Wiener index[2] *WW*, and relations between *WWW* and *WW* were established. In this note it will be shown how the *WWW* can be computed from the Laplacian eigenvalues of the underlying molecular graph.

The Laplacian graph spectral theory has found recently many chemical applications, see, for instance, the papers[3–11] and the references quoted therein. Details of this theory can be found in several reviews.[12–15]

The Laplacian matrix $L(G)$ of a graph G with n vertices, $v_1, v_2, \ldots v_n$, is a square matrix of order n whose (i,j)-entry is defined as

$$L(G)_{ij} = \begin{cases} \delta_i & \text{if } i = j \\ -1 & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

where δ_i denotes the degree (= number of first neighbors) of the i-th vertex of G. The eigenvalues of the Laplacian matrix, denoted by $\mu_1, \mu_2, \ldots, \mu_n$, are said to be the Laplacian eigenvalues of the graph G and to form its Laplacian spectrum.

The Laplacian eigenvalues are labeled so that

$$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n.$$

Then for all graphs, $\mu_n = 0$, and for connected graphs (among which are all molecular graphs), $\mu_{n-1} > 0$.

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The Laplacian characteristic polynomial is $\psi(G,x) = \det[x\,I - L(G)]$. It can be written in the coefficient form as:

$$\psi(G,x) = \sum_{k=0}^{n-1} (-1)^k c_k x^{n-k}$$

According to the Kel'mans theorem,[3,8,16,17] the k-th coefficient of the Laplacian polynomial can be computed from the structure of the graph G by means of the formula

$$c_k = \sum_F \Gamma(F)$$

where the summation goes over all spanning forests F of G, possessing k disconnected components, and where $\Gamma(F)$ is equal to the product of the number of vertices of the components of F. In the case of a tree T, the straightforward application of the Kel'mans theorem gives:

$$\begin{aligned} c_n &= 0 \\ c_{n-1} &= n \\ c_{n-2} &= \sum_{adj} n_1 n_2 \\ c_{n-3} &= \sum_{u,v} n_1 n_2 n_3 \end{aligned} \tag{1}$$

where the notation is same as in the preceding paper.[1] Thus, it can immediately be realized that:

$$c_{n-2} = W(T) \tag{2}$$

$$c_{n-3} = WWW(T). \tag{3}$$

Using the Vieta identities and bearing in mind that $\mu_n = 0$, the coefficients c_{n-1}, c_{n-2}, and c_{n-3} are expressed in terms of Laplacian eigenvalues as:

$$\begin{aligned} c_{n-1} &= \mu_1 \times \mu_2 \times \ldots \times \mu_{n-1} \\ c_{n-2} &= \sum_i \mu_1 \times \mu_2 \times \ldots \times \mu_{i-1} \times \mu_{i+1} \times \ldots \times \mu_{n-1} \\ c_{n-3} &= \sum_{i<j} \mu_1 \times \mu_2 \times \ldots \times \mu_{i-1} \times \mu_{i+1} \times \ldots \times \mu_{j-1} \times \mu_{j+1} \times \ldots \times \mu_{n-1} \end{aligned}$$

i.e.,

$$\begin{aligned} c_{n-1} &= \prod_k \mu_k \\ c_{n-2} &= \left(\prod_k \mu_k\right)\left(\sum_i \frac{1}{\mu_i}\right) \\ c_{n-3} &= \left(\prod_k \mu_k\right)\left(\sum_{i<j} \frac{1}{\mu_i \mu_j}\right) \end{aligned}$$

Combining the latter identities with Eqs. (1)–(3), one obtains:

$$W(T) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i} \tag{4}$$

$$WWW(T) = n\sum_{i<j}\frac{1}{\mu_i\mu_j} \tag{5}$$

Formula (4), which is an expression for the Wiener index in terms of Laplacian eigenvalues, is a previously known result.[3,4] The analogous formula (5) is being reported here for the first time. It can be simplified as:

$$\begin{aligned} WWW(T) &= \frac{n}{2}\left(\sum_{i=1}^{n-1}\sum_{j=1}^{n-1}\frac{1}{\mu_i\mu_j} - \sum_{i=1}^{n-1}\frac{1}{(\mu_i)^2}\right) \\ &= \frac{n}{2}\left[\left(\sum_{i=1}^{n-1}\frac{1}{\mu_i}\right)\left(\sum_{j=1}^{n-1}\frac{1}{\mu_j}\right) - \sum_{i=1}^{n-1}\frac{1}{(\mu_i)^2}\right] \\ &= \frac{n}{2}\left[\left(\frac{W(T)}{n}\right)^2 - \sum_{i=1}^{n-1}\frac{1}{(\mu_i)^2}\right] \end{aligned}$$

which finally results in the identity:

$$WWW(T) = \frac{W(T)}{2n} - \frac{n}{2}\sum_{i=1}^{n-1}\frac{1}{(\mu_i)^2}. \tag{6}$$

Formula (6), combined with (4), is particularly suitable for computer-aided numerical calculation of the hyper-Wiener index. All the results reported in the preceding work[1] were obtained by means of this formula.

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ИЗВОД

ХИПЕР-ВИНЕРОВ ИНДЕКС И ЛАПЛАСОВ СПЕКТАР

ИВАН ГУТМАН

Природно-математички факултет у Крагујевцу

Хипер-Винеров индекс *WWW* хемијског стабла *T* дефинисан је као сума производа $n_1n_2n_3$, преко свих парова *u*, *v* чворова стабла *T*, где n_1 и n_2 означавају број чворова који леже са две стране пута који повезује *u* и *v*, а n_3 је број чворова између *u* и *v*. Добивена је формула која омогућава да се *WWW* израчуна из Лапласових сопствених вредности стабла *T*.

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