J. Serb. Chem. Soc. *65*(11)799–801(2000) UDC 519.1/.4:339.124/.126.34/.184
JSCS–2806 *Original scientific paper*

No Hückel graph is hyperenergetic

I. GUTMAN,[a#] Y. HOU,[b] H. B. WALIKAR,[c] H. S. RAMANE[d] and P. R. HAMPIHOLI[d]

[a]*Faculty of Science, University of Kragujevac, P. O. Box 60, YU-34000, Kragujevac, Yugoslavia,* [b]*Department of Mathematics, University of Science and Technology of China, Hefei, Anhui 230026, China,* [c]*Department of Mathematics, Karnatak University Campus, Post Bag 3, Belgaum - 509 001 India, and* [d]*Gogte Institute of Technology, Udyambag, Belgaum - 590 008, India*

(Received 10 July 2000)

If G is a molecular graph with n vertices and if $\lambda_1, \lambda_2, ..., \lambda_n$ are its eigenvalues, then the energy of G is equal to $E(G) = |\lambda_1| + |\lambda_2| + ... + |\lambda_n|$. If $E(G) > 2n - 2$, then G is said to be hyperenergetic. We show that no Hückel graph (= the graph representation of a conjugated hydrocarbon within the Hückel molecular orbital model) is hyperenergetic.

Keywords: total π-electron energy, energy of graph, hyperenergetic graphs.

The concept of hyperenergetic graphs was introduced in a recent work.[1] A graph G with n vertices is said to be hyperenergetic if its energy $E(G)$ satisfies the relation $E(G) > 2n - 2$. As usual, $E(G) = |\lambda_1| + |\lambda_2| + ... + |\lambda_n|$, where $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of G. The energy of a graph is a quantity closely related to the Hückel molecular orbital total π-electron energy.[2]

Although the existence of hyperenergetic graphs has been known for quite some time,[3] their systematic design was first achieved by three of the present authors,[4] followed by others.[1,5–7] All the hitherto known hyperenergetic graphs possess a large number of edges and, from a chemical point of view, may be considered as cluster graphs.[1] Among the ordinary molecular graphs representing conjugated molecules, so-called Hückel graphs,[2,8] not a single hyperenergetic species has been detected. We now show that this necessarily has to be the case: Hückel graphs cannot be hyperenergetic.

We first deduce an auxiliary result.

Theorem 1. A graph with n verices and m edges, such that $m < 2n - 2$ cannot be hyperenergetic.

Proof. In order to show the validity of Theorem 1 we recall the recently obtained upper bound for the total π-electron energy[9]

Serbian Chemical Society active member.

$$E(G) \le \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} \tag{1}$$

which holds for all (n, m)-graphs. Now, whenever the condition

$$\frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} < 2n - 2 \tag{2}$$

is satisfied, then because of Eq. (1) the graph G cannot be hyperenergetic.

The inequality (2) is easily transformed into

$$2n^3 - 4n^2 + 2n - 3mn + 2m^2 + 4m - mn^2 > 0$$

which is simplified as

$$2m^2 - m(n-1)(n+4) + 2n(n-1)^2 > 0. \tag{3}$$

Considering the right-hand side of (3) as a polynomial in the variable m we conclude that it is positive for $m < m_1$ and $m > m_2$, where m_1 and m_2 are the two solutions of the equation

$$2m^2 - m(n-1)(n+4) + 2n(n-1)^2 = 0.$$

By direct calculation we get

$$m_1 = 2(n-1)\ ;\ m_2 = n(n-1)/2$$

The condition $m > n(n-1)/2$ is impossible, because the complete graph has $n(n-1)/2$ edges, which is the maximal number of edges that an n-vertex graph may possess. There remains the condition $m < 2(n-1)$ which is just what has been stated in Theorem 1.

We are now prepared to prove our main result:

Theorem 2. No Hückel graph is hyperenergetic

Proof. As is well known,[2,8] every vertex of a Hückel graph has a degree (= number of first neighbors) of at most 3. Consequently, an n vertex Hückel graph has at most $3n/2$ edges. (Exactly $3n/2$ edges have the molecular graphs of fullerenes.)

By Theorem 1 we know that whenever $m < 2n-2$, then the respective graph cannot be hyperenergetic. Now,

$$\frac{3n}{2} = 2n - 2 - \frac{n-4}{2}$$

and for $n > 4$ we see that $3n/2 < 2n - 2$. In other words, all Hückel graphs with more than four vertices have fewer than $2n - 2$ edges and are thus not hyperenergetic.

The fact that graphs with 4 or fewer vertices are also not hyperenergetic is easily verified by direct checking.

ИЗВОД

НИЈЕДАН ХИКЕЛОВ ГРАФ НИЈЕ ХИПЕРЕНЕРГЕТСКИ

И. ГУТМАН,[а] J. HOU,[б] H. B. VALIKAR,[ц] H. S. RAMANE[д] и P. R. HAMPIHOLI[д]

[а]*Природно-математички факултет у Крагујевцу*, [б]*Одсек за математику, Кинески Универзитет науке и технологије, Хефеј, Кина*, [ц]*Одсек за математику, Универзитет Карнатак, Белгаум, Индија* и [д]*Технолошки институт Гогте, Белгаум, Индија*

Нека је G молекулски граф са n чворова и нека су $\lambda_1, \lambda_2, ..., \lambda_n$ његове сопствене вредности. Енергија графа G је $E(G) = |\lambda_1| + |\lambda 2| + ... + |\lambda_n|$. Ако је $E(G) > 2n - 2$ кажемо да је граф G хиперенергетски. Показано је да ниједан Хикелов граф (= графовска репрезентација конјугованог молекула у оквиру Хикеловог молекулско орбиталног модела) није хиперенергетски.

(Примљено 10. јула 2000)

REFERENCES

1. I. Gutman, *J. Serb. Chem. Soc.* **64** (1999) 199
2. I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986
3. D. Cvetković, I. Gutman, *J. Comput. Chem.* **7** (1986) 640
4. H. B. Walikar, H. S. Ramane, P. R. Hampiholi, in *Graph Connections,* R. Balakrishnan, H. M. Mulder, A. Vijayakumar, Eds., Allied Publishers, New Delhi, 1999, pp. 120–123
5. I. Gutman, T. Soldatović, D. Vidović, *Chem. Phys. Letters* **297** (1998) 428
6. I. Gutman, L. Pavlović, *Bull Acad. Serbe Sci. Arts (Cl. Math. Natur.)* **118** (1999) 35
7. J. H. Koolen, V. Moulton, I. Gutman, D. Vidović, *J. Serb. Chem. Soc.* **65** (2000) 571
8. A. Graovac, I. Gutman, N. Tinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer-Verlag, Berlin, 1977
9. J. H. Koolen, V. Moulton, I. Gutman, *Chem. Phys. Lett.* **320** (2000) 213.