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Note

NOTE

Bicyclic molecular graphs with the greatest energy

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Abstract: The molecular graph Q_n is obtained by attaching hexagons to the end vertices of the path graph $P_{n\text{-}12.}$ Earlier empirical studies indicated that Q_n has greatest energy among all bicyclic n-vertex (molecular) graphs. Recently, Li and Zhang proved that Q_n has greatest energy among all bipartite bicyclic graphs, with the exception of the graphs $R_{a,b}$, $a + b = n$, where $R_{a,b}$ is the graph obtained by joining the cycles C_a and C_b by an edge. This result is now completed by showing that Q_n has the greatest energy among all bipartite bicyclic n-vertex graphs.

Keywords: total π-electron energy; graph energy; bicyclic molecular graphs.

INTRODUCTION

The HMO total π-electron energy E is an important quantum-chemical characteristic of large polycyclic conjugated molecules.[1–4] A closely related quantity is the graph energy (also denoted by E), equal to the sum of the absolute values of the eigenvalues of the underlying molecular graph.[4,5] The question which molecular graph (within some pertinently defined class) has the greatest E value is of evident chemical relevance and has been much studied.[1,6–13]

In 2001, by means of a computer-aided empirical search, it was established[8] that the graph Q_n (depicted in Fig. 1) is most probably the maximum-energy specie among n-vertex bicyclic molecular graphs. Recently, Li and Zhang[11] offered a mathematical result that almost completely proved this finding. Namely, they showed that Q_n has the greatest energy among bipartite bicyclic n-vertex graphs, with the exception of the graphs $R_{a,b}$, $a + b = n$. The structures of the graphs Q_n and $R_{a,b}$ are shown in Fig. 1.

COMPLETING THE RESULT OF LI AND ZHANG

For odd n, the graphs $R_{a,b}$, $a + b = n$, are not bipartite. Therefore, for odd n, it is know that Q_n is the maximum-energy bicyclic bipartite graph and there re-

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mains nothing to be added to the proof of Li and Zhang. In view of this, in what follows, it is assumed that n is even.

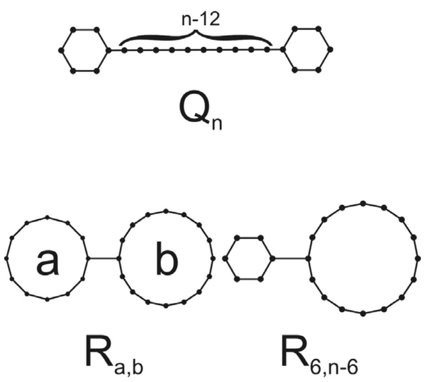

Fig. 1. The molecular graphs considered in this note. All these graphs are assumed to possess n vertices and that $n \geq 12$. Therefore $a + b = n$.

In order to complete the result of Li and Zhang,[11] appropriate computer-based investigations were undertaken. First it was necessary to determine which among the graphs $R_{a,b}$, $a + b = n$, has the greatest energy. As bipartite graphs are under consideration,[5] the parameters a and b must be even. In view of the earlier collected knowledge on the Hückel ($4m + 2$)-rule (for details see[14–16]), it could be anticipated that $E(R_{a,b})$ will be maximal for $a = 6$, $b = n - 6$ (or, what is the same: $a = n - 6$, $b = 6$). This, indeed, was confirmed by our calculations, performed until $a + b = 50$.

A comparison of the energies of Q_n and $R_{6,n-6}$ was now required. For this the quantity $\Delta(n) = E(Q_n) - E(R_{6,n-6})$, the dependence of which on n is shown in Fig. 2, was computed.

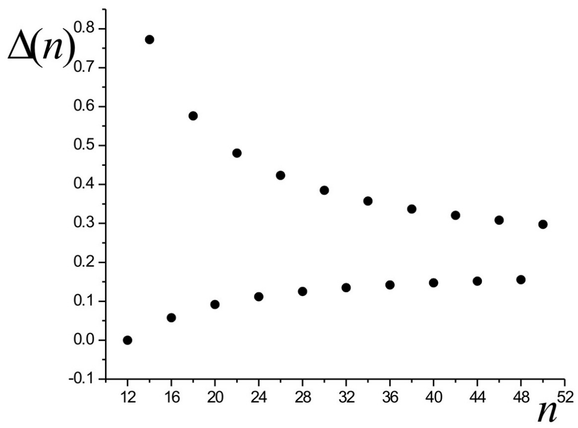

Fig. 2. The dependence of $\Delta(n) = E(Q_n) - E(R_{6,n-6})$ on the number n of vertices of the molecular graphs considered. For details see text.

As another consequence of the Hückel ($4m + 2$)-rule, the data points for $n \equiv 0 \pmod 4$, *i.e.,* for n = 12, 16, 20, 24,…, lie below the data points for $n \equiv 2 \pmod 4$, *i.e.*, for n = 14, 18, 22, 26,… For $n = 12$, the molecular graphs Q_n and

$R_{6,n-6}$ coincide and therefore $\Delta(12) = 0$. For all other (even) values of n, $\Delta(n)$ is greater than zero. Moreover, as seen from Fig. 2, in the limit case $n \to \infty$, $\Delta(n)$ tends to a value that lies between 0.2 and 0.3.

By this it was verified that for all even values of n, $n > 12$, $E(Q_n) > E(R_{6,n-6})$. Consequently, $E(Q_n) > E(R_{a,b})$ for any even value of a and b, $a + b = n$. Together with the result of Li and Zhang[11], this implies that the earlier guess[8] that Q_n, the molecular graph of the α,ω-diphenylpolyene, has the greatest energy among all bicyclic graphs was correct.

ИЗВОД

БИЦИКЛИЧНИ МОЛЕКУЛСКИ ГРАФОВИ СА НАЈВЕЋОМ ЕНЕРГИЈОМ

БОРИС ФУРТУЛА, СЛАВКО РАДЕНКОВИЋ и ИВАН ГУТМАН

Природно–математички факултет Универзитета у Крагујевцу

Молекулски граф Q_n се добија додавањем по једног хексагона на крајње чворове пута $P_{n\text{-}12}$. Ранија емпиријска проучавања указала су на то да Q_n има највећу енергију међу свим бицикличним (молекулским) графовима са n чворова. Недавно су Li и Zhang доказали да Q_n има највећу енергију међу свим бипартитним бицикличним графовима, са изузетком графова $R_{a,b}$, $a + b=n$, где је $R_{a,b}$ граф добијен повезивањем циклова C_a и C_b једном граном. Сада је овај резултат комплетиран тиме што је показано да Q_n има највећу енергију међу свим бипартитним бицикличним графовима са n чворова.

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