NOTE

Bicyclic molecular graphs with the greatest energy

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(Received 6 December 2007)

Abstract: The molecular graph $Q_n$ is obtained by attaching hexagons to the end vertices of the path graph $P_{n-12}$. 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 established8 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 Zhang11 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-
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 \( n \equiv 0 \) (mod 4), \( i.e.\), for \( n = 12, 16, 20, 24, \ldots \), lie below the data points for \( n \equiv 2 \) (mod 4), \( i.e.\), for \( n = 14, 18, 22, 26, \ldots \). 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 $a,\omega$-diphenylpolyene, has the greatest energy among all bicyclic graphs was correct.

**REFERENCES**