

Partitioning of π -Electrons in Rings of Fibonacenes

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The partitioning of π -electrons into rings of benzenoid hydrocarbons is examined in the case of fibonacenes. It is demonstrated that the π -electron contents (EC s) of the hexagons of fibonacenes satisfy the following peculiar regularities: Let h be the number of hexagons, and $EC(i)$ the electron content of the i -th hexagon. Then $EC(i)$ is maximal for $i = 1$ and $i = h$, and minimal for $i = 2$ and $i = h - 1$. Going from the end towards the center of the fibonacene chain, $EC(1) > EC(3) > EC(5) > \dots$ and $EC(2) < EC(4) < EC(6) < \dots$ and $EC(1) > EC(2) < EC(3) > EC(4) < EC(5) > EC(6) < \dots$. For large values of h , the asymptotic values of $EC(1)$ and $EC(2)$ are 5.146 and 3.798, whereas of the central ring(s) 4 π -electrons.

Key words: Benzenoid Hydrocarbon; Fibonacene; Partition of π -Electrons;
 π -Electron Content (of a Ring).