OPEN PROBLEMS IN MATHEMATICAL CHEMISTRY

GENERALIZATION OF EXTREMAL HEXAGONAL ANIMALS (POLYHEXES)

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Received 19 December 1991

A very useful relation for polyhexes, viz.

$$n_i \leq 2h+1-\left\lceil (12h-3)^{1/2} \right\rceil, \tag{1}$$

was given explicitly by Gutman [1] as a simple deduction from an analysis of Harary and Harborth [2]. Here, h and n_i are the numbers of hexagons and internal vertices, respectively. The ceiling function is employed; $\lceil x \rceil$ is the smallest integer not smaller than x. The upper bound (1) of n_i is realized in "extremal animals" [2]. It is noted that the Harary–Harborth analysis which led to eq. (1) was based on the solution [3] of an open problem posed by Reutter [4] in the form of a conjecture.

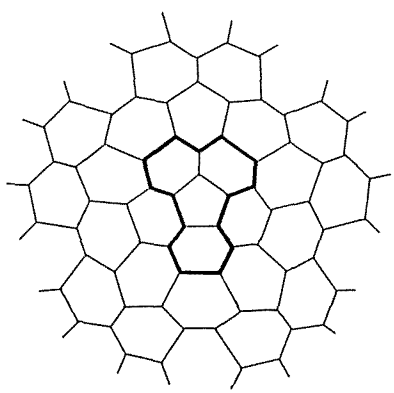

Fig. 1. The monopentahexagonal lattice with the contour (heavy line) defining the $C_{16}H_{10}$ fluoranthene graph.

Let a geometrically planar, simply connected mono-q-polyhex be defined by a cycle on a mono-q-hexagonal lattice in analogy with the current definition of geometrically planar, simply connected polyhexes (benzenoids) [1]. The mono-q-hexagonal lattice is similar to the hexagonal lattice; it consists of exactly one q-gon and otherwise hexagons. In fig. 1, the example with $q = 5$ is depicted, the monopentahexagonal lattice. The cycle should embrace the unique q-gon, in fig. 1 the pentagon.

Many hydrocarbons correspond to the mono-q-polyhex graphs, e.g. the (q)circulenes. In this set of homologous molecules, $C_{20}H_{10}$ corannulene [5] is (5)circulene, while $C_{24}H_{12}$ coronene is chemically indistinguishable from (6)circulene. Also $C_{28}H_{14}$ (7)circulene has been synthesized [6], and a synthesis of $C_{32}H_{16}$ (8)circulene has been attempted [7].

The following conjecture is proposed for mono-q-polyhexes:

$$n_i \le 2h' - \left\lceil (1/2)(8qh' + q^2)^{1/2} - (q/2) \right\rceil, \tag{2}$$

where h' is the number of hexagons outside the unique q-gon. The upper bound (2) is supposed to be realized in the appropriate extremal systems. In the words of Reutter [4]: "Man beweise oder widerlege diese Vermutung."

The special case (1) emerges from (2) by inserting $h' = h - 1$ and $q = 6$. Another important special case is $q = 5$ for monopentapolyhexes, which pertain to the many known fluoranthenoid/fluorenoid hydrocarbons (including corannulene). Let

$$r = h' + 1 \tag{3}$$

denote the number of polygons (or "rings"). Then, if the conjecture (2) is sound, one has

$$n_i \le 2r - \left\lceil (1/2)(40r - 15)^{1/2} - (1/2) \right\rceil. \tag{4}$$

References

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