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Counterexamples to Cyvin's conjecture

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A conjuctured bound for the number of internal vertices in a simply connected mono-q-polyhex is disproved

Introduction

Let C be a cycle in the regular hexagonal lattice in the plane. The structure consisting of all vertices, edges and hexagons interior to or on C is called a *polyhex* (or a *hexagonal animal*). Polyhexes are of interest to chemists since they correspond to benzenoids. A *mono-q-hexagonal lattice* in the plane contains a single q-gon ($q = 3, 4, 5$ or $q \geqslant 7$) but all other faces are hexagons. It is impossible for such a lattice to be constructed solely from regular polygons but it will be assumed that at each vertex precisely three of the polygons meet. For a cycle C on such a lattice, the analogue of a polyhex is called a *mono-q-polyhex*, it being assumed that the q-gon is inside C. The case $q = 5$ in particular is of interest to chemists since many known fluoranthenoid and fluorenoid hydrocarbons correspond to monopentapolyhexes.

Recently S.J. Cyvin [1] conjectured that the number n of internal vertices in a simply connected mono-q-polyhex satisfies the following inequality:

$$n \leqslant 2h - \lceil \{\sqrt{(q^2 + 8qh)} - q\}/2 \rceil, \tag{1}$$

where h is the number of hexagons and $\lceil x \rceil$ denotes the smallest integer which is not less than x. In this paper it is shown that for any fixed $h \geqslant 2$ the conjecture is wrong provided q is sufficiently large and for any fixed $q \geqslant 9$ it is wrong for certain values of h.

NOTATION

Let

$$\alpha(h, q) = \sqrt{(q^2 + 8qh)} - q$$

and

$$\beta(h,q) = 2h - \alpha(h,q)/2 .$$

Also let $\gamma(h,q)$ denote the right hand side of inequality (1). It is easy to show that

$$\gamma(h,q) = \lfloor \beta(h,q) \rfloor ,$$

where $\lfloor x \rfloor$ denotes the integer part of x.

LEMMA

For fixed h, the number $\beta(h,q) \to 0$ as $q \to \infty$.

Proof

It suffices to show that $\alpha(h,q) \to 4h$ as $q \to \infty$. Now

$$\begin{aligned}\alpha(h,q) &= \sqrt{(q^2+8qh)} - q \\ &= \frac{\{\sqrt{(q^2+8qh)} - q\}\{\sqrt{(q^2+8qh)} + q\}}{\sqrt{(q^2+8qh)} + q} \\ &= \frac{8qh}{\sqrt{(q^2+8qh)} + q} \\ &= \frac{8h}{\sqrt{(1+8h/q)} + 1} \\ &\to 8h/2 = 4h .\end{aligned}$$

□

COROLLARY

Since $\gamma(h,q) = \lfloor \beta(h,q) \rfloor$ is an integer, it follows that $\gamma(h,q) = 0$ for q sufficiently large. [In the counterexamples below it suffices to note that $\gamma(h,q) < h - 1$ for q sufficiently large.]

COUNTEREXAMPLES

For any $h \geqslant 2$ and $q \geqslant h+1$ the mono-q-polyhex $Q(h,q)$ with the h hexagons adjoining h consecutive edges of the q-gon (see fig. 1) has $n = h - 1$ so $Q(h,q)$ is a counterexample. [The condition $q \geqslant h+1$ is not important since if $q \leqslant h$ then it is easy to construct a counter example with $n > h - 1$ by completely encircling the q-gon with hexagons.]

The simplest cases are (see fig. 2) $h = 2, q = 10$ for which $n = 1$ but $\gamma(2,10) = 0$ and (see fig. 3) $h = 3, q = 9$ for which $n = 2$ but $\gamma(3,9) = 1$.

More generally, the following results hold.

(a) For fixed $h \geqslant 2$ Cyvin's conjecture is false for all $q > (h+1)^2/(h-1)$.

(b) For $q = 9$ Cyvin's conjecture is false for $h = 3$ and 4 and for fixed $q \geqslant 10$ the conjecture is false for all h satisfying

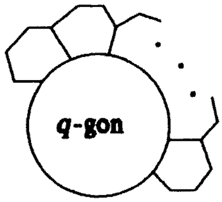

Fig. 1. $Q(h,q)$.

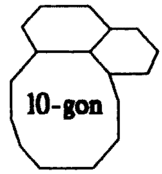

Fig. 2. $Q(2,10)$.

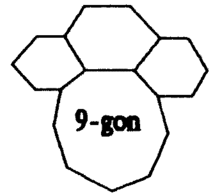

Fig. 3. $Q(3,9)$.

$$2 \leqslant h < \{(q-2) + \sqrt{(q^2 - 8q)}\}/2 . \tag{2}$$

Proof

The mono-q-polyhexes $Q(h,q)$ provide counterexamples when

$$h - 1 > \beta(h,q) . \tag{3}$$

It is straightforward to show that (3) is equivalent to

$$q > (h+1)^2/(h-1) \tag{4}$$

and that (4) is equivalent to

$$h^2 + (2-q)h + q + 1 < 0 . \tag{5}$$

The roots of the quadratic equation

$$h^2 + (2-q)h + q + 1 = 0$$

are

$$\{(q-2) \pm \sqrt{(q^2 - 8q)}\}/2$$

and they are real and distinct if and only if $q > 8$. Inequality (5) then holds for values of h strictly between the two roots. When $q = 9$ the roots are 2 and 5 but for $q \geqslant 10$ the smaller root lies strictly between 1 and 2 so the lower bound for h may be replaced by 2 to give (2). □

Summary

The present paper shows that Cyvin's conjecture is false for infinitely many pairs (h,q) but it leaves undecided the status of the conjecture for infinitely many other pairs satisfying neither condition (a) nor condition (b). In particular no light is shed on the cases $q = 3, 4, 5, 7, 8$ some of which are of particular interest to chemists.

The case $q = 6$ is excluded above, but substituting $q = 6$ into (1) gives

$$n \leqslant 2h + 3 - \lceil \sqrt{(12h + 9)} \rceil . \tag{6}$$

Inequality (6) gives the best possible bound for n for polyhexes with $h + 1$ hexagons; the equivalent inequality

$$n \leqslant 2h + 1 - \lceil \sqrt{(12h - 3)} \rceil ,$$

where h is the total number of hexagons in the polyhex was given explicitly by Gutman [2].

Postscript

Since this paper was originally submitted, Mohar [3], using a very different approach, has proved Cyvin's conjecture for $q < 6$, disproved it for $q > 6$ and has shown that (6) gives the best possible bound for n not just in the case when $q = 6$ but for all $q \geqslant 6$.

References

[1] S.J. Cyvin, J. Math. Chem. 9 (1992) 389.
[2] I. Gutman, Bull. Soc. Chim. Beograd. 47 (1982) 453.
[3] B. Mohar, University of Ljubljana, Institute of Mathematics, Physics and Mechanics Preprint Series 31 (1993) 396.