Open problem

Generalization of extremal animals once again

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I have noted with pleasure the mathematical activity which was triggered by my conjecture on mono-q-polyhexes [1]. It became clear through private communications with E.K. Lloyd that the conjecture is sound for $q \le 6$, but fails for q > 6. The present note deals with polygonal systems which (for $q \ne 6$) are different from the mono-q-polyhexes.

Consider a system, P_q , of simply connected q-gons where any two q-gons either share exactly one edge or are disjointed. Then q = 6 represents the simply connected polyhexes, for which the Harary-Harborth formula [2,3]

$$(n_i)_{\max} = 2r + 1 - \left[(12r - 3)^{1/2} \right] \tag{1}$$

is sound. Here r and n_i denote the number of hexagons (or rings) and the number of internal vertices, respectively. The system P_q is by definition extremal when $n_i = (n_i)_{\max}$. It is reasonable to assume that, when q > 6, one extremal P_q is generated for every r (number of polygons) during a spiral walk in analogy with the situation for polyhexes (q = 6) [2]; see fig. 1. My attempts to find $(n_i)_{\max}$ for P_q when q > 6 gave some surprises.

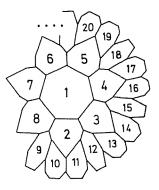


Fig. 1. Illustration of the spiral walk for polyheptagonal (P_7) systems.

Let me first report briefly a facile derivation which gives a clue to eq. (1). Consider k-fold circumscribed benzene (one hexagon), which is a special extremal P_6 system, and denote its number of hexagons and number of internal vertices by r_k and $(n_i)_k$, respectively. It is easily found [4]

$$r_k = 3k^2 + 3k + 1, \quad (n_i)_k = 6k^2.$$
 (2)

Herefrom

$$k = \frac{1}{2} \pm \frac{1}{6} (12r_k - 3)^{1/2}, \qquad (3)$$

where the minus sign should be applied. On inserting this k into the right-hand side of (2) one obtains

$$(n_i)_k = 2r_k + 1 - (12r_k - 3)^{1/2}.$$
(4)

This expression is indeed consistent with eq. (1), although (1), of course, does not follow immediately from (4).

When attempting to do something of the same for k-fold circumscribed heptagon (cf. fig. 1) I arrived at

$$r_k = 7F_{2k} - 6, \quad (n_i)_k = 7(2F_{2k} - F_{2k-1} - 2),$$
(5)

in terms of the Fibonacci numbers ($F_{-1} = 0, F_0 = F_1 = 1$, etc.). This is an interesting result, derived previously by Harborth [5], but stops effectively a derivation of an expression for $(n_i)_{max}$ when q = 7.

In precise terms, the open problem reads: Find the maximum of internal vertices, $(n_i)_{max}$, as a function of the number of polygons, r, in simply connected polygonal systems (P_q) consisting of q-gons where q > 6.

References

- [1] S.J. Cyvin, J. Math. Chem. 9 (1992) 389.
- [2] F. Harary and H. Harborth, J. Combin. Inf. Sys. Sci. 1 (1976) 1.
- [3] I. Gutman, Bull. Soc. Chim. Beograd 47 (1982) 453.
- [4] J. Brunvoll and S.J. Cyvin, Z. Naturforsch. (a) 45 (1990) 69.
- [5] H. Harborth, Applications of Fibonacci Numbers, Vol. 3, eds. G.E. Bergum, A.N. Phillippou and A.F. Horadam (Kluwer Academic, Dordrecht, 1990) p. 123.