Journal of Mathematical Chemistry 13(1993)213–215

Open problems in mathematical chemistry

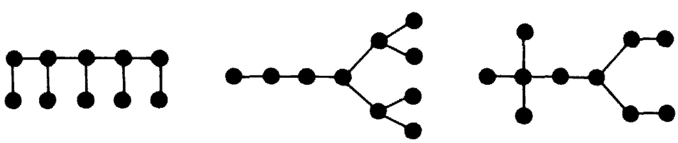
Benzenoid graphs with equal maximum eigenvalues

I. Gutman and S. Marković

Faculty of Science, University of Kragujevac, P.O. Box 60, 34000 Kragujevac, Yugoslavia

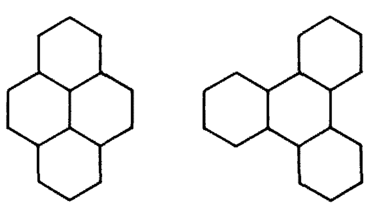
Received 4 May 1992

The maximum graph eigenvalue (x_1) is a quantity of interest in both mathematics (for a review, see ref. [1]) and in chemical graph theory (see ref. [2]). There is a plethora of molecular graphs having equal maximum eigenvalues. Such are, for instance, the molecular graphs of 3,4,5-trimethylheptane (G_1), 2-methyl-3-isopropylhexane (G_2) and 2,2-dimethyl-4-ethylhexane (G_3). Their characteristic polynomials can be written in the form $(x^2-1)(x^4-3x^2+1)(x^4-5x^2+1)$, $x^2(x^2-2)^2(x^4-5x^2+1)$ and $x^2(x^2-1)(x^2-3)(x^4-5x^2+1)$, respectively. Consequently, the maximum eigenvalues of G_1, G_2 and G_3 are equal to the largest root of the equation $x^4-5x^2+1=0$.



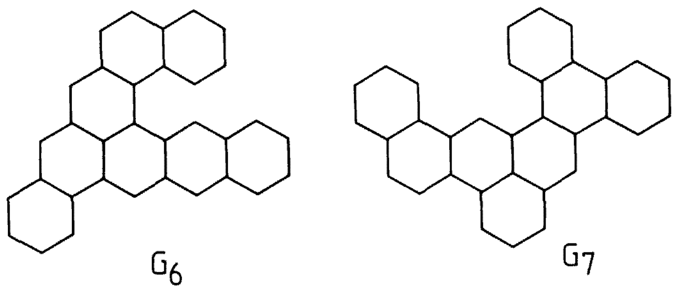
G_1 G_2 G_3

Recently, we tried to find benzenoid graphs (see ref. [3]) having equal maximum eigenvalues. It was easy to show that the molecular graphs of pyrene (G_4) and triphenylene (G_5) have such a property. This is because their characteristic polynomials are factored as $(x^2-1)(x^2-4)(x^6-5x^4+6x^2-1)(x^6-9x^4+18x^2-9)$ and $(x^6-6x^4+9x^2-3)^2(x^6-9x^4+18x^2-9)$, respectively, and because x_1 is equal to the largest root of the equation $x^6-9x^4+18x^2-9=0$.



G_4 G_5

We also tried to find benzenoid isomers whose x_1-values coincide. (Recall that the respective graphs have equal numbers of vertices and edges.) This task, however, proved to be less easy. First of all, the number of such benzenoid isomers seems to be very small. Among all benzenoid graphs with eight or less hexagons, we found only a single pair which, according to computer testing, could have the required property. This pair is G_6, G_7. The calculated maximum eigenvalues are equal to 2.6369724380 and 2.6369724369, respectively.



PROBLEM

Prove or disprove that G_6 and G_7 have equal maximum eigenvalues.

PROBLEM

Find (further) isomeric benzenoid graphs whose maximum eigenvalues coincide.

Remark

The referees suggested two approaches towards the solution of our problems.

(a) If two graphs G_a and G_b have equal maximum eigenvalues, then their characteristic polynomials have a non-trivial greatest common divisor (gcd) and the maximum eigenvalue is a zero of the gcd. Provided the gcd is a polynomial with integer coefficients, then there exists a simple procedure for its determination. The procedure requires integer arithmetic and, thus, consists of a finite number of steps. This is exactly how we treated the graphs G_1, G_2 and G_3 as well as G_4 and G_5, namely we demonstrated that they possess non-trivial gcd's.

Unfortunately, the gcd need not be an integer-coefficient polynomial (as may be the case with the graphs G_6 and G_7) and then its finding is not feasible.

(b) It may look possible to use the Sturm sequence of the product of the characteristic polynomials of G_a and G_b in order to establish whether, for a pertinently chosen constant t, in the interval $(x_1 - t, x_1 + t)$ there are two distinct zeros (implying $x_1(G_a) \neq x_1(G_b)$) or only one (implying $x_1(G_a) = x_1(G_b)$). The problem is that in order to construct the Sturm sequence of a polynomial, we must eliminate its multiple zeros. This is achieved by dividing the first two members of the Sturm sequence. However, in order to perform such a division in practice, we would have to know in advance whether the two (closely lying) zeros are equal or not.

Hence, the use of the Sturm-sequence technique seems to be of little value for the solution of our problem.

References

[1] D. Cvetković and P. Rowlinson, Lin. Multilin. Algebra 28(1990)3.
[2] N. Trinajstić, *Chemical Graph Theory*, Vol. 2 (CRC Press, Boca Raton, 1983) pp. 108–110.
[3] N. Trinajstić, *Chemical Graph Theory*, Vol. 1 (CRC Press, Boca Raton 1983) pp. 23, 24.