MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **70** (2013) 471-472

ISSN 0340 - 6253

BOOK REVIEW

Graph Energy

by

Xueliang Li, Yongtang Shi & Ivan Gutman

Springer, New York, 2012, XII + 266 pp. ISBN 978-1-4614-4219-6

The energy of a graph is the sum of absolute values of eigenvalues of the adjacency matrix of the graph.This definition was given by the third author (I.G.) in 1978. Motivation came from theoretical chemistry but the intention was to initiate mathematical studies of this graph invariant. No significant work on this subject appeared in about next twenty years.

As stated a little bit mysteriously in Preface, "sometime around the turn of the century, a dramatic change occurred, and graph energy started to attract the attention of a remarkably large number of mathematicians, all over the globe". The reviewer will offer below his explanation of this phenomenon. Anyhow, the number of published papers on graph energy is nowadays of order of several hundred. Only in years 2008-2011 the average number of such papers was around 50 per year.

The book consists of the following chapters: 1. Introduction, 2. The chemical connection, 3. The Coulson integral formula, 4. Common proof methods, 5. Bounds for the energy of graphs, 6. The energy of random graphs, 7. Graphs extremal with regard to energy, 8. Hyperenergetic and equienergetic graphs, 9. Hypoenergetic and strongly hypoenergetic graphs, 10. Miscellaneous, 11. Other graph energies.

The bibliography contains 574 references.

As explained in Chapter 2, graph energy is related to the Hückel molecular orbital (HMO) theory, an approximative method for solving the Schrödinger equation for a class of organic compounds called conjugated hydrocarbons. Within this theory the graph energy coincides with the total π-electron energy in some (majority but not all) cases.

The energy is a non-smooth function and this fact, together with a discrete character of the underlying structure (graphs), makes it difficult, but also challenging, to study problems which appear. For example, the authors emphasize, as they call, Grand Open Problem (see p.192) to characterize graphs on n vertices with maximal energy. Solution is known for $n = 4k^2$, k an integer, and extremal graphs are strongly regular which have three distinct eigenvalues. Tools from calculus suggest that extremal graphs should have a small number of distinct eigenvalues but then the discrete structure of graphs prevents to find solution: simply - desired graphs do not exist.

Another difficult open problem is presented on p. 201: how to verify that two graphs are equienergetic, i.e. have the same energy. The problem can be formulated without referring to graphs: Given two polynomials with integral coeeficients, how to check whether they have the same sum of absolute values of their zeros.

In reviewer's opinion the paper (reference [53] in the book)

G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs, 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39** (1999) 984–996,

had an essential influence on the further development of the subject. This paper offered several conjectures on graph energy obtained by the use of the computer package AutoGraphiX for finding extremal graphs with respect to given graph invariants.

Among other things, a conjecture on unicyclic graphs with maximal energy (Conjecture 7.6 on p. 153 in the book) attracted much attention. The conjecture was difficult to prove (22 pages in the book). This conjecture was unusual and attractive for a mathematician. While a mathematician (perhaps not a chemist) would expect that the cycle is extremal, the computer found that, with a finite number of exceptions, the graph consisting of a hexagon with an appended path is extremal.

The paper [53] established that among graphs on 10 vertices maximal energy has a strongly regular graph (complement of the Petersen graph). This attracted researchers working in the area of strongly regular and related graphs and we now have the Koolen-Moulton upper bound for the energy of graphs with n vertices. The order of magnitude in this bound ($n^{3/2}$) was numerically predicted in [53].

To conclude, the book presents an interesting and quickly developing area of research and will attract mathematicians and chemists interested in the theory and applications of graph eigenvalues (spectral graph theory).

Dragoš Cvetković