Geometry of Chemical Graphs: Polycycles and Two-faced Maps (Encyclopedia of Mathematics and its Applications)

Michel Deza, Mathieu Dutour Sikiri?

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Polycycles and symmetric polyhedra appear as generalisations of graphs in the modelling of molecular structures, such as the Nobel prize winning fullerenes, occurring in chemistry and crystallography. The chemistry has inspired and informed many interesting questions in mathematics and computer science, which in turn have suggested directions for synthesis of molecules. Here the authors give access to new results in the theory of polycycles and two-faced maps together with the relevant background material and mathematical tools for their study. Organised so that, after reading the introductory chapter, each chapter can be read independently from the others, the book should be accessible to researchers and students in graph theory, discrete geometry, and combinatorics, as well as to those in more applied areas such as mathematical chemistry and crystallography. Many of the results in the subject require the use of computer enumeration; the corresponding programs are available from the author's website.

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