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Geometry of Chemical Graphs: Polycycles and Two-faced Maps

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Relationships among mathematics and physics are old and well known. However, already Arthur Cayley in the 19th century realized that chemistry can inspire interesting mathematical questions. In the seventies of the 20th century a bunch of chemists realized that discrete mathematics, and especially graph theory, offer powerful tools to analyze molecular properties and reactivity in a quantitative manner. A new field of chemistry, *mathematical chemistry*, was established. Mathematicians entered this field later but today they make a large community as well.

The authors of the present book, Michel Deza of Ecole Supérieure in Paris and Mathieu Dutour Sikirić of the «R. Bošković» Institute in Zagreb, are pure mathematicians but with a strong interest in chemical problems. Their book appears as No. 119 in the series *Encyclopedia of Mathematics and Its Applications*. The volumes of the series are encyclopedic references and guides to major mathematical topics. It is a great pleasure to see that *chemical graphs* are recognized as an important subject in mathematics.

The book treats polycycles and two-faced maps.

Two-faced map and specifically, *({a,b,},k)*-map is any *k*-valent map with only *a*- and *b*-gonal faces for given integers $2 \leq a < b$. It becomes immediately clear why such maps are of interest to chemists and materials scientists: *fullerenes* are finite 3-valent maps with only 5- and 6-gonal faces. However, besides spherical fullerenes mathematicians are able to study embeddings of fullerenes in torus, Klein bottle and projective plane as well as infinite plane fullerenes. That at least one spherical fullerene with n vertices exists for all even $n \geq 20$ except for $n = 22$ is known to chemists after discovery of fullerenes in 1985 but the fact was known to mathematicians B. Gruenbaum and T. S. Motzkin already in 1963.

When restriction on 6-gonal faces is relaxed, one speaks of *fulleroids* and a chapter is devoted to them, especially their icosahedral realizations. Fulleroids are also a subject of extensive research in chemistry.

A *(r,q)-polycycle* is a simple plane 2-connected (locally finite) graph with degree at most *q* such that all interior vertices are of degree *q* and all interior faces are (combinatorial) *r*-gones. It is clear that many related pages there are of interest to chemists as *e.g.* benzenoids make just a special class of polycycles.

The book contains nineteen chapters: Preface; 1. Introduction; 2. Two-faced maps; 3. Fullerenes as tilings of surfaces; 4. Polycycles; 5. Polycycles with given boundary; 6. Symmetries of polycycles; 7. Elementary polycycles; 8. Applications of elementary decompositions to (r, q)-polycycles; 9. Strictly face-regular spheres and tori; 10. Parabolic weakly face-regular spheres; 11. Generalities on 3-valent face-regular maps; 12. Spheres and tori, which are aRi; 13. Frank-Kasper spheres and tori; 14. Spheres and tori, which are bR1; 15. Spheres and tori, which are bR2; 16. Spheres and tori, which are bR3; 17. Spheres and tori, which are bR4; 18. Spheres and tori, which are bRj for $j \geq 5$; 19. Icosahedral fulleroids.

It is organized in such a way that each chapter can be read independently from the others.

The book contains some 180 references. About a quarter of them belong to mathematicians and a few chemists who regularly publish in *MATCH Communications in Mathematical and in Computer Chemistry*, have visited University of Kragujevac and attended the *MATH/CHEM/COMP* meetings in Dubrovnik. The leading scientists among them in citations are G. Brinkmann and P. W. Fowler and are followed by G. Caporossi, A. Dress and P. Hansen. Once or twice are quoted the papers of A. T. Balaban, J. Brunvoll, M. Brusquet-Mélou, B. N. Cyvin, S. J. Cyvin, M. S. Delaney, J. R. Dias, M. N. Diudea, M. Fujita, J. E. Graver, R. B. King, E. C. Kirby, D. J. Klein, B. Mohar, A. Rassat, R. Tošić, C. H. Sah, and H. Zhu. Among these papers many of them have been published in *Journal of Chemical Information and Computer Science*, four in *MATCH Communications in Mathematical and in Computer Chemistry*, and one in *Croatica Chemica Acta*.

A series of new results is presented in this clearly written and nicely organized book. Many of them are obtained by computer enumeration and the related web sites are given in the book. It makes a useful and enjoyable reading not only for researchers and students in graph theory and mathematical chemistry but also in chemistry in general, crystallography, physics and materials sciences.

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