Geometry of Chemical Graphs

Polycycles and symmetric polyhedra appear as generalizations of graphs in the modeling of molecular structures, such as the Nobel prize winning fullerenes, occurring in chemistry and crystallography. 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. Organized 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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Geometry of Chemical Graphs: Polycycles and Two-faced Maps

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Contents

Preface

Platonic solids have been studied since antiquity and in a multiplicity of artistic and scientific contexts. More generally, "polyhedral" maps are ubiquitous in chemistry and crystallography. Their properties have been studied since Kepler. In the present book we are going to study classes of maps on the sphere or the torus and make a catalog of properties that would be helpful and useful to mathematicians and researchers in natural sciences.

In particular, we are studying here two new classes of maps, interesting for applications, especially in chemistry and crystallography (on the sphere or the torus) generalizing Platonic polyhedra. *Polycycles* are 2-connected plane graphs having prescribed combinatorial type of interior faces and the same degree q for interior vertices, while at the most q for boundary vertices. *Two-faced maps* are the maps having at most two types of faces and the same degree of vertices. Many examples and various generalizations are given throughout the text. Pictures are given for many of the obtained graphs, especially when a full classification is possible. A lot of the presentation is necessarily compact but we hope to have made it as explicit as possible.

We are interested mainly in enumeration, symmetry, extremal properties, face-regularity, metric embedding and related algorithmic problems. The graphs in this book come from broad areas of geometry, graph theory, chemistry, and crystallography. Many new interesting spheres and tori are presented.

The book is organized as follows. Chapters 1 and 2 give the main notions. After reading them, other chapters can be read almost independently.

Chapters 4–8 present the theory of polycycles. In Chapter 4, we explain the general notion of the (r, q)-polycycle, present the cases where classification is possible and the cell-homomorphism into the regular tiling $\{r, q\}$. In Chapter 5, the problem of how the boundary of an (r, q)-polycycle determines it, or not, is addressed. In Chapter 6, we consider the possible symmetries of (r, q)-polycycles and how we can classify these with a symmetry group transitive on faces and/or vertices.

Chapter 7 presents a way to decompose a generalized polycycle into elementary components. This powerful technique is used in Chapters 8, 12, 13, 14, and 18.

The second main subject – k-valent two-faced maps – is treated in Chapter 3 and Chapters 9–19. Chapter 3 deals with our main example, fullerenes, while Chapter 9 classifies strictly face-regular maps on sphere or torus. In Chapters 10–18, we consider a weaker notion of face-regularity. Chapter 19 treats 3-valent two-faced maps with icosahedral symmetry.

Many simple questions (some, possibly, easy) are raised; we hope that this book will be instrumental in their solutions. Much of the results have been obtained (and could only have been obtained) though computer enumeration; the corresponding programs are available from [Du07].

We are grateful to many people for their help with this book, especially, to Jacques Beigbeder, Gunnar Brinkmann, Olaf Delgado Friedrichs, Maja Dutour Sikirić, Patrick Fowler, Jack Graver, Marie Grindel, Viatcheslav Grishukhin, Gil Kalai, Stanislav Jendrol, and Mikhail Shtogrin.

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