

Geometry of Chemical Graphs: Polycycles and Two-faced Maps

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Preface

We study here two new, interesting for applications, especially, in Chemistry and Crystallography, classes of maps (on sphere or torus) generalizing Platonic polyhedra. *Polycycles* are 2-connected plane graphs having unique combinatorial type of interior faces and the same degree q for interior vertices, while at most q for boundary vertices. *Two-faced maps* are the maps, having at most two types of faces and the same degree of vertices.

We are interested mainly in enumeration, symmetry, extremal properties, face-regularity, metric embedding and related algorithmic problems.

The lists of 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 organised as follows. Chapters 1 and 2 give main notions. After reading them, each other chapter can be read almost independently.

Chapters 4–8 present theory of polycycles. In Chapter 4, we explain the general notion of (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 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 one can classify those with a symmetry group transitive on faces and/or vertices.

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

The second main subject - k -valent two-faced maps - is treated in Chapters 3 and 9–19. Chapter 3 deals with our main example, fullerenes, while Chapter 9 classify 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 solution. Much of the results have been obtained and could only be obtained through computer enumeration; the corresponding programs are available from [Du07].

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Contents

Preface	1
1 Introduction	7
1.1 Graphs	7
1.2 Topological notions	8
1.2.1 Maps	8
1.2.2 Orientability and classification of surfaces	10
1.2.3 Fundamental groups, coverings and quotient maps	11
1.2.4 Homology and Euler-Poincaré characteristic	13
1.3 Representation of maps	14
1.4 Symmetry groups of maps	16
1.5 Types of regularities of maps	20
1.6 Operations on maps	23
2 Two-faced maps	25
2.1 The Goldberg-Coxeter construction	28
2.2 Description of the classes	31
2.3 Computer generation of the classes	35
3 Fullerenes as tilings of surfaces	37
3.1 Classification of finite fullerenes	37
3.2 Toric and Klein bottle fullerenes	38
3.3 Projective fullerenes	40
3.4 Plane 3-fullerenes	40
4 Polycycles	43
4.1 (r, q) -polycycles	43
4.2 Examples	45
4.3 Cell-homomorphism and structure of (r, q) -polycycles	47
4.4 Angles and curvature	49
4.5 Polycycles on surfaces	51
5 Polycycles with given boundary	55
5.1 The problem of uniqueness of (r, q) -fillings	55
5.2 $(r, 3)$ -filling algorithms	59

6	Symmetries of polycycles	63
6.1	Automorphism group of (r, q) -polycycles	63
6.2	Isohedral and isogonal (r, q) -polycycles	63
6.3	Isohedral and isogonal $(r, q)_{gen}$ -polycycles	69
7	Elementary polycycles	71
7.1	Decomposition of polycycles	71
7.2	Parabolic and hyperbolic elementary $(R, q)_{gen}$ -polycycles	74
7.3	Kernel-elementary polycycles	77
7.4	Classification of elementary $(\{2, 3, 4, 5\}, 3)_{gen}$ -polycycles	80
7.5	Classification of elementary $(\{2, 3\}, 4)_{gen}$ -polycycles	84
7.6	Classification of elementary $(\{2, 3\}, 5)_{gen}$ -polycycles	85
7.7	Appendix 1: 204 Sporadic elementary $(\{2, 3, 4, 5\}, 3)$ -polycycles	87
7.8	Appendix 2: 57 sporadic elementary $(\{2, 3\}, 5)$ -polycycles	93
8	Applications of elementary decompositions to (r, q)-polycycles	97
8.1	Extremal polycycles	98
8.1.1	Extremal $(5, 3)$ -polycycles	99
8.1.2	Extremal $(3, 5)$ -polycycles	102
8.1.3	Parabolic and hyperbolic extremal (r, q) -polycycles	102
8.2	Non-extensible polycycles	104
8.3	2-embeddable polycycles	109
9	Strictly face-regular spheres and tori	113
9.1	Strictly face-regular spheres	114
9.2	Non-polyhedral strictly face-regular $(\{a, b\}, k)$ -spheres	122
9.3	Strictly face-regular $(\{a, b\}, k)$ -planes	124
9.3.1	Case determination	129
9.3.2	Proof and description of 33 parameter sets	134
10	Parabolic weakly face-regular spheres	151
10.1	Face-regular $(\{2, 6\}, 3)$ -spheres	151
10.2	Face-regular $(\{3, 6\}, 3)$ -spheres	151
10.3	Face-regular $(\{4, 6\}, 3)$ -spheres	152
10.4	Face-regular $(\{5, 6\}, 3)$ -spheres (fullerenes)	153
10.5	Face-regular $(\{3, 4\}, 4)$ -spheres	159
10.6	Face-regular $(\{2, 3\}, 6)$ -spheres	161
11	Generalities on 3-valent face-regular maps	163
11.1	General $(\{a, b\}, 3)$ -maps	166
11.2	Remaining general questions	167
12	Spheres and tori, which are aR_i	169
12.1	Maps aR_0	169
12.2	Maps $4R_1$	171
12.3	Maps $4R_2$	175
12.4	Maps $5R_2$	182
12.5	Maps $5R_3$	182

13 Frank-Kasper spheres and tori	195
13.1 Euler formula for $(\{a, b\}, 3)$ -maps bR_0	195
13.2 The major skeleton, elementary polycycles and classification results	198
14 Spheres and tori, which are bR_1	201
14.1 Euler formula for $(\{a, b\}, 3)$ -maps bR_1	201
14.2 Elementary polycycles	202
15 Spheres and tori, which are bR_2	209
15.1 $(\{a, b\}, 3)$ -maps bR_2	209
15.2 $(\{5, b\}, 3)$ -tori bR_2	211
15.3 $(\{a, b\}, 3)$ -spheres with a cycle of b -gons	214
16 Spheres and tori, which are bR_3	221
16.1 Classification of $(\{4, b\}, 3)$ -maps bR_3	221
16.2 $(\{5, b\}, 3)$ -maps bR_3	224
17 Spheres and tori, which are bR_4	231
17.1 $(\{4, b\}, 3)$ -maps bR_4	231
17.2 $(\{5, b\}, 3)$ -maps bR_4	234
18 Spheres and tori, which are bR_j for $j \geq 5$	249
18.1 Maps bR_5	249
18.2 Maps bR_6	255
19 Icosahedral fullerooids	257
19.1 Construction of I -fullerooids and infinite series	258
19.2 Restrictions on the p -vectors	261
19.3 From the p -vectors to the structures	263

