

# Preface

The central actors in the present book are the *zigzags* and *central circuits* of three- or four-regular plane graphs, which allow to obtain a double covering or covering of the edgeset. This book, a companion of the authors' book [DeDu08], mainly focuses on specific classes of bifaced plane graphs, that is, those without faces of negative curvature. It contains, as a particular case, the *fullerenes*, that is, three-regular plane graphs with faces of size five or six, which are prominent chemistry-relevant graphs. The class also contains the *octahedrites*, that is, four-regular plane graphs with faces of size three or four. We also consider three classes of graphs, which are self-dual. For all those graphs, we consider how to enumerate them, their possible symmetry groups, their connectivity, and other structural properties. We also study the *icosahedrites*, that is, five-regular plane graphs with faces of size three or four; these have faces of negative curvature and so, their number grows exponentially. Finally, we consider *disk-fullerenes*, that is, three-regular partitions of a disk by five- and six-gons.

For all these classes of graphs, we treat the notion of zigzags and central-circuits, sometimes, at the same time. We consider simplicity of circuits, possible configuration, tightness, and enumeration of the tight graphs with simple circuits. We also address extremal questions, such as the maximum number of circuits of tight graphs.

For the classes of graphs with maximal symmetry, such as the fullerenes of icosahedral symmetry, a special construction called *Goldberg-Coxeter construction* allows to describe them explicitly in terms of two integer parameters  $k$  and  $l$ . This construction is studied systematically for three-, four-, and six-valent graphs and allow us to describe many classes in a simple way. We study the zigzags and central-circuits of the obtained graphs and build a new  $(k, l)$ -product algebraic formalism that allows us to describe the zigzags and central-circuits of the obtained graphs explicitly.

For classes of graphs with non-maximal symmetry, more complex description is needed. We explain how this can be done in practice by presenting the formalism of hyperbolic complex geometry derived by William Thurston in [Thur98].

For dimensions higher than two, the possible similar structures are more complicated. In that case, we limit ourselves to zigzags and compute them for several infinite families of complexes and the regular, semiregular, and regular-faced polytopes.

Michel-Marie Deza  
Mathieu Dutour Sikirić  
Mikhail Ivanovitch Shtogrin

## References

- [DeDu08] Deza, M., Dutour Sikirić, M.: Geometry of Chemical Graphs: polycycles and two faced maps, *Encyclopedia of Mathematics and its Applications*, vol. 119. Cambridge University Press, Cambridge (2008)
- [Thur98] Thurston, W.P.: Shapes of polyhedra and triangulations of the sphere. In: Rivin, J., Rourke, C., Series, C. (eds.) *Geometry and Topology Monographs 1*, The Epstein Birthday Schrift, pp. 511–549. Geometry and Topology Publishing, Coventry (1998)

Geometric Structure of Chemistry-Relevant Graphs

Zigzags and Central Circuits

Deza, M.-M.; Dutour Sikiric, M.; Shtogrin, M.I.

2015, XI, 211 p. 161 illus., 1 illus. in color., Hardcover

ISBN: 978-81-322-2448-8