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Multi-shell Polyhedral Clusters

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Preface

Nanoworld is the world seen at the size of 10^{-9} m; searching matter at this depth started since 1970 when Eiji Osawa had enounced the conjecture that the truncated icosahedron could be a molecule, later called C_{60}. Then, in 1985, Kroto, Curl, and Smalley got spectral evidence that C_{60}, which shows a single peak in ^{13}C-NMR, is a real molecule. They were awarded the Nobel Prize in 1995 for this historical discovery. Macroscopic synthesis of C_{60} came later, in 1990, by the work of Kraetschmer and collaborators. Iijima reported in 1991 the synthesis of nanotubes; the period after these pioneering discoveries is commonly called the "Nanoera." Development of computers and technology enabled researchers and industry to go further in research and applications, promoting an explosive development of electronics, optoelectronics, telecommunications, education, etc. Thereafter, the most important event (for the actual book) was the recognition of quasi-crystals as ordered, nonperiodic matter, the class to which the multi-shell clusters belong. Dan Shehtman was the Noble Prize winner for these results in 2011. . .then the book was started to be written. . .

Topology is the mathematical study of shapes; the multi-shell clusters concerned herein are referred to as sets of shapes, arranged, in an abstract space, in increasing rank (as Egon Schulte proposed in 1980), rather than in the geometrical higher dimensional space. Cluster models representing primary atomic arrangement are needed to understand the actual structure and then the undergoing transformations, both in concept and experimental realization and in the computational treatment. However, there is little reference to crystallographic entities, e.g., real crystal networks and quasi-crystals. Also, this book does not provide all possible structures of a given set of restrictive conditions; it rather gives chosen, representative examples. This book about multi-shell clusters could be more inspiring for architects or visual artists in making monumental, artistic works, by its aesthetic message.

The structure of this book is as follows:

An introduction to the Chemical Graph Theory is made in the first chapter. It is a description through the eye of a chemist of the basic notions of Graph Theory: definitions, topological matrices and indices, counting polynomials, etc.

Chapter 2 describes some of the most important operations on maps that enabled the design of the multi-shell clusters, as is shown in the following chapters.

In Chap. 3, rigorous definitions in polyhedra and polytopes of higher rank are given with a view to helping in the effort of counting structural elements and naming and extracting mathematical and physicochemical properties of multi-shell clusters. Some examples of polytope realization are given at the end of this chapter.

Chapter 4 deals with the complexity and methods of investigation and characterization of multi-shell clusters, such as centrality index counted on layer matrices and the ring signature index, calculated on rings around each vertex/atom of the cluster. Theory about these descriptors is given as well as case studies providing data on topology, defined on connectivity rather than geometry.

From Chaps. 5–9, the topological study is directed to multi-shell clusters classified according to the point group symmetry of the parent Platonic clusters, used as seeds in the design of more complex clusters with the aid of map operations.

Chapter 10 speaks about chiral multi-tori, spongy structures, the complexity of which is given by the high genus surface in which they are embedded.

Chapter 11 opens a gate to the spongy hypercubes, developed on the Platonic solids. The designed structures were characterized by topological (figure) counting and by Omega and Cluj counting polynomials.

Finally, Chap. 12 provides a bound to the real world by energy computation, in an attempt to find multi-shell cluster (or corresponding networks) candidates to the status of real chemical/mineral clusters.

Chapters 2, 5–10, and 12 have Atlas sections that detail the discussed structures; the number of these figures is listed in separate files, in each chapter, while the figure number is associated with the name of clusters within all the text, tables, and figures included, for an easier identification.

The book includes personal research results of the author, in connection with his activity within the Topo Group Cluj, Romania. It is addressed to students and researchers in the interdisciplinary field of Chemistry, Physics, and Mathematics as well as to architects and visual artists. Hin-files of the structures illustrated in this book are deposed online, at www.esmc.ro, available on request.

I was aided in this effort by my younger colleagues, Dr. Csaba L. Nagy and Dr. Atena Pirvan-Moldovan, Faculty of Chemistry and Chemical Engineering, “Babes-Bolyai” University, Cluj, Romania, with quantum chemical and symmetry calculation, figure design, and error checking, while writing the book, which I highly appreciate. Many thanks are addressed to Dr. Attila Bende (Molecular and Biomolecular Physics Department, National Institute for R&D of Isotopic and Molecular Technologies, Cluj, Romania), Dr. Beata Szefler (Department of Physical Chemistry, Faculty of Pharmacy, Collegium Medicum, Nicolaus Copernicus University, Bydgoszcz, Poland), Dr. Zahra Khalaj (Department of Physics, Shahr-e-Qods Branch, Islamic Azad University, Tehran, Iran), and Dr. Igor Baburin (Technische Universität Dresden, Theoretische Chemie, Germany) for a fruitful collaboration.

Cluj-Napoca, Romania Mircea Vasile Diudea
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Contents

List of Abbreviations

d	Dual
l	Leapfrog
m	Medial
t	Truncated
CO	Cuboctahedron
DCO	Dual cuboctahedron
ID	Icosidodecahedron
hP	Half polyhedron
MC	Medial cube
LDCO	Leapfrog (of dual) of cuboctahedron
MDCO	Medial (of dual) of cuboctahedron
MMC	Medial (of medial) of cube
RCO	Rhombicuboctahedron
RID	Rhombicosidodecahedron
SC	Snub cube
SD	Snub dodecahedron
TC	Truncate cube
TCO	Truncate cuboctahedron
TID	Truncate icosidodecahedron
TMC	Truncate (of medial) of cube
TO	Truncate octahedron
TT	Truncate tetrahedron
XAYb	Figure at the bottom of the main figure XAY