

Periodic Nanostructures

Developments in Fullerene Science

Volume 7

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Budapest, Hungary*

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Periodic Nanostructures

by

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Foreword

Some twenty years ago, an article in *Nature* (London) announced the synthesis of the first fullerene. This fullerene was named C_{60} , and is also commonly known as *Buckminsterfullerene*. C_{60} was isolated *via* the self-assembled products of graphite heated by plasma. Later, the synthesis of nanotubes by the laser vaporization of graphite, led to a further increase in the family of nanostructures and heralded unprecedented perspectives for a new science and technology to impact humanity.

The coalescence reactions (illustrated by electronic microscopy) have shown that the nanoworld is continuous, giving rise to zero- (fullerenes), one- (tubules), two-(graphite) and three-(diamond, spongy carbon) dimensional carbon allotropes. Peapods are nanotubes doped with fullerenes (zero-dimensional cages) or longer capsules, formed inside the tube by coalescence of spherical units. Hetero-atomic nanostructures, containing boron, nitrogen, germanium, selenium, etc. have also been synthesized and studied.

Foam-like carbon structures, related to 'schwarzites', have been well documented and represent infinite periodic minimal surfaces of negative curvature. They contain polygons with dimensions larger than hexagons (w.r.t. to the graphite), that induce the negative curvature. Units of such structures appear as nanotube junctions, produced in an electron beam, with wide potential applications in molecular electronics. Self-assembling supra-molecular structures, of various tessellation, and diamond architectures, have also been recently proposed. The periodicity of close repeat units of such structures is more evident in these structures, but is also present in all the carbon allotropes.

Depending on the lattice tessellation, heteroatom type, and/or doping, metal nanostructures (nanotubes in particular) can be metallic or semiconductors. Therefore their properties can be changed by chemical functionalization. This has led to the improved performance of Li-ion batteries, capacitors, and field electron emitters in displays. Their use as tips in scanning tunneling microscopy (STM)

and atomic force microscopy (AFM) has introduced a new generation of nanoscale biological/chemical/physical devices.

This book is organized as follows.

Chapter 1 introduces the reader to the realm of periodic fullerenes, obtainable by coalescence reactions. It presents literature data and the authors own results on nanostructure building, and semiempirical and strain energy calculations. Novel dimeric and oligomeric structures predicted to appear via the coalescence of C_{60} molecules and the cages that could result by loss of carbon atoms from the starting molecules are the main subjects discussed herein.

Chapter 2 presents one of the most intensively studied carbon allotropes (entirely covered by a benzenoid lattice) namely the polyhex torus. Original methods of construction and tiling modification, nomenclature and correspondence to other nomenclatures are presented. Criteria for metallic and aromatic character properties are tabulated. Rules to identify identical polyhex toroidal graphs within families of chiral embedding isomers (furnished by the authors building method) are formulated in terms of the net dimensions. Resonance energy of polyhex tori is evaluated in the context of a generalized Clar theory of aromaticity.

Chapter 3 introduces a new class of toroidal structures, named Distinct Walled Tori (DWT), so called to indicate the varying number of atoms on the inner and outer walls, respectively. The energetics and aromaticity for various types of DWTs derived from armchair nanotubes or conical domains are presented. Diameter doubling of single-walled carbon nanotubes and zigzag nanotubes are also discussed.

Chapter 4 begins with a background on Graph Theory followed by defining some of the most discussed counting polynomials and the more recently proposed Omega and Cluj polynomials. Some theorems in the two latter named polynomials are discussed and demonstrated. Hosoya, Cluj, and Omega polynomials are detailed and used in the topological characterization and stability prediction of nanostructures: spherical, tubular, and toroidal. A *factorization* procedure, for describing the chiral polyhex tori in terms of Omega polynomial is presented.

Chapter 5 deals with the study of planar and 3D surfaces by various polygonal faces. Operations on maps and geometrical-topological transformation of a parent covering, are systematically introduced, from the simplest, through to composites, and up to generalized operations, which enable the embedding of various coverings in any surface. General analytical relations among the parameters of transformed and parent maps are presented. Molecular realizations of the proposed operations or sequences of operations are illustrated. Stone-Wales edge-rotations (related to map operations) are presented as possible routes of isomerization, enabling changes in the nanostructure tessellation.

Chapter 6 offers a detailed discussion on the aromatic character of fullerenes, with classical and non-classical covering. It is shown that aromatic character is a multi-conditional molecular property which can be dependent upon energetics, electronic structure, magnetic response, geometric characteristics, or chemical behaviour.¹⁶⁻¹⁸ It is shown that having a varied aromaticity criteria results in a random ordering of molecules. Generalized perfect Clar structures, with the 2-

factor designed as corannulenic or corazulenic disjoint flowers have been proven. Sequences of classical or single generalized map operations were used to obtain these coverings (also given as π -electron partitions within Kekulé valence structures). As a structural/geometric parameter of aromaticity, the HOMA index enabled an evaluation of local aromatic character of the featured supra-faces and thus generated evidence for several dominant Kekulé valence structures. The described operations and structures are believed to be helpful in the process of molecular structure elucidation and in guiding researchers in finding novel nanostructured materials.

Chapter 7 discusses triply periodic nanostructures and associated units which, by a self-assembly process, provide architectures of negative curvature, also known as schwarzites (or spongy structures). A short introduction to the theory of triply periodic minimal surfaces is offered. Unit blocks built up by opening map operations could model the junctions of carbon nanotubes; these can be synthesized by “nanowelding”, that is, crossing tubes in an electron beam. Junctions are rationalized according to the building operation. A gallery of junctions and triply periodic architectures is offered in the appendices. This book is aimed at scientists working in the field of nanoscience and nanotechnology, Ph.D. and MSc. degree students, and others interested in amazing nanoarchitectures, which could inspire the cities of the future.

* * *

Although each author contributed to the entire book, Chapters 1 and 3 were written by C. L. N. and Chapters 2, 4 to 7 by M. V. D. Each author takes responsibility only for the materials outlined in the chapters written by himself. The authors acknowledge the help of Dr. Aniela Vizitiu (contributing with objects and calculations to the sections: 3.2 and 7.4.3 to 7.4.6) and Dr. Katalin Nagy (with contributions to the Gallery). Many thanks are addressed to Prof. Tibor Braun, Hungarian Academy of Sciences, for his valuable advice and encouragement during the editing of this book.

Cluj, Winter, 2006

Mircea V. Diudea

Csaba L. Nagy

Gallery of Carbon Nano Junctions and Derived Infinite Lattices

Abbreviations used:

T – tetrahedron

C – cube

D – dodecahedron

$Le_{1,1}$

$Le_{2,2}$

$Q_{2,0}$

$Q_{3,0}$

$Ca_{2,1}$

$Ca_{3,2}$

nf_s – negative face of size s

Op – open

$Op_{1,1}$ – consecutive open

Op_{2a} – alternating open

A – array

D – supra dodecahedron

 $Op(Le_{1,1}(T)); nf_9$


 $Op(Le_{1,1}(T))-TU(3,0); v = 24$

 $Le_{1,1}(Op(Le_{1,1}(T)))-TU(3,3); v = 36$

 $Le_{2,2}(Op(Le_{1,1}(T)))-TU(6,6); v = 72$

 $Q_{2,0}(Op(Le_{1,1}(T)))-TU(6,0); v = 48$


 $Q_{3,0}(Op(Le_{1,1}(T))) - TU(9,0); v = 72$

 $Ca_{2,1}(Op(Le_{1,1}(T))) - TU(6,3); v = 120$
 $Op(Q_{2,0}(T)); nf_8$

 $Op(Q_{2,0}(T)) - TU(3,0); v = 28$

 $Le_{1,1}(Op(Q_{2,0}(T))) - TU(3,3); v = 48$

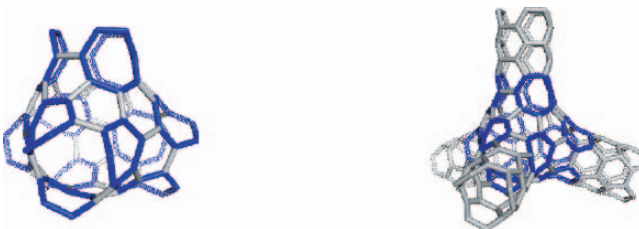

 $L_{e_{2,2}}(Op(Q_{2,0}(T)))-TU(6,6); v = 120$

 $Q_{2,0}(Op(Q_{2,0}(T)))-TU(6,0); v = 64$

 $Q_{3,0}(Op(Q_{2,0}(T)))-TU(9,0); v = 180$

 $Ca_{2,1}(Op(Q_{2,0}(T)))-TU(6,3); v = 148$


 $Ca_{3,2}(Op(Q_{2,0}(T)))-TU(9,6); v = 268$
 $Op(Ca_{2,1}(T)); nf_7$

 $Op(Ca_{2,1}(T))-TU(3,0); v = 40$

 $Le_{1,1}(Op(Ca_{2,1}(T)))-TU(3,3); v = 84$

 $Le_{2,2}(Op(Ca_{2,1}(T)))-TU(6,6); v = 264$


 $Q_{2,0}(Op(Ca_{2,1}(T)))-TU(6,0); v = 112$

 $Q_{3,0}(Op(Ca_{2,1}(T)))-TU(9,0); v = 216$

 $Ca_{2,1}(Op(Ca_{2,1}(T)))-TU(6,3); v = 160$

 $Ca_{3,2}(Op(Ca_{2,1}(T)))-TU(9,6); v = 496$

 $Op_{2a}(S_2(T)); nf_7$

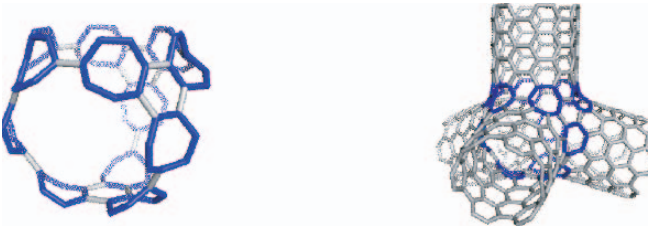

 $Op_{2a}(S_2(T))-TU(3,3); v=52$

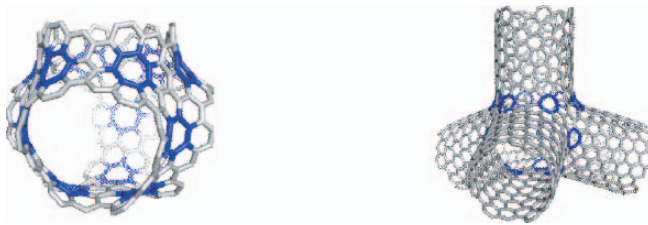
 $Le_{1,1}(Op_{2a}(S_2(T)))-TU(9,0); v=120$

 $Q_{2,0}(Op_{2a}(S_2(T)))-(6,6); v=184$

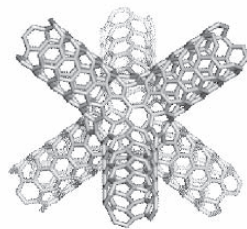
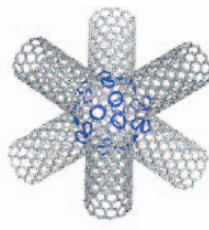
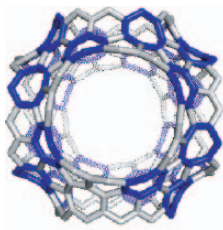
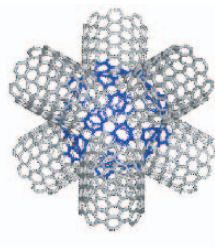
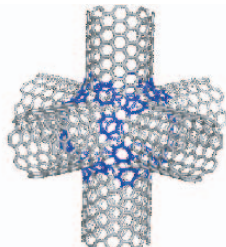
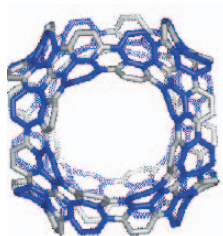
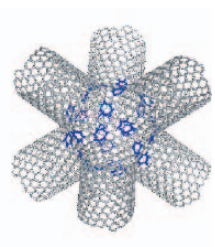
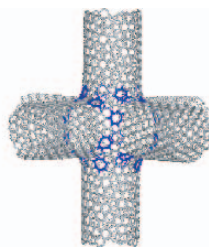
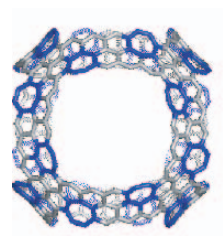
 $Ca_{2,1}(Op_{2a}(S_2(T)))-TU(12,3)$

 $Op_{1,1}(S_2(T)); nf_7$

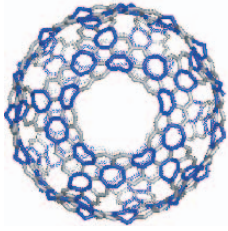

 $Op_1(S_2(T))-TU(6,0); v = 52$

 $Le_{1,1}(Op_1(S_2(T)))-TU(6,6); v = 84$

 $Q_{2,0}(Op_1(S_2(T)))-TU(12,0); v = 112$

 $Ca_{2,1}(Op_1(S_2(T)))-TU(12,6); v = 268$

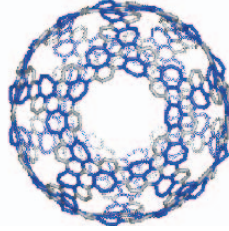
 $Op_{2a}(S_2(C)); nf_7$


 $Op_{2a}(S_2(C))-TU(4,4); v = 104$

 $Le_{1,1}(Op_{2a}(S_2(C)))-TU(12,0); v = 240$

 $Q_{2,0}(Op_{2a}(S_2(C)))-TU(8,8); v = 368$

 $Ca_{2,1}(Op_{2a}(S_2(C)))-TU(16,4); v = 368$

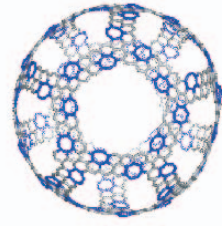
$Op_{2a}(S_2(D)); n_f7$



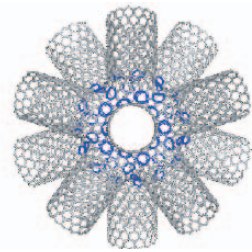
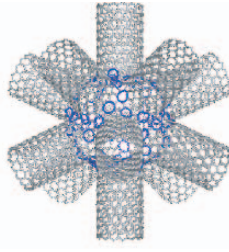
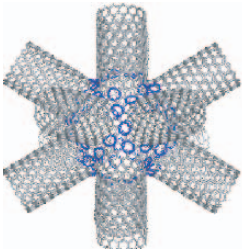
$Le_{1,1}(Op_{2a}(S_2(D)))-TU(15,0)$
 $v = 600$



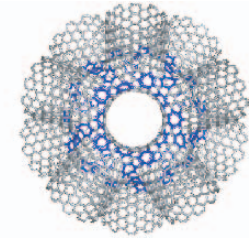
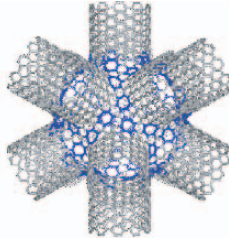
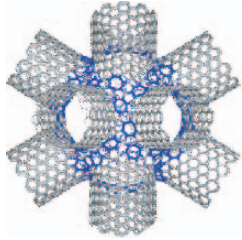
$Q_{2,0}(Op_{2a}(S_2(D)))-TU(10,10)$
 $v = 684$



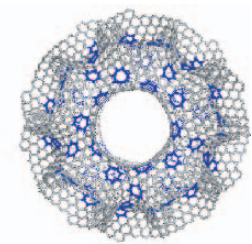
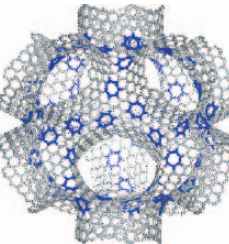
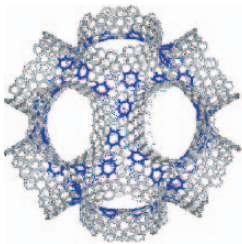
$Ca_{2,1}(Op_{2a}(S_2(D)))-TU(20,5)$
 $v = 918$



$Le_{1,1}(Op_{2a}(S_2(D)))-TU(15,0)$

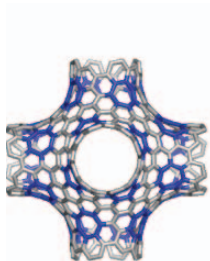
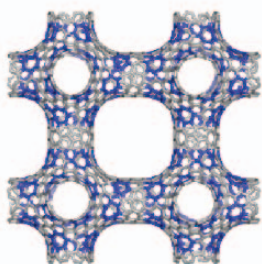
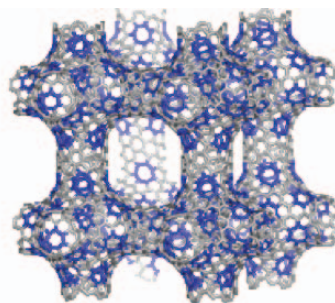
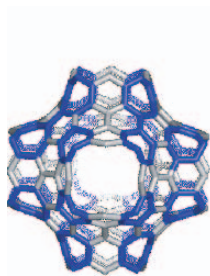
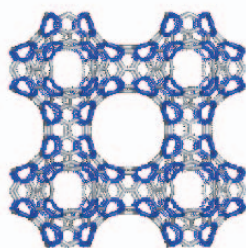
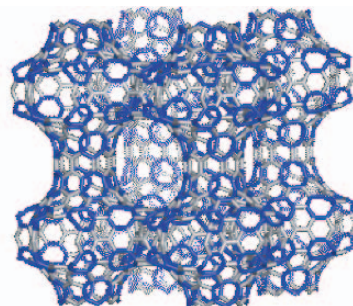
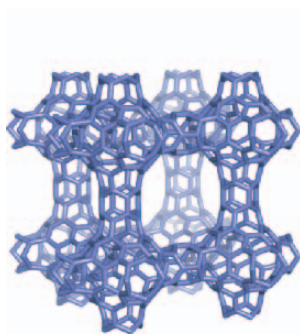
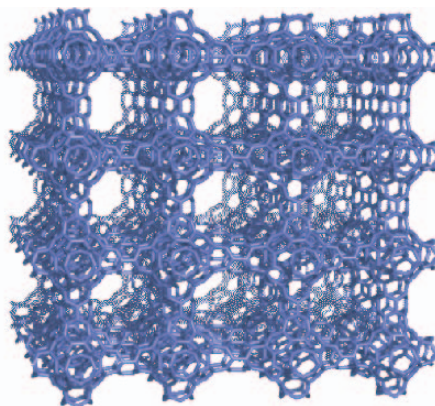


$Q_{2,0}(Op_{2a}(S_2(D)))-TU(10,10)$

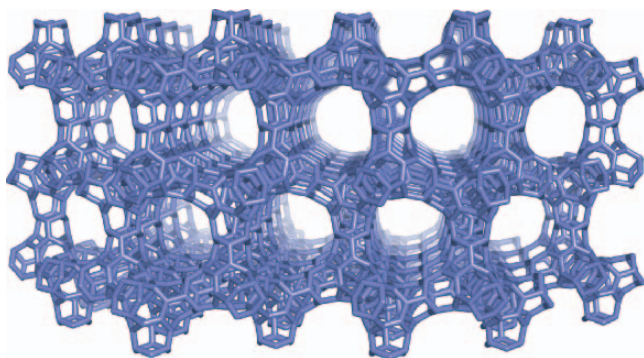


$Ca_{2,1}(Op_{2a}(S_2(D)))-TU(20,5)$

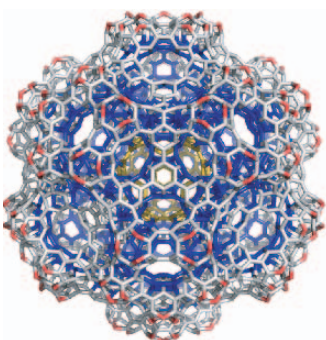
 P-type networks


 $Ca_{2,1}R(Op(Ca_{2,1}S(C)))$

 $4 \times Ca_{2,1}R(Op(Ca_{2,1}S(C)))$

 $8 \times Ca_{2,1}R(Op(Ca_{2,1}S(C)))$

 $Op(Le_{1,1}(Le_{1,1}(Le_{1,1}(C))))$

 $4 \times Op(Le_{1,1}(Le_{1,1}(Le_{1,1}(C))))$

 $8 \times Op(Le_{1,1}(Le_{1,1}(Le_{1,1}(C))))$

 $4 \times Op(Le_{1,1}(Le_{1,1}(C)))$

 $16 \times Op(Le_{1,1}(Le_{1,1}(C)))$

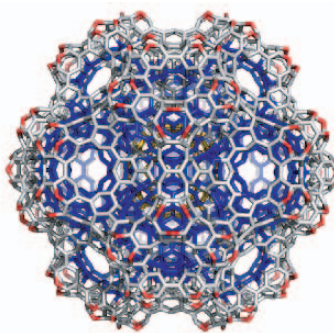
 D- and FRD-type networks



$126 \times Op(Ca_{2,1}(T)); v = 3816$



$v = 3120-3$; 3-fold axis



$v = 3120-2$; 2-fold axis

$A(D(Op(Le(T))))$; $[D(Op_1(Le_{1,1}(T)))]$

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