BABEŞ-BOLYAI UNIVERSITY CLUJ-NAPOCA
FACULTY OF CHEMISTRY AND CHEMICAL ENGINEERING
FACULTY OF MATHEMATICS AND COMPUTER SCIENCE

PhD Thesis Summary

Molecular/Crystalline Nanostructures Design

PhD Supervisors:
Prof. Dr. Mircea V. Diudea
Prof. Dr. Bazil Pârv

PhD Candidate: Virginia-Ramona Hatfaludi
(căs. Bucilă)

Cluj-Napoca
2013

UNIUNEA EUROPEANĂ
GUVERNUL ROMÂNIEI MINISTERUL MUNCII, FAMILIEI PROTECȚIEI SOCIALE ȘI PERSOANELOR VARSTNICE AMPOSDRU
Fondul Social European POSDRU 2007-2013
Instrumente Structurale 2007-2013
MINISTERUL EDUCAȚIEI NAȚIONALE
OIPOSDRU
UNIVERSITATEA BABEȘ-BOLYAI CLUJ-NAPOCA

Acknowledgements:

This work was possible with the financial support of the Sectoral Operational Programme for Human Resources Development 2007-2013, co-financed by the European Social Fund, under the project number POSDRU/107/1.5/S/76841 with the title „Modern Doctoral Studies: Internationalization and Interdisciplinarity".

FONDUL SOCIAL EUROPEAN
Investeşte în
OAMENI
Parteneri:
UNIVERSITATEA „ALEXANDRU IOAN CUZA" din IAŞI
universität wien
Universitat Regensburg

TABLE OF CONTENTS:

Keywords: nanostructures, operation on maps, covering, program, software, graph, polynomial, networks, Omega polynomial

Introduction

The thesis presents the main theoretical aspects and personal contributions to crystallographic classification and complex analysis of some given nano crystalline structures, built using map operations.

From 69 nano crystalline 3-periodic structures that were studied, 39 turned out to be new topologies (4 new 3,4-c net structures, 10 new 3-c net structures, 1 new 4-c net structure and other 24 new nets) and from the 1-periodic structures studied all turned out to be new topologies.

To analyze these stuctures, the TOPOS program was used, particularly the AutoCN (to edit the adjacency matrix), IsoCryst (to visualize the geometrical crystal structures and do the topological analysis) and ADS programs. For each net category (3-c, 4-c, 3,4-c) the topos parameters, point symbol, stochiometry were outlined.

Also, another program, named Systre, was used to determine the ideal symmetry of a crystalline net (optimal embedding) and to analyze the topological structure.. To visualize new topologies, we used the 3dt program.

To transfer the studied nano crystalline structures in TOPOS two programs needed to be created.

The new topologies discovered this way were already introduced in the data base of this program and are already available to users.

A new topology discovered is introduced in data base collections of different computational programs used by chemists and it is of real help to chemists in the metal organic net domain, who have an interest in discovering of new nets and to those with interest in new forms of carbon.

In this summary, the numbering of the chapters and the bibliographical references are kept as in the thesis.

Original contributions

Chapter III. 3-periodic structures

The personal contributions refer to the classification of the structures contained in this chapter and to their crystallographic description. A part of the obtained results are contained in the paper submitted for publication: Virginia Bucilă, Monica Ştefu and Beata Szefler Octahedral CNT Junctions as P-Type Networks, *Studia Univ. Babes-Bolyai Chemia*, 2013.

The figure on the left represents the image obtained with the help of TOPOS and the unit cell is also represented, and the figure on the right represents the structure from the original .hin file.

In four of the structures, we presented the visualization with the 3dt program.

In this summary, an example (without Topos parameters) is presented for each category: 3,4-c, 3-c, 4-c and others.

3,4-c

6. NEW: diu2 (Cube, Polygonal P4, Unit, co-net, hexagon 6, X cut edges) CP4UCo6X

Point symbol for net: $\{6^3\}4\{6^4.8^2\}3\{6^5.8\}6$

3,4,4-c net with stoichiometry (3-c)4(4-c)9; 3-nodal net

VS [6.6.6] [$6.6.6.6.6_2.8_2$] [$6_2.6_2.6_2.6_2.8.8$]

New topology

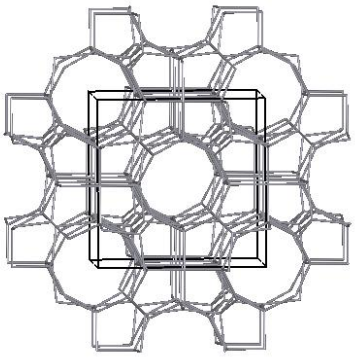
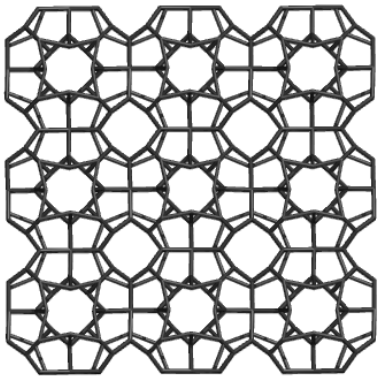
 p4u_corecell P4U_Core_6E_333B	 P4U_Core_6E_333B
Diudea's name **diu2**	CP4UCo6X

Fig.3. 1 NEW: diu2 (Cube, Polygonal P4, Unit, co-net, hexagon 6, X cut edges) CP4UCo6X

3-c

5. NEW diu8=CQOp2a

Point symbol for net: (8^3)
3,3-c net with stoichiometry (3-c)4; 2-nodal net
VS $[8.8.8_2]$ [8.8.8]
New topology

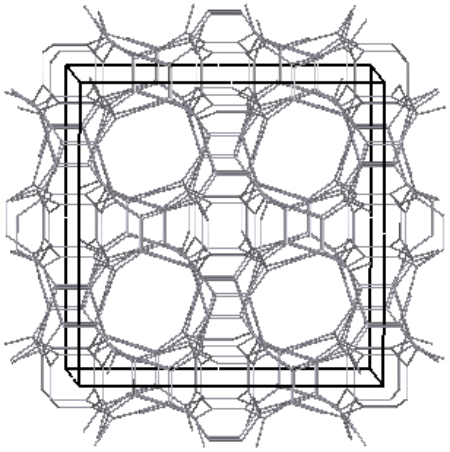
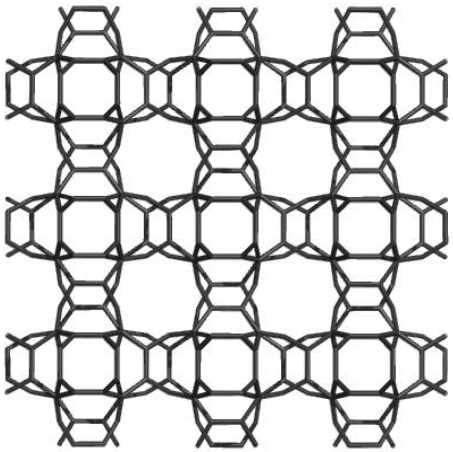
 CCA12cell CCA12_R[8_2]_333_1080	 CCA12_R[8_2]_333_1080
Diudea,s name **diu8**	CQOp2a

Fig.3. 2 NEW diu8=CQOp2a

4-c

6. mgz-x-d L5

Point symbol for net: $(5^5.6)12(5^6)5$
4,4,4,4,4,4,4-c net with stoichiometry (4-c)34; 7-nodal net
Topological type: mgz-x-d
VS [5.5.5.5.5.5] [5.5.5.5.5.5] [5.5.5.5.5.6] [5.5.5.5.5.6] [5.5.5.5.5.6] [5.5.5.5.5.5] [5.5.5.5.5.6]

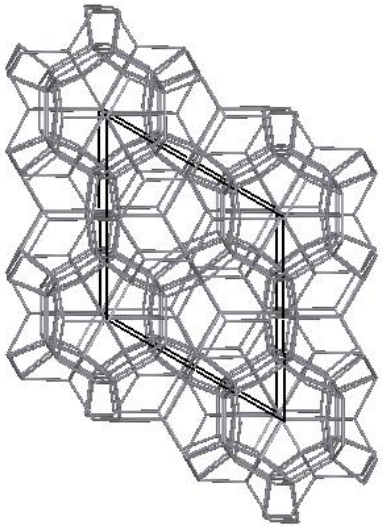
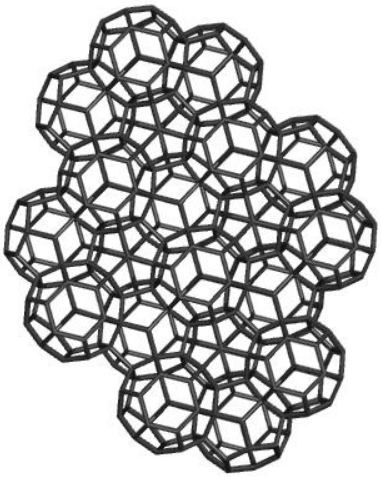
 mgz-x-d	 L5_28_222_1224C
Diudea's name	L5

Fig.3. 3 mgz-x-d L5

others

33. NEW CP4R_444_5248

Point symbol for net: $\{4.5^{10}.6.7^2.8\}3\{4.5^5\}6\{5^3\}4\{5^5.8\}6$
3,3,4,4,4,6-c net with stoichiometry (3-c)4(4-c)12(6-c)3; 6-nodal net
VS $[5.5.5.5.5_2.8_2]$ $[5.5.5.5.5.8_2]$ $[4.5.5.5.5.5.5.5.5.5.8.8_2.*.*]$
New topology

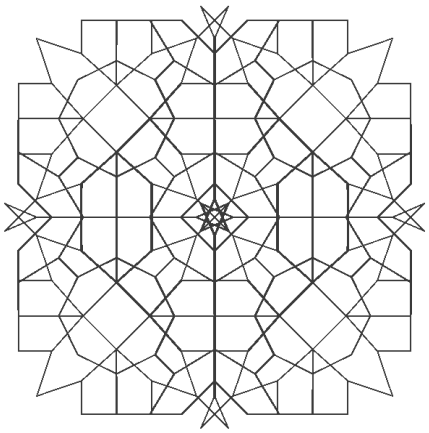
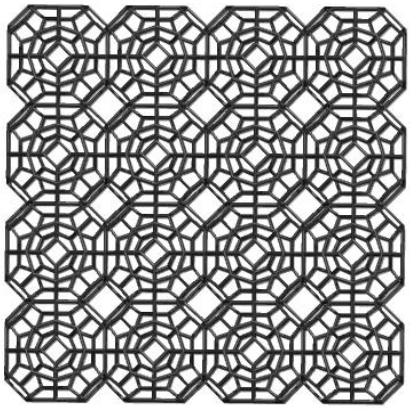
 CP4Rcell	 CP4R_444_5248

Fig.3. 4 NEW CP4R_444_5248

The visualization of the analyzed topologies with the 3dt program

The 3dt program of the Gavrog project, offers a visualization qualitatively better and more detailed of the image, and therefore, I considered useful a vizualization of the studied structures in 3D format.

For each example I attached the image realized by Jmol[88], Topos[72] and 3dt[89].

In this summary there are two examples presented:

Example 1. CQOp2a, Point symbol for net: (83), 3-c net with stoichiometry (3-c)4; 2-nodal net; VS [8.8.82] [8.8.8] ;Known also as “etk” or 83P; diu8

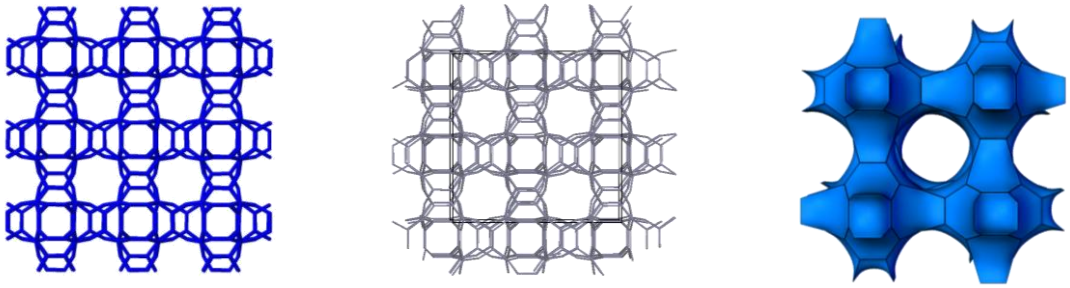


Fig.3. 5

Example 2. CP4UCo6X, Point symbol for net: (63)4(64.82)3(65.8)6, 3,4-c net with stoichiometry (3-c)4(4-c)9; 3-nodal net; VS [6.6.6] [6.6.6.6.62.82] [62.62.62.62.8.8] ;New topology; diu2

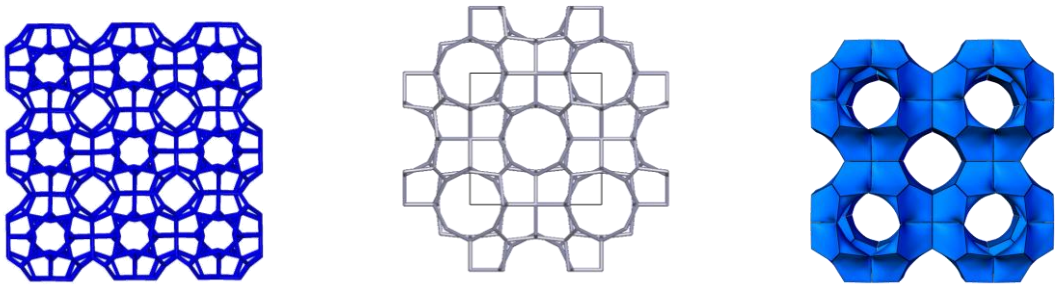


Fig.3. 6

Chapter IV. 1-Periodic Nanostructures

Computational details

The personal contributions refer to the classification of the structures contained in this chapter and to their crystallographic description The obtained results are contained in the paper: M.V. Diudea, V.R. Bucilă, D.M. Proserpio, 1-Periodic Nanostructures, *MATCH Communications in Mathematical and in Computer Chemistry*, 2013, 70(2), p.545-564.

By the aid of TOPOS, program package for multipurpose crystallochemical analysis, we classified the 1-periodic structures assigning them to a space group compatible with the structure and computing the Point Symbol. All the structures are new and never described before in TOPOS databases.

We used three programs: atom.exe, hinzalign.exe and hin2topos.exe in order to transfer the studied structures to TOPOS.

The program atom.exe enabled to find the direction/orientation of the structure. The three input parameters are: a_0, δ, α, where a_0 is an atom of the structure to be the origin of the new coordinates while δ (metric) and α (angular) are tolerance parameters.

For an atom a, let E_a be the set of edges incident to a. For two atoms, a, a′ we define the "vertex similarity" as the cardinality of $E_a \cap_s E_{a'} = \{e_a \mid e_a \in E_a, \exists\, e_{a'} \in E_{a'}, \mid e_a - e_{a'} \mid \leq \delta; \angle(e_a, e_{a'}) \leq \alpha\}$.

The program collects a set $S(a_0)$ of atoms of maximal similarity to a_0. The atoms in $S(a_0)$ are candidates to be paired with a_0 to form the repetitive vector. The vector is chosen according to various criteria, like "shortest", "longest" etc.

Given a vector ν, the program hinzalign.exe first rotates the coordinate system such that the z axis becomes parallel to ν. The coordinates of each atom are recalculated based on the new (rotated) coordinate system. Next, the coordinate system is translated with the origins in the atom a_0 (i.e., in the new (translated) coordinate system, a_0 will be (0,0,0)).

The resulting .hin-file was converted to a TOPOS file using the third program, called hin2topos.exe.

The images obtained with the TOPOS program have to be similar to the original structure in order to be correctly interpreted.

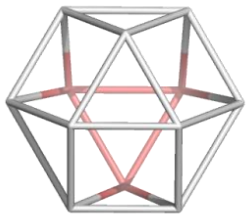
For each structure, the coordination of the nodes (3-c, 4-c and so on), the number of topologically independent nodes (*n*-nodal), and the Point Symbol (PS) is given. [85]

Structure design

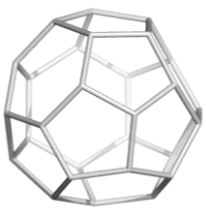
The hypothetical structures herein discussed were designed by using CVNET[23] and NANO STUDIO[90]. The units used in construction of more complex structures are presented in Fig.4.1. Five such units, denoted here U_1, form a hyper pentagonal ring R5. A dodecahedron having in lieu of its pentagonal faces the hyper-pentagons R_5 hyper-faces) is a spongy structure, named in the following U_{20}, to remember the 20 simple cages/units composing it. Next, by identifying the hyper-faces of two units U_{20} one obtains 1-periodic structures. There are experimental data showing that in alloys like AlMn, AlFe, AlCuCo, and AlCoNi, with a diffraction pattern of tenfold rotational symmetry, have also a 1-dimensional translational periodicity along the tenfold rotational axis. This symmetry is also called "axial" symmetry. The rod-like structures herein discussed have been characterized in crystallographic terms by using the TOPOS software[72].

Truncated Tetrahedron
TT_12 (3.6^2)

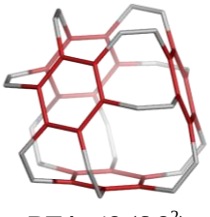
Truncated Octahedron
TO_24 (4.6^2)



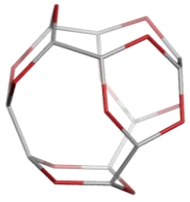
Cuboctahedron
CO_12 $(3.4)^2$



C_{28} ; $(5^3)_4(5^2.6)_{24}$



BTA_48 (6.8^2)



BTZ_24; (6.9^2)

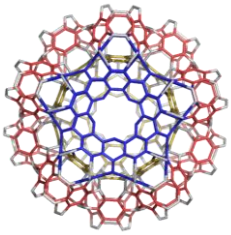
By S_2(T) By spanning $Le(P_4(T))$ By Op(Le(T))

Fig.4. 1 Units U1 used in construction of complex structures

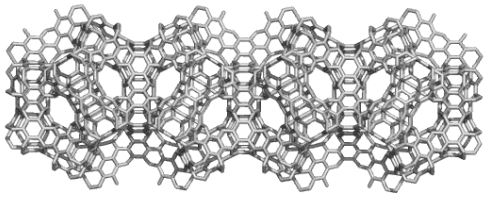
In this chapter, eleven new 1-periodic networks are listed, together with their crystallographic description and the map operation used in their design.

In this summary there are two examples presented.

The U_{20} structures in Fig. 2 and 3 are built up from BTA_48 and BTZ_24 (Fig. 4.1, bottom row), structures called "polybenzenes". [92-94] The unit $BTZU_{20}$_480 was shown to self-arrange in a more complex spherical arrays.



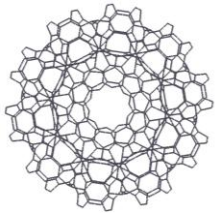
$BTAU_{20}$_780



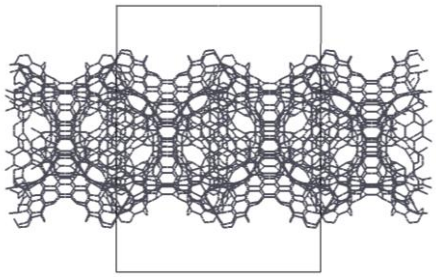
BTA_{20}_4_2490

The unit U_1 is BTA_48 (Fig. 4.1)

designed by spanning $Le(P_4(T))$



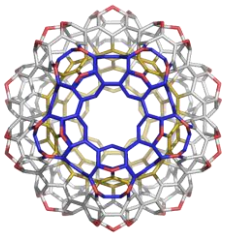
TOPOS view



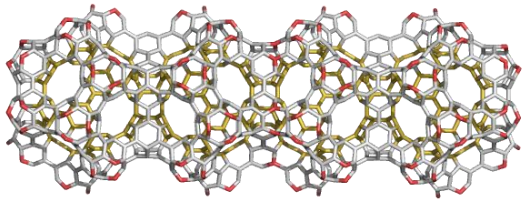
BTA_{20}_*k* is a 3-c 27-nodal

PS $(6.8^2)_{11}(6^2.8)_{26}(6^3)_{14}$

Fig.4. 2 BTA_{20}_*k* rod-like structure



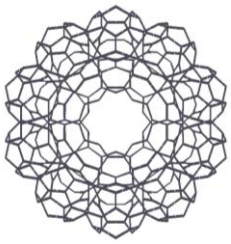
$BTZU_{20}$_480



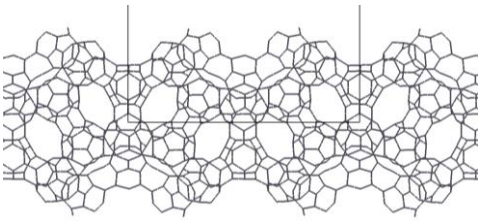
BTZ_{20}_4_1560

The unit U_1 is BTZ_24 (Fig. 4.1)

designed by spanning S_2(T)



TOPOS view



BTZ_{20}_*k* is 3-c net 20-nodal

PS $(5.6.8)_2(5.8^2)_3(6.8^2)_6$

Fig.4. 3 BTZ_{20}_*k* rod-like structure

Chapter V. Omega polynomial in crystal-like structures

The Omega polynomial $\Omega(x)$ [106-108] is defined on the ground of opposite edge strips ops $S_1, S_2, ..., S_k$ in the graph. Denoting by *m*, the number of ***ops*** of cardinality/length $s=|S|$, then we can write

$$\Omega(x) = \sum_s m \cdot x^s$$

The first derivative (in $x=1$) can be taken as a graph invariant or a topological index:

$$\Omega'(1) = \sum_s m \cdot s = \left|E(G)\right|$$

An index, called Cluj-Ilmenau $CI(G)$, was defined on $\Omega(x)$:

$$CI(G) = \left\{ [\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)] \right\}$$

In tree gaphs, the Omega polynomial simply counts the non-opposite edges, being included in the term of exponent $s=1$.

On the ground of strips *s*, the Sadhana[109] polynomial and corresponding index[110] can be defined:

$$Sd(x) = \sum_s m \cdot x^{e-s}$$

$$Sd'(G,1) = \sum_s m \cdot (e-s) = Sd(G)$$

Omega polynomial was thought to describe the covering of polyhedral nano-structures or the tiling of crystal-like lattices, as a complementary description of the crystallographic one.

Next, only the folowing sections are presented: Crystalline networks designed by leapfrog and chamfering, Lattices built by Op(Trs(P4(Oct))), Nets based on Dyck graphs and Conclusions

Crystal networks designed by leapfrog and chamfering

In this section we present four infinitely periodic networks, of which repeating units can be designed by applying leapfrog Le and chamfering Q map operations on the Cube C. [27,45] The units are the small cages C_{24} and C_{32}, with vertex symbol (4.6^2) and $(4.6^2)(6^3)$, respectively.

The lattice CLe_4 (Fig.5.1) is a triple periodic net built up from C_{24} = CLe_24,, by identifying the (4,4) faces. It is the well-known sodalite **sod** net, a uninodal 4-c net,

belonging to the *Im-3m* group and having the net symbol ($4^2.6^4$) and topological type sod/SOD; 4/4/c1; sqc970. Note the repeating unit CLe_24 is just the truncated Octahedron.

By applying the Chamfering Q operation on the Cube, results in the repeating unit CQ_32. Next, by identifying (4,4), (4,6) or (6,6) faces it results in different networks CQ_4, $CQ_{4,6}$ or CQ_6 even the starting object is one and the same. Fig.5.2 shows the net CQ_4 (known as **tfg** or sqc9223), a triple periodic 2-nodal lattice. of the group *Pm-3m* (http://epinet.anu.edu.au); its net point symbol is ($4.6^4.8$)3(6^3)2, 3,4-c net with stoichiometry (3-c)2(4-c)3.

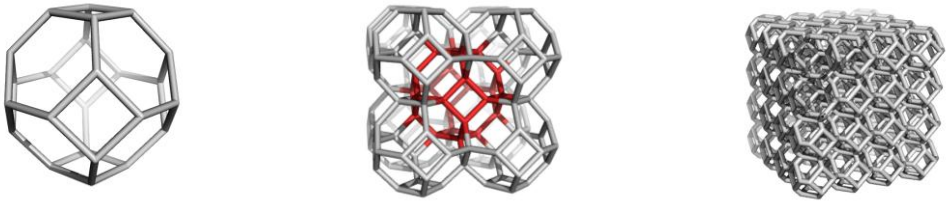


Fig.5. 1 CLe4=sod, a triple periodic lattice, belonging to the Im-3m group, designed by Le(C) and identifying (4,4) faces: the unit CLe_24; (vertex symbol 4.62) (left) and two cubic domains of the net, 2,2,2_144 (middle) and 4,4,4_960 (right); the last number counts the atoms in a given domain

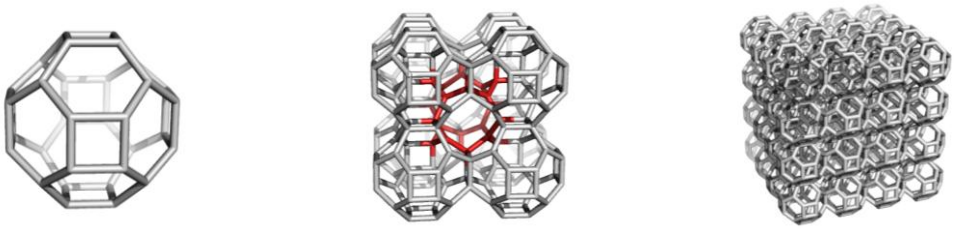


Fig.5. 2 CQ_4=*tfg*, sqc9223, group *Pm*-3*m*, a triple periodic lattice designed by *Q*(C) and identifying (4,4) faces: the unit CQ_32, vertex symbol (4.6^2)(6^3)) (left) and two cubic domains, 2,2,2_208 (middle) and 4,4,4_1472 (right)

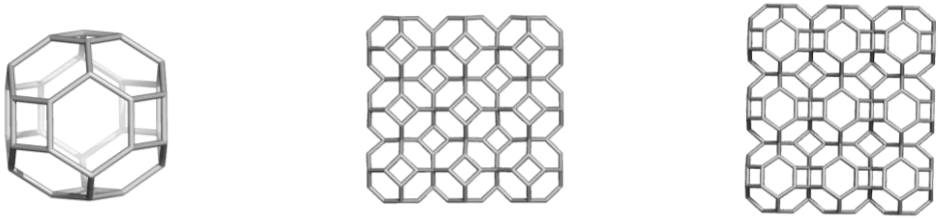


Fig.5. 3 CQ4,6=sqc8121, group P4/mmm, a triple periodic net designed by Q(C(a,b,c) and identifying (4,6) faces: the unit CQ_32 (left) and two cubic domains, 3,3,3_576 (a) (middle) and 3,3,3_576 (b,c) (right)

The net $CQ_{4,6}$ is a 3-nodal 4,4,4-c net of the group *P*4/*mmm*, with stoichiometry (4-c)2(4-c)(4-c) and point symbol for net: (4.6^5)($4^2.6^4$)($4^3.6^3$)2. Its topological specification is sqc8121 (epinet.anu.edu.au).

Finally, the net CQ_6 (Fig. 8.4) is also known as **ast** net, group *Fm-3m*; it is a triple periodic 4,4-c, 2-nodal net, built by identifying (6,6) faces of C_{32} unit. The point symbol for net is $(4^3.6^3)4(6^6)$ and stoichiometry (4-c)4(4-c); its topological type is: ast/octadecasil/AST; sqc3869.

Analytical formulas to calculate the Omega polynomial were developed for either incomplete (*a*,*b*,*c*), $a \geq b \geq c$ or complete (*a*,*a*,*a*) cubic domains; other net parameters like number of vertices, edges and rings are given, function of *a* that is the number of repeating units on one direction in a cubic domain.

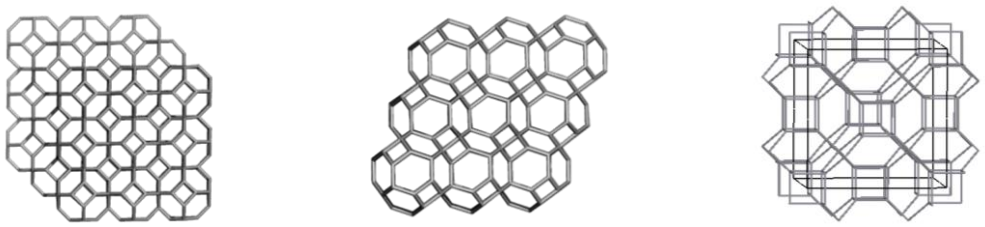


Fig.5. 4 CQ_6 net =ast, group Fm-3m, a triple periodic net designed by Q(C) and identifying f_6 faces: DP_333_492 domain(left); TP_333_484 domain (middle) and the unit cell (right)[111]

Net	Formulas
G=*CLe*$_4$(*a*,*b*,*c*); $a \geq b \geq c$:	$\Omega(G,X) = 4\sum_{i=1}^{c-1} X^{4ai+2i} + 2(b-c+1)X^{(4a+2)c} + 4\sum_{i=1}^{c-1} X^{4bi+2i} + 2(a-c+1)X^{(4b+2)c} + 4\sum_{i=1}^{b-1} X^{4ci+2i} + 2(a-b+1)X^{(4c+2)b}$
G= *CLe*$_4$ (*a*,*a*,*a*):	$\Omega(G,X) = 12\sum_{i=1}^{a-1} X^{2i(2a+1)} + 6X^{2a(2a+1)}$ $\Omega'(G,1) = 12a^2(2a+1)$
G=*CQ*$_4$(*a*,*b*,*c*); $a \geq b \geq c$:	$\Omega(G,X) = 4abcX^6 + aX^{4bc+2b+2c} + bX^{4ac+2a+2c} + cX^{4ab+2a+2b}$
G= *CQ*$_4$ (*a*,*a*,*a*):	$\Omega(G,X) = 4a^3X^6 + 3aX^{4a(a+1)}$ $\Omega'(G,1) = 12a^2(3a+1) = e(G) = \mid E(G) \mid$ $v(G) = \mid V(CQ_4) \mid = 4a^2(3+5a)$ $R_4 = 3a^2(1+3a)$; $R_6 = 12a^3$
G=*CQ*$_{4,6}$(*a*,*b*,*c*); $a \geq b \geq c$:	

$$\Omega(G,X)=4\sum_{i=1}^{b-1}X^{2(3c+1)i}+2(a-b+1)X^{2(3c+1)b}+$$
$$4\sum_{i=1}^{c-1}X^{2(2a+1)i}+2(b-c+1)X^{2(2a+1)c}+$$
$$4\sum_{i=1}^{c-1}X^{2(2b+1)i}+2(a-c+1)X^{2(2b+1)c}+cX^{4ab+2a+2b}$$

G=$CQ_{4,6}$ (a,a,a):

$$\Omega(G,X)=4\sum_{i=1}^{a-1}X^{2i(3a+1)}+8\sum_{i=1}^{a-1}X^{2i(2a+1)}+2X^{2a(3a+1)}+4X^{2a(2a+1)}+aX^{4a(a+1)}$$
$$\Omega'(G,1)=16a^2(2a+1)=e(G)=|E(G)|$$
$$v(G)=|V(\mathrm{CQ}_{4,6})|=16a^2(1+a)$$
$$R_4=a(4-7a+9a^2);\quad R_6=2a(2-3a+7a^2)$$

G=CQ_6 (a,a,a) DP:

$$\Omega(x)=2\left[\sum_{i=1}^{a-1}x^{(2a-2)+(4a+4)i}+\sum_{i=1}^{a}x^{2i^2+6i}+2\sum_{i=1}^{a-1}x^{2a+(2a+2)i}+\sum_{i=1}^{\frac{2a-7-(-1)^a}{4}a}x^{(2a^2+6a)+4(a-1-i)i}\right]$$
$$+(2a+2)\,x^{2a(a+2)}+a\,x^{4a(a+1)}+$$
$$\frac{3+(-1)^a}{2}\,x^{(3a^2+4a+\frac{1-(-1)^a}{2})}+1\,x^{4a^2+6a-2}$$
$$CI(G)=400a^6+\frac{7756}{5}a^5+\frac{2648}{3}a^4-\frac{3532}{3}a^3+\frac{2384}{6}a^2-\frac{1408}{15}a+8$$
$$e(G)=|E(G)|=\Omega'(G,1)=20a^3+40a^2-14a+2$$
$$v(G)=|\mathrm{V(CQ6\_DP)}|=10\mathrm{a}^3+26a^2-4a$$
$$\mathrm{R}(4)=6\mathrm{a}^3+20a^2+18a+6;\quad R(6)=10\mathrm{a}^3+36a^2+33a+12$$

G=CQ_6 (a,a,a) TP:

$$\Omega(x)=2\left[\sum_{i=1}^{a}x^{i^2+4i+1}+3\sum_{i=1}^{a-1}x^{2a+(4a+2)i}+\sum_{i=1}^{\frac{2a-7-(-1)^a}{4}}x^{a^2+4a+1+2(a-1)i-2i^2}\right]$$
$$+\frac{3+(-1)^a}{2}\,x^{\frac{6a^2+12a+5-(-1)^a}{4}}+3a\,x^{2a(a+2)}+3\,x^{4a(a+1)}$$
$$CI(G)=400a^6+\frac{6969}{5}a^5+917a^4-650a^3-116a^2+\frac{86}{5}a+6$$
$$e(G)=|E(G)|=\Omega'(G,1)=20a^3+36a^2-6a-2$$
$$v(G)=|\mathrm{V(CQ6\_TP)}|=10\mathrm{a}^3+24a^2-2$$
$$\mathrm{R}(4)=6\mathrm{a}^3;\quad R(6)=10\mathrm{a}^3+3a^2-3a+2$$

Data in this section refer to R_{max}[6]. If faces instead of rings are considered, the polynomial is different. Data were calculated by the original program Nano Studio[90], developed at the TOPO Group Cluj. Examples are given for each discussed lattice, both for polynomials and indices, in the following tables.

Tabel 5. 1 Examples for $CLe_4(a,b,c)$ lattice

$CLe_4(a,b,c)$_atoms	Omega polynomial	*CI*_Index
111_24	$6x^{6}$	1,080
222_144	$12x^{10}+6x^{20}$	54,000
422_272	$4x^{10}+4x^{14}+4x^{18}+6x^{20}+6x^{28}+2x^{36}+2x^{44}$	363,408
442_512	$4x^{14}+8x^{18}+4x^{28}+12x^{36}+4x^{42}+2x^{56}+2x^{80}$	1,353,664
444_960	$12x^{18}+12x^{36}+12x^{54}+6x^{72}$	2,900,448
	Sadhana polynomial	*Sd*_Index
111_24	$6x^{30}$	180
222_144	$6x^{220}+12x^{230}$	4,080
422_272	$2x^{572}+2x^{580}+6x^{588}+6x^{596}+4x^{598}+4x^{602}+4x^{606}$	16,632
442_512	$2x^{1104}+2x^{1128}+4x^{1142}+12x^{1148}+4x^{1156}+8x^{1166}+4x^{1170}$	41,440
444_960	$6x^{1656}+12x^{1674}+12x^{1692}+12x^{1710}$	70,848

Tabel 5. 2 Examples for $CQ_4(a,b,c)$ lattice

$CQ_4(a,b,c)$_atoms	Omega polynomial	*CI*_Index
111_32	$4x^{6}+3x^{8}$	1,968
222_208	$32x^{6}+6x^{24}$	108,288
331_240	$36x^{6}+6x^{20}+1x^{48}$	141,456
332_444	$72x^{6}+6x^{34}+2x^{48}$	521,688
333_648	$108x^{6}+9x^{48}$	1,141,776
444_1472	$256x^{6}+12x^{80}$	6,144,000
	Sadhana polynomial	*Sd*_Index
111_32	$3x^{40}+4x^{42}$	288
222_208	$6x^{312}+32x^{330}$	12,432
331_240	$x^{336}+6x^{364}+36x^{378}$	16,128
332_444	$2x^{684}+6x^{698}+72x^{726}$	57,828
333_648	$9x^{1032}+108x^{1074}$	125,280
444_1472	$12x^{2416}+256x^{2490}$	666,432

$CQ_4(a,a,a)$	*e*(G)	*v*(G)	*CI*_Index
111	48	32	1,968
222	336	208	108,288
333	1,080	648	1,141,776
444	2,496	1,472	6,144,000

Lattices built by Op(Trs(P4(Oct)))

The lattices below are constructed by using the units designed with the sequence $Op(Trs(P_4(Oct)))$, where Oct is the Octaedronul. The net in the top row of Fig. 5.5 was made by identifying ("Id"-net) the opposite faces of non-optimized units, thus appearing a more "mathematical" network. The net in the bottom of this figure is realized by joining ("Jn"-net) energetically optimized structures, the net being a more "chemical" one.[113] These networks show only hexagonal faces/rings and have large

hollows, as those encountered in zeolites, natural alumino-silicates widely used in synthetic chemistry as catalysts.

Omega polynomial was evaluated on a cubic domain, the analytical formulas being listed below.

Examples are given in the following tables.

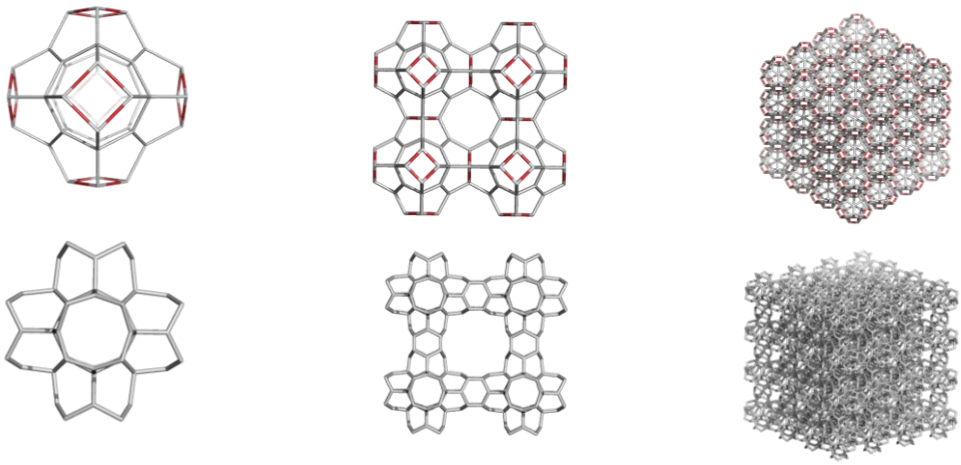


Fig.5. 5 Top row: Unit designed by *Op*(*Trs*(P_4(*Oct*))) and the net constructed by identifying ("Id"-net) the opposite faces of non-optimized units, thus being a "mathematical" network. Bottom row: a more "chemical" network constructed by joining ("Jn"-net) the energetically optimized units; the right column shows these hypothetical networks in the corner view of a cubic domain *a*,*a*,*a* where *a* is the number of repeating units on a given dimension of 3D space.

Tabel 5. 3 Examples of Omega polynomial in *Op*(*Trs*(*P*4(Oct)))_*Id* crystal-like network

k	Polinom Omega; $R_{max}[6]$	*v*	*e*	*CI*
1	$24x^3+6x^4$	68	96	8,904
2	$48x^3+48x^4+48x^5+12x^8$	448	672	448,416
3	$72x^3+162x^4+144x^5+72x^8$	1,404	2,160	4,654,152
4	$96x^3+384x^4+288x^5+216x^8$	3,200	4,992	24,892,032
5	$120x^3+750x^4+480x^5+480x^8$	6,100	9,600	92,104,200
6	$144x^3+1296x^4+720x^5+900x^8$	10,368	16,416	269,387,424

Omega polynomial in *Op*(*Trs*(P_4(*Oct*)))_*Id* crystal-like network

$$\Omega(R_{\max}[6];Id,x) = a_3x^3 + a_4x^4 + a_5x^5 + a_8x^8$$

$$a_3 = 24k\ ;\ a_4 = 6a^3;\ a_5 = 24a(a-1)\ ;\ a_8 = 6k(k-1)^2$$

$$\Omega(R_{\max}[6];Id,x) = 24ax^3 + 6a^3x^4 + 24a(a-1)x^5 + 6a(a-1)^2x^8$$

$$\Omega'(R_{\max}[6];Id,1) = |E(G)| = e(G) = 24a^2(3a+1)$$

$$\Omega''(R_{\max}[6];Id,1) = 24a^2(17a-8)$$

$$CI(R_{\max}[6];Id) = 24a^2(216a^4 + 144a^3 + 24a^2 - 20a + 7)$$

$$v(Id) = 44a^3 + 24a^2$$

Tabel 5. 4 Examples of Omega polynomial in *Op*(*Trs*(P_4(*Oct*)))_*Jn* crystal-like networks

k	Polinom Omega; F_{max}[6]	*v*	*e*	*CI*
1	$24x^3+6x^4$	68	96	8,904
2	$48x^3+60x^4+48x^9$	544	816	660,576
3	$72x^3+216x^4+72x^9+72x^{15}$	1,836	2,808	7,858,728
4	$96x^3+528x^4+96x^9+96x^{15}+96x^{21}$	4,352	6,720	45,077,376
5	$120x^3+1050x^4+120x^9+120x^{15}+120x^{21}+120x^{27}$	8,500	13,200	174,045,000
6	$144x^3+1836x^4+144x^9+144x^{15}+144x^{21}+144x^{27}+144x^{33}$	14,688	22,896	523,826,784

Omega polynomial in în *Op*(*Trs*(P_4(*Oct*)))_*Jn* crystal-like networks

$$\Omega(F_{\max}[6]; Jn, x) = a_3x^3 + a_4x^4 + a_3\sum_{i=2}^{k} x^{3(2i-1)}$$

$a_3 = 24k$; $a_4 = 6a[a(a-1)/2 + a^2]$

$$\Omega(F_{\max}[6]; Jn, x) = 24ax^3 + 6a[a(a-1)/2 + a^2]x^4 + 24a\sum_{i=2}^{a} x^{3(2i-1)}$$

$$\Omega'(F_{\max}[6]; Jn,1) = |E(G)| = e(G) = 12a^2(9a-1)$$

$$\Omega''(F_{\max}[6]; Jn,1) = 36a^2(8a^2 + a - 3)$$

$$CI(F_{\max}[6]; Jn) = 24a^2(486a^4 - 108a^3 - 6a^2 - 6a + 5)$$

$$v(Jn) = 68a^3$$

Dyck graph based networks

The networks making the subject of this section were built up by units that are representations of the celebrate Dyck graph.[114] This graph consists of 32 vertices of valence 3, it has 48 edges, 12 octagons R[8], girth 6, diameter 5, and the chromatic number 2; it is non-planar and has the genus g = 1 (i.e., there exists an embedding of the graph on the torus). Cycle counting on the finite representation revealed 12 octagons and 16 hexagons. As a unit of the infinite lattice, it shows 12 octagons and the genus is g=3. [3]

The Dyck graph units are designed as: the zig-zag isomer Z-56 (Fig.5.6, left) by the sequence *Op(Q(C))*, performed on the Cube C while the armchair isomer A-56 (Fig.5.6,middle), by the sequence *Op2a(Q(C))*. There is a third unit, that makes co-net with the above A-isomer, designed by *Op2a(Ca(C))* and denoted A-104 (Fig. 5.6 right). All these units have the genus g=3, the last one being a chiral unit, made by the pro-chiral operation Ca ="Capra"(Rom)=Goat (Eng). The chirality induced by Ca-operation approaches the unity, according to Petitjean theory. [115]

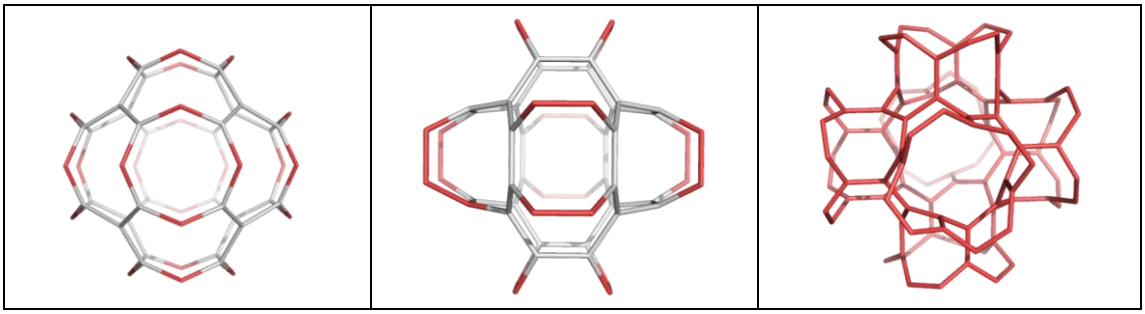


Fig.5. 6 Dyck graph units: zig-zag Z-56, R[8]=12 (left); armchair A-56, R[8]=12 (middle); armchair A-104, R[8]=24 (right).

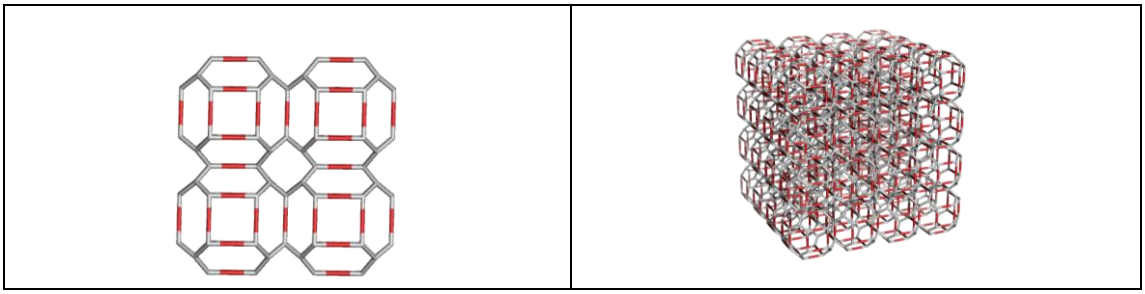


Fig.5. 7 Dyck Z-56 based network as a "mathematical" non-optimized "Id"-lattice: 222_352 (left) and 444_2432 (right)

Conclusions

A network embedded in the P-type surface can be considered a decoration of this surface; basically, it belongs to the space group *Pm*-3*m*. Among many such P-networks there are some ones (having as repeating units) representations of celebrate structures, e.g. P-(7,3) network represents the Klein tessellation while P-(8,3) network is the representation of Dyck graph the last one being registered by Topo Group Cluj (as diu8, TOPOS). Construction of these networks/decorations was made by using sequences of map operations (implemented in the CVNET software for the repeating units while their assembly/embedding was done by the aid of Nano Studio program, both of them developed at TOPO Group Cluj. Topology of these networks was described by Omega polynomial (also developed in Cluj), as a complement to the crystallographic classical description.

Chapter VI. Original software programs

The personal contributions refer to the design and implementation in C of the programs.

A periodic structure is formed by repeating a base structure through translation along a direction (for 1-periodic structures) or more directions (three directions for 3-periodic structures). The programs designed, presented next, help in finding the repeating directions (atom.c) and in the processing of the structure. The ahin.c program colors some atoms in the structure so that the directions found by atom.c can be vizualized. The hinZalign.c program reorients the structure, so that the direction specified by a given vector becomes the direction of the z axis. It is used mostly for 1-periodic structures.

The program for finding the unit vectors of a periodic structure:

If the base structure that generates the periodic structure through repetition were known and if every instance of the base structure in the periodic structure were identified, than the vectors that show the distance and direction between any two instances of the base structure are possible unit vectors. The purpose of the program is to find up to three unit vectors, without knowing and without identifying the base structure. Taking a random atom as reference, it belong to a base structure. As the base structure repeats, so does the reference atom and the corresponding atoms are somewhat similar to the reference atom. By identifying the similar atoms to the reference atom, we can determine the vectors between two instances of the base structure. The program does just that, it calculates the unit vectors after finding the similar atoms to a reference atom.

The program can be run as follows: atom.exe «file» «delta» «alpha» [«atom0» [«n»]]. The file «file» contains the crystalline structure to be analyzed, in „hin” format. «delta» and «alpha» are tolerance parameters. «atom0» designates the reference atom, by default the first atom in the structure. For some selection criteria for unit vectors, the program searches up to «n» solutions, if not specified «n» is chosen as 1.

General conclusions

Graph theory is useful in describing crystalline networks.

Recent publications in crystallography use graph theory more in describing the crystalline state of the matter.

The triple periodic structures were generated using CVNET[23] and Nano Studio[90] based on map operations.

At the TOPO Cluj group, there were generated 69 crystalline networks, subsequently there were analyzed at Università degli Studi di Milano, under the supervision of prof. Davide M Proserpio. Among them, 39 are originals new structures that were recorded with the names diu1, diu2, etc.

The investigation was done using the original programs atom, hin and hinzalign, hin2off and TOPOS, the latter developped at the University of Samara, Russia by prof Vladislav Blatov's group.

The structures that show 1 periodicity can be associated with cvasicrystal networks, having axial symmetry. The topology of these structures were presented in crystallographic terms.

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