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CELL@CELL HIGHER DIMENSIONAL STRUCTURES

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ABSTRACT. Local domains of *n*-spaces surrounded by the common Euclidean 3D-space may exist in complex chemical (mineral or synthetic) structures. In this paper, two classes of the simplest clusters embedded in n-dimensional spaces higher than three are designed by operations on maps and their properties discussed.

Keywords: *graph, n-dimensional space, n-cube, torus, cluster*

INTRODUCTION

The gravitational theory (general relativity) describes our universe having the geometry of three-dimensional space with the fourth-dimension being the time. The so-called 3 + 1 space gives an accurate description of the universe we observe. A stellar black hole is believed to be formed by the gravitational collapse of a massive star (from five to several tens of the solar mass). Understanding the universe led us to the need of learning about spaces of dimensions higher than three. The aim of finding domains of *n*-spaces surrounded by the common Euclidean 3D-space, in complex chemical (mineral or synthetic) structures promoted our efforts towards a systematic design of n-dimensional hyper-structures. Let, for the beginning, introduce to some basic mathematical notions.

A ***convex hull*** (envelope) [1-3] of a set *X* of points in the Euclidean space is the smallest convex set that contains *X*. A set of points is called convex if it contains all the line segments connecting each pair of its points. The convex hull of a finite set *S* of points is the set of all its convex combinations; in a convex combination, each point x_i is weighted by a coefficient α_i such that the coefficients are all non-negative and their sum is one. For each choice of coefficients, the resulting convex combination is a point in the convex hull, and the whole convex hull can be generated by choosing coefficients in all possible ways. One can write the convex hull as the set:

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$$\left\{ \sum_{i=1}^{|S|} \alpha_i x_i \mid (\forall_i : \alpha_i \geq 0) \wedge \sum_{i=1}^{|S|} \alpha_i = 1 \right\} \quad (1)$$

The convex hull of a finite point set $S \in \mathbf{R}^n$ forms a convex polygon, for n = 2, or, in general, a convex polytope in $\mathbf{R}^n$. Every convex polytope in $\mathbf{R}^n$ is the convex hull of its vertices.

There are six regular 4D-polytopes, also called polychora: 5-Cell {3,3,3}; 8-Cell {4,3,3}; 16-Cell {3,3,4}; 24-Cell {3,4,3}; 120-Cell {5,3,3} and 600-Cell {3,3,5}. Five of them can be associated to the Platonic solids but the sixth, the 24-cell has no close 3D equivalent; it consists of 24 octahedral cells, 6 cells meeting at each vertex. Among them, 5-Cell and 24-Cell are self-cage-dual while the others are pairs: (8-Cell & 16-Cell); (120-Cell & 600-Cell). In the above, {p, q, r,…} are the Schläfli symbols: the symbol {p} denotes a regular polygon for integer p, or a star polygon for rational p; the symbol {p, q} denotes a 3D-object tessellated by p-gons while q is the vertex-figure (i.e. the number of p-gons surrounding each vertex); the symbol {p, q, r} describes a 4D-structure, in which r 3D-objects join at any edge (r being the edge-figure) of the polytope, and so on. The Schläfli symbol has the nice property that its reversal gives the symbol of the dual polyhedron. The 4D polytopes have been first described by Schläfli [4].

In dimensions 5 and higher, there are only three kinds of convex regular polytopes no non-convex regular polytopes exists. Let us give some details, in the following.

The ***n-simplex***[1], with Schläfli symbol {3^{n-1}}, and the number of its k-faces $\binom{n+1}{k+1}$, is a generalization of the triangle or tetrahedron to arbitrary dimensions. A simplex is an n-dimensional polytope, which h is the convex hull of its n+1vertices. For example, a 0-simplex is a point, a 1-simplex is a line segment, a 2-simplex is a triangle, a 3-simplex is a tetrahedron, and a 4-simplex is a 5-cell. A simplex may be defined as the smallest convex set containing the given vertices. A regular n-simplex may be constructed from a regular (n − 1)-simplex by connecting a new vertex to all original vertices by the common edge length.

The convex hull of any nonempty subset of k+1 points that define an n-simplex is called a *face* of the simplex; faces are simplexes themselves. In particular, the convex hull of a subset of size k+1 (of the n+1 defining points) is a k-simplex and is called a k-face of the n-simplex. The 0-faces (i.e., the points themselves) are called the *vertices*, the 1-faces are called the *edges*, the (n − 1)-faces are called the *k-faces* (or *facets)*, and the sole n-face is the whole n-simplex itself.

The ***hypercube*** [1] is a generalization of the 3-cube to *n*-dimensions; it is also called an *n*-cube and commonly denoted Q_n. It is a regular polytope with mutually perpendicular sides, thus being an orthotope. It has the Schläfli symbol $\{4,3^{n-2}\}$ and k-faces given by $2^{n-k}\binom{n}{k}$. Figure 1 illustrates the 4-cube, i.e., 8-Cell or Tesseract, as painted by the Italian painter Juseppe Zaccuri, Milano.

Figure 1. HyperCube by Juseppe Zaccuri, Milano

The ***n-orthoplex* or cross-polytope** [1] has the Schläfli symbol $\{3^{n-2},4\}$ and k-faces $2^{k+1}\binom{n}{k+1}$; it exists in any number of dimensions and is the dual of *n*-cube. The cross-polytope is the convex hall of its vertices; its facets are simplexes of the previous dimensions, while its vertex figures are other cross-polytopes of lower dimensions.

To investigate an *n*-dimensional polytopes, a formula, also due to Schläfli [4], is used

$$\sum_{i=0}^{n-1}(-1)^i f_i = 1-(-1)^n \tag{2}$$

For n=4, eq (2) reduces to the well-known Euler [5] relation

$$v-e+f=2(1-g) \tag{3}$$

with *v*, *e*, *f* and *g* being the vertices, edges, 2-faces and the genus, respectively; *g*=0 for the sphere and *g*=1 for the torus.

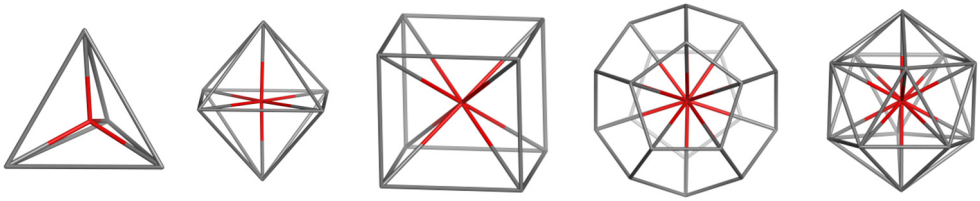
RESULTS AND DISCUSSION

The n-dimensional spaces may be locally present in minerals or artificial chemicals [6]. Some 4-dimensional 13-atom clusters: MaMb12 or M13, M=Fe, Pd, Ru, Rh was found to show giant magnetic moments [7]. Other simple molecules as B4Cl4, $Co(CO)_4^-$, etc. may be described in dimensions higher than three. In this respect, two simplest classes of clusters showing dimensionality higher than three will be introduced as follows.

P-Centered Clusters

Body centered clusters derived from the Platonic solids are easily drawn, as shown in Figure 2; their figure count is given in Table 1. These small clusters, excepting DoP.21, were next transformed by operations on maps [8-10] in their 2-dual, medial (i.e. rectified) and truncated derivatives (Figures 3 to 6). P-centered clusters represent cell-duals of polyhedra with the same number of cells around a central one; they are objects of Euclidean 4D-space, as shown by the figure count (Tables 2 to 5) cf. eq (2). This idea can be extended to objects other than Platonics.

The name of clusters can be made in at least three ways, as shown in the bottom of figures and tables; the “endohedral” @ symbol was used, starting from the core and going radially, to the exterior, the suffix number counting the points/atoms in the whole structure.

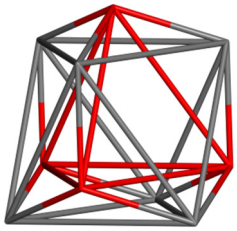


TP.5	OctP.7	CP.9	DoP.21	IcoP.13
P@T.5	P@Oct.7	P@C.9	P@Do.21	P@Ico.13
P@T4@T.5	P@T8@Oct.7	P@(Py4)6@C.9	P@(Py5)12@Do.21	P@T20@Ico.13

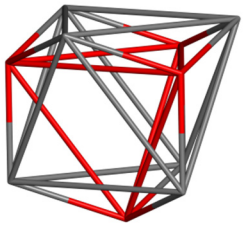
Figure 2. Body centered clusters derived from the Platonic solids

Table 1. Figure count for clusters in Figure 2

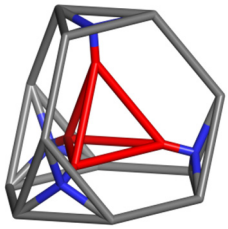
Cluster	v	e	f_3	f_5	f_6	f	p1	p2	p3	M	c	Sum(f)	Sym	p_k; (M)
TP	5	10	10	0	0	10	4	0	0	1	5	0	3	T; 0; 0 (T)
OctP	7	18	20	0	0	20	8	0	0	1	9	0	4	T;0;0 (Oct)
CP	9	20	12	6	0	18	0	6	0	1	7	0	4	0;Py4; 0 (C)
DoP	21	50	30	0	12	42	0	12	0	1	13	0	5	0;Py5;0 (Do)
Icop	13	42	50	0	0	50	20	0	0	1	21	0	5	T; 0; 0 (Ico)



Du(TP).10
T@Oct.10



Med(TP).10
T@Oct.10

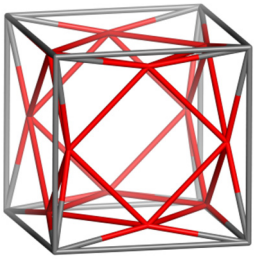


Tr(TP).20
T@(TT4;T4)@TT.20

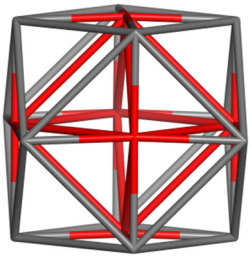
Figure 3. TP-derived structures

Table 2. Figure count for clusters derived from TP cluster

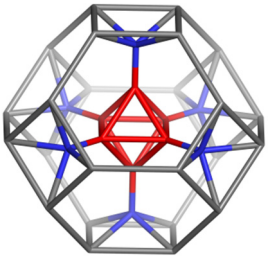
T-structure	v	e	f_3	f_5	f_6	f	p1	p2	p3	M	c	Sum(f)	Sym	p_K; (M)
TP.5	5	10	10	0	0	10	4	0	0	1	5	0	3	T; 0; 0 (P; T)
Du(TP).10	10	30	30	0	0	30	4	4	0	2	10	0	3	T; Oct= AP_3; 0 (T;Oct)
Med(TP).10	10	30	30	0	0	30	4	4	0	2	10	0	3	T; Oct= AP_3; 0 (T;Oct)
Tr(TP).20	20	40	20	0	10	30	4	4	0	2	10	0	3	T;TT; 0 (T; TT)



Du(OctP).20
CO@((AP4)6;T8)@C.20



Med(OctP).18
Oct@(Oct8;(Py4)6)@CO.18

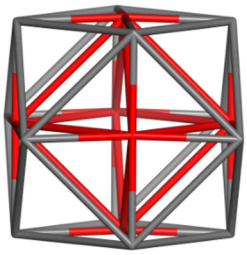


Tr(OctP).36
Oct@(TT8;(Py4)6)@TO.36

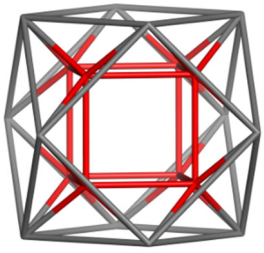
Figure 4. OctP-derived structures

Table 3. Figure count for clusters derived from OctP cluster

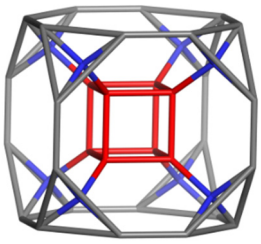
Oct-structure	v	e	f_3	f_5	f_6	f	p_1	p_2	p_3	M	c	Sum(f)	Sym	p_K; (M)
OctP.7	7	18	20	0	0	20	8	0	0	1	9	0	4	T;0;0 (P;Oct)
Du(OctP).20	20	60	44	12	0	56	8	6	0	2	16	0	4	T;Ap4;0 (CO;C)
Med(OctP).18	18	60	52	6	0	58	8	6	0	2	16	0	4	Oct; Py4 (Oct; CO)
Tr(OctP).36	36	78	32	6	20	58	8	6	0	2	16	0	4	TT;Py4;0 (Oct;TO)



Du(CP).18
Oct@(Oct8;(Py4)6)@CO.18



Med(CP).20
C@((AP4)6;T8)@CO.20

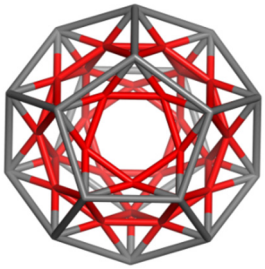


Tr(CP).40
C@((HTO)6;T8)@TC.40

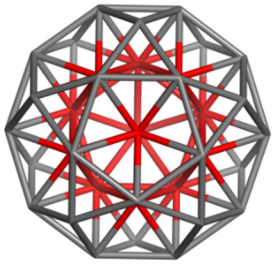
Figure 5. CP-derived structures

Table 4. Figure count for clusters derived from CP cluster

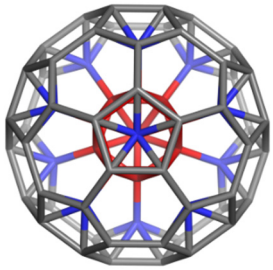
C-structure	v	e	f_3	f_5	f_6	f	p_1	p_2	p_3	M	c	Sum(f)	Sym	p_k; (M)
CP.9	9	20	12	6	0	18	0	6	0	1	7	0	4	0;Py4; 0 (P;C)
Du(CP).18	18	60	52	6	0	58	8	6	0	2	16	0	4	Oct; Py4 (Oct; CO)
Med(CP).20	20	60	44	12	0	56	8	6	0	2	16	0	4	T;Ap4;0 (C; CO)
Tr(CP).40	40	80	32	6+6	12	56	8	6	0	2	16	0	4	T;HTO;0 (C; TC)



Du(IcoP).50
ID@((AP5)12;T20)@Do.50
Med(DoP).50=Do@((AP5)12;T20)@ID.50



Med(Icop).42
Ico@(Oct20;(Py5)12)@ID.42



Tr(Icop).84
Ico@(TT20;(Py5)12)@C60.84

Figure 6. IcoP-derived structures

Table 5. Figure count for clusters derived from IcoP cluster

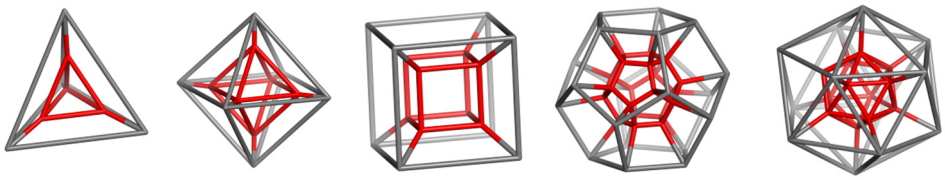
Ico-structure	v	e	f_3	f_5	f_6	f	p_1	p_2	p_3	M	c	Sum(f)	Sym	p_k; (M)
IcoP.13	13	42	50	0	0	50	20	0	0	1	21	0	5	T; 0; 0 (P; Ico)
Du(IcoP).50	50	150	110	24	0	134	20	12	0	2	34	0	5	T;AP5;0 (ID30;Do20)
Med(Icop).42	42	150	130	60	12	142	20	12	0	2	34	0	5	Oct; Py5;0 (Ico;ID30)
Tr(Icop).84	84	192	80	0	62	142	20	12	0	2	34	0	5	TT; Py5; 0 (Ico;C60)

Note that Tr(Icop).84 is related to the Samson cluster, that consists of twenty truncated tetrahedra TT (Friauf polyhedra), icosahedrally arranged, with a central atom inside each TT, all together counting 104 points/atoms [11-13]; the central shell forms an icosahedron. It is related to intermetallic phases. Intermetallics [14] represent compounds involving two or more metals, e.g.Laves phases (AB_2), e.g., $MgCu_2$, $MgZn_2$ and $MgNi_2$, size packing phases, such as Frank-Kasper, phases, etc. They can display desirable magnetic, superconducting and chemical properties, due to their strong internal order and mixed (metallic and covalent/ionic bonding, respectively). Intermetallics have promoted novel materials development.

Cell-in-Cell Clusters

Let now introduce the selective truncation operation (for general map operations, the reader is invited to consult refs [8-10, 15]: it leaves unchanged the non-marked points/atoms. In this simple way, cell-in-cell clusters can be designed (Figure 7); the figure count for these structures is listed in Table 6.

Further examples are shown in Figures 8 and 9 while their figure count is given in Table 7. Observe the double-shell torus T(4,12)Q4T5.96 (Figure 9, left), with a square tube section; every sector can be counted as an n-cube (see Figure 9, right). It was proposed by Diudea [16] as a model for the galactic black holes.

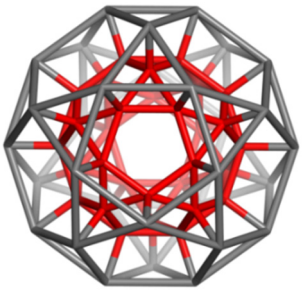


T@T.8 T@(P3)4@T.8 | Oct@Oct.12 Oct@(P3)8@Oct.12 | C@C.16 C@C6@C.16 | Do@Do.40 Do@((P5)12@Do.40 | Ico@Ico.24 Ico@((P3)20@Ico.24

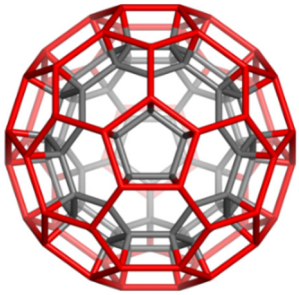
Figure 7. Selectively truncated body centered clusters of the Platonic solids

Table 6. Figure count for selectively truncated body centered clusters Trs(P@M); M= Platonic solids

	Trs(P@M)	v	e	f_3	f_4	f_5	f	p_k	M	Cell	Sum(f)	Sym	p_k; M
1	.T@T.8	8	16	8	6	0	14	4	2	6	0	3	P3 (T;T)
2	Oct@Oct_12	12	30	16	12	0	28	8	2	10	0	4	P3 (Oct;Oct)
3	C@C.16	16	32	0	24	0	24	6	2	8	0	4	P4 (C;C)
4	Do@Do.40	40	80	0	30	24	54	12	2	14	0	5	P5 (Do;Do)
5	Ico@Ico.24	24	72	40	30	0	70	20	2	22	0	5	P3 (Ico;Ico)

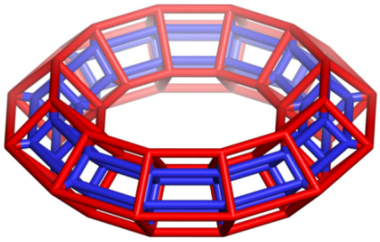


ID@ID.60
ID@((P5)12;(P3)20)@ID.60

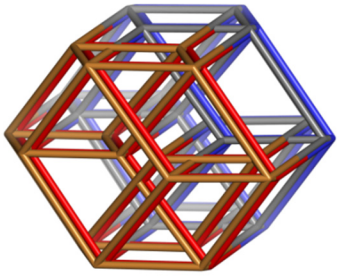


C_{60}@C_{60}.120
C_{60}@((P5)12;(P6)20)@C_{60}.120

Figure 8. Other "cell-in-cell" structures



T(4,12)Q4T5.96



Q6(TU(4,8)Q6T7.64

Figure 9. A double-wall torus with the square section and 12 units Q4 (left); a detailed Q6 unit (right)

Table 7. Figure count for the objects in Figures 4 and 5

Structure	0	1	f3	f4	f5	f6	2	p3	p5	p6	m	3	4	5	Sum(f)
ID@ID.60	60	150	40	60	24	0	124	20	12	0	2	34	0	0	0
C_{60}@C_{60}.120	120	240	0	90	24	40	154	0	12	20	2	34	0	0	0
T(4,12)Q_4T_5.96	96	240	0	216	0	0	216	0	0	0	0	84	12	0	0*
Q6.64	64	192	0	240	0	0	240	0	0	0	0	160	60	12	0

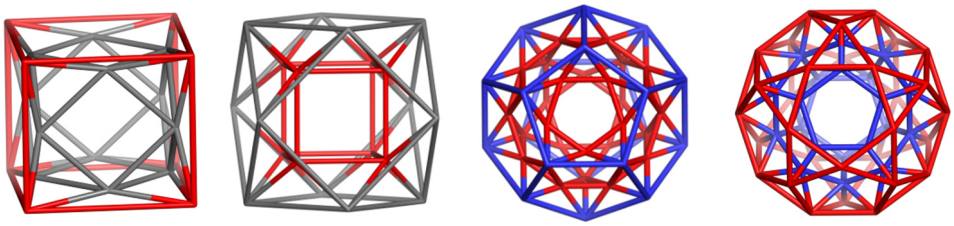
* in case of Torus, the right member of (2) gives all time zero, because the torus is a surface of genus g=1.

It is the time to show a lower bound for the clusters existing in dimensions higher than three:

Theorem. A cluster of points/atoms with at least two (concentric) shells belongs to n-spaces higher than tridimensional.

Proof. A polytope is convex if any of its *k*-facets is shared by at least two *k*+1-facets. In particular, for *n*=4, *k* =2 while *k*+1 is a 3-facet, i.e. a cell. In other words, any 2-facet must share at least two 3-facets: the actual cell and the whole envelope. Next, the cluster is bound by 3-facets, thus the polytope is of dimension 3+1=4. This condition is already reached in P-centered clusters (Figure 2; Table 1), as much as in the "cell-in-cell" double-shell clusters (Figure 7). This is a lower bound condition and the theorem is demonstrated.

At the end, two pairs of clusters are presented: Med(CP).20 & Du(OctP).20 (Figure 10, left) and Med(DoP).50 & Du(IcoP).50 (Figure 10, right); they illustrate the sphere inversion event and is equivalent to tesseract moving on the fourth dimension (i.e. the time), a proof in addition that double-shell clusters belong to higher-dimensional spaces.



CO@C.20
CO@((AP4)6;T8)@C
Med(CP).20

C@CO.20
C@((AP4)6;T8)@CO
Du(OctP).20

ID@Do.50
ID@((AP5)12;T20)@Do
Med(DoP).50

Do@ID.50
Do@((AP5)12;T20)@ID
Du(IcoP).50

Figure 10. Sphere inversion by 4D-clusters: moving on the fourth dimension

COMPUTATIONAL DETAILS

The design and properties of the studied structures was performed by our original CVNET [17] and Nano Studio [18] software programs.

CONCLUSIONS

Some 4D-and higher-dimensional structures have been designed by using operations on maps, and their topological properties discussed. Multi-shell clusters appear frequently in minerals/chemicals and such analysis as we performed here could help in structure elucidation efforts.

There is a trend in Chemistry, Physics and even Astronomy to consider the *n*-dimensional spaces locally mixed/interlaced with the actually perceptible 3-dimensional Euclidean space. It seems that 3D-space and nD-spaces

simultaneously exist, as a manner of highly organizing the matter. The difficulty of visualization of the higher dimensions arises from the fact that only projections of the whole nD-structure can be seen in 3D- or even 2D-spaces.

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