Iranian J. Math. Chem. 9 (1) March (2018) 1 − 8

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

Hypercube Related Polytopes

MIRCEA V. DIUDEA •

Department of Chemistry, Faculty of Chemistry and Chemical Engineering, Arany Janos Str. 11, 400028, "Babes−Bolyai" University, Cluj, Romania

ARTICLE INFO

Article History:

Received 14 November 2017
Accepted 27 November 2017
Published online 11 December 2017
Academic Editor: Ali Reza Ashrafi

Keywords:

Polyhedron
n-Polytope
24-Cell
Rhombellane
Rank

ABSTRACT

Body centered structures are used as seeds for a variety of structures of rank 3 and higher. Rhombellane structures are introduced and their design and topological properties are detailed.

1 INTRODUCTION

A regular polyhedron is a polyhedron having congruent regular polygons as faces, arranged in the same manner around identical vertices; its symmetry group acts transitively on its flags, a regular polyhedron being vertex-, edge- and face-transitive [1]. They show three symmetry groups: *tetrahedral*; *octahedral* (or cubic) and *icosahedral* (or dodecahedral). Any shapes with icosahedral or octahedral symmetry will also include the tetrahedral symmetry.

There are five regular polyhedra, known as Platonic polyhedral solids: *tetrahedron* (T), *cube* (C), *octahedron* (O), *dodecahedron* (D) and *icosahedron* (I), written as {3,3}; {4,3}; {3,4}; {5,3} and {3,5} by using the basic Schläfli [2] symbols {p,q} where *p* is the number of vertices in a given face while *q* is the number of faces containing a given vertex.

• Corresponding Author (Email address: diudea@gmail.com)
DOI: 10.22052/ijmc.2017.101019.1318

They show pair duals: (cube & octahedron) and (dodecahedron & icosahedron) while the tetrahedron is selfdual.

Generalization of a polyhedron to *n*-dimensions is called a polytope [1,3]. Regular 4-polytopes are written as $\{p,q,r\}$ and have cells of the type $\{p,q\}$, faces $\{p\}$, edge figures $\{r\}$ and vertex figures $\{q,r\}$; it means that *r*-polyhedra (of the type $\{p,q\}$) meet at any edge of the polytope. There are six regular 4-polytopes: 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 3D equivalent. Among them, 5-cell and 24-cell are selfduals while the others are pairs: (8-cell & 16-cell); (120-cell & 600-cell).

A 5-polytope is written as $\{p,q,r,s\}$, where $\{p,q,r\}$ is the 4-face type, $\{p,q\}$ is the cell type, $\{p\}$ is the face type; $\{s\}$ is the face figure, $\{r,s\}$ is the edge figure and $\{q,r,s\}$ is the vertex figure. The three types of convex regular polytopes in dimensions 5 and higher, are as follows.

The *n-simplex* [1,4], with the Schläfli symbol $\{3^{n-1}\}$, and the number of its *k*-faces $\binom{n+1}{k+1}$; it is a generalization of the triangle or tetrahedron to *n*-dimensions. A regular *n*-simplex may be constructed from a regular $(n-1)$-simplex by connecting a new vertex to all original vertices.

The *hypercube* Q_n is a generalization of the 3-cube to *n*-dimensions; it has the Schläfli symbol $\{4,3^{n-2}\}$ and the number of *k*-faces given by $2^{n-k}\binom{n}{k}$. The hypercube can be constructed by the Cartesian product graph of *n* edges: $(P_2)^{\square n} = Q_n$; the Q_4 hypercube is called 8-cell or also tesseract.

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 is the dual of *n*-cube. The cross-polytope faces are simplexes of the previous dimensions, while its vertex figures are other cross-polytopes of lower dimensions.

For general surfaces, Euler [5] characteristic χ can be calculated as an alternating sum of figures of rank *k* [6–8]:

$$\chi(S) = f_0 - f_1 + f_2 - f_3 + ...,$$

It may be used for checking the consistency of a proposed structure.

An abstract polytope is a structure which considers only the combinatorial properties of a classical polytope: angles and edge lengths are disregarded. No space, such as Euclidean space, is required to contain an abstract polytope [7], which is a partially ordered set (poset). Every polytope has a dual, of which partial order is reversed; the dual of a dual is isomorphic to the original. A polytope is self-dual if it is the same as (*i.e.* isomorphic to) its dual. Any abstract polytope may be realized as a geometrical polytope having the same topological structure.

[1,1,1]Propellane is an organic molecule, first synthesized in 1982 [9]; by *IUPAC* rules, it is named tricyclo[1.1.1.0^{1,3}]pentane, a hydrocarbon with formula C_5H_6. The length of central bond separating the triangles is 160 pm, much longer than 154 pm, the average length of sp^3 C-C bond; this bond may be considered non-effective and the propellane consisting of squares/rhombs, a triangle-free structure.

Rhombellation is a procedure enabling the design of generalized rhombellanes, performed as follows: join by a point (called "rbl-point") the two vertices lying opposite diagonal in each rhomb of an all rhomb-map (considered the zero-generation, Rh_0). Then, add new vertices opposite to the parent vertices and join each of them with the rbl-vertices lying in the proximity of each parent vertex, thus local Rh-cells being formed. The process can continue, considering the envelope Rh_n as "Rh_0" for Rh_{n+1}, in this way shell by shell being added to the precedent structure. Since the two diagonals may be topologically different, each generation may consist of two isomers.

Proposition [10]. *A structure is a rhombellane if all the following conditions are obeyed:*

a) *All strong rings are squares/rhombs;*
b) *Vertex classes consist of all non-connected vertices;*
c) *Omega polynomial has a single term: 1X^|E|;*
d) *Line graph of the original graph shows a Hamiltonian circuit*;
e) *Structure contains at least one* $K_{2.3}$ *subgraph.*

A fast detected condition is $\Omega(x) = 1x^e$, in words: all the edges in G are topologically parallel. Omega polynomial is defined as: $\Omega(x) = \Sigma_s m x^s$, m being the number of opposite edge strips, *ops*, of length s, in a graph G. There are graphs with a single *ops*, which is a Hamiltonian circuit. For such graphs, omega polynomial has a single term: $\Omega(x) = 1x^s$; $s = e = |E(G)|$. Hamiltonicity is an *np*-complete problem, being here a corollary of a single *ops* in the omega polynomial; however, not any graph having a Hamiltonian circuit has all the edges topologically parallel (see the case of cube and cuboctahedron). By construction, the rhombellanes have all classes of vertices not connected to each other within a same class. The smallest rhombellane is $K_{2.3}$, *i.e.*, the complete bipartite graph (corresponding to the [1,1,1]propellane molecule); any $K_{2.n}$ graph fulfills all the above conditions. A $K_{2.n}$ graph consists of $n(n\text{-}1)(n\text{-}2)/6$ $K_{2.3}$ substructures. There are graphs with more than two vertex classes obeying the above conditions; the proposed rhombellation operation enables the design of such graphs.

Rhombellanes represent *n*-partite graphs, both by topology and coloring [11,12]. Some crystal networks also fulfill the above criteria; among these, only the *dia* net is full rhombellanic.

2 BODY–CENTERED CLUSTERS

Body centered clusters, derived from the Platonic solids (here denoted by MP^n), represent cell-duals of polyhedra having n-cells around a central cell; they are objects of Euclidean 4D-space [13]; this idea can be extended to objects other than Platonics (Figure 1); extension of P central point to a same cell leads to "cell-in-cell" clusters (Figure 2). Such body centered clusters have been used to design a plethora of polyhedral or non-polyhedral objects, and also periodic networks [14].

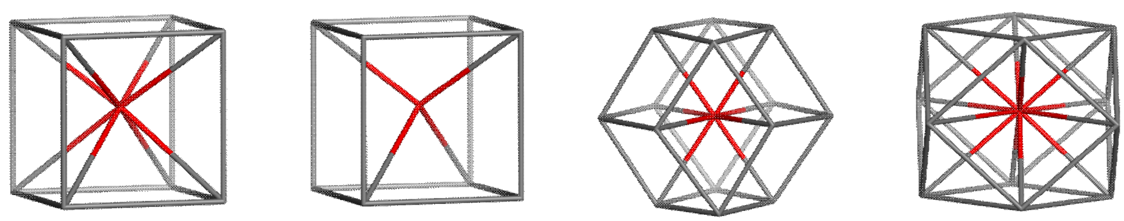


Figure 1. Seeds for some periodic networks.

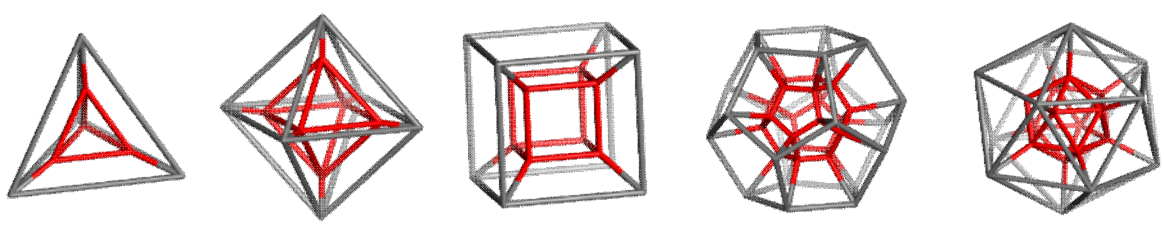


Figure 2. Cell-in-cell clusters of the Platonic solids.

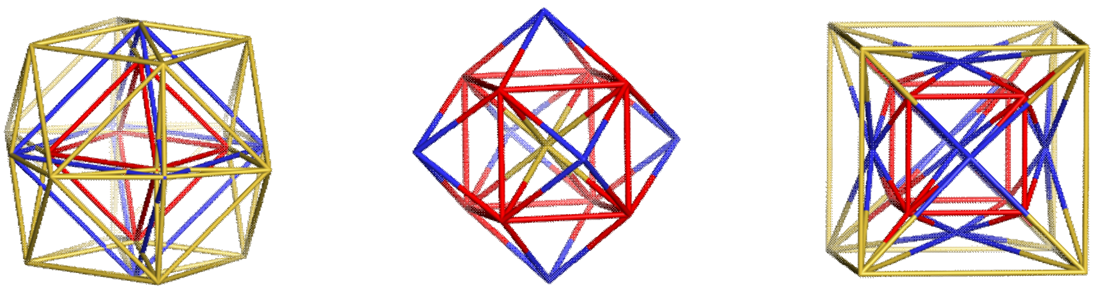
3. THE 24–CELL

The 24-cell (Figure 3, left) is a convex regular 4-polytope, also called "icositetrachoron", "octaplex", or polyoctahedron", as it consists of 24 octahedral cells, with six of them meeting at each vertex and three at each edge; its vertex figure is a cube. The 24-cell is the unique self-dual regular polytope, (of which dual is) neither a polygon nor a simplex; by this reason, it has no analogue in 3D.

The vertex figure at a given vertex comprises all the figures incident on that vertex; edges, faces, etc. A vertex figure of an n-polytope is an $(n-1)$-polytope (*e.g.*, the vertex figure of a 4-polytope is a 3-polytope, or a polyhedron) [14].

The first 8 vertices of 24-cell are the vertices of a regular 16-cell while the remaining 16 are the vertices of the dual 8-cell, or the tesseract, $Q_4.16$. This suggests the construction either by *rectification* of 16-cell (*i.e.*, *medial* *m*(16-cell)) or by *dualization* of 8-cell (*i.e.*, *d*(8-cell)). There are several 3D projections of 24-cell, of which envelopes are the rhombic dodecahedron Rh_{12}, cuboctahedron CO, hexagonal bi-antiprism, elongated hexagonal bipyramid or a tetrakis hexahedron (*i.e.*, stellated cube *st*(C) – Figure 3, middle).

Starting from the idea of MP^n clusters, and keeping in mind the projection of 24-cell with a *st*(C) envelope, a construction of 24-cell as all-body-centered hypercube $Q_4.8CP^8.24$ is proposed here, by joining eight CP^8 units (Figure 3, right). In our best knowledge, this construction was not yet reported in literature.



24-Cell.24 Cuboctahedron orthogonal projection

$st(CP^8).15$

$Q_4.8CP^8.24$

Figure 3. 24-Cell appearance.

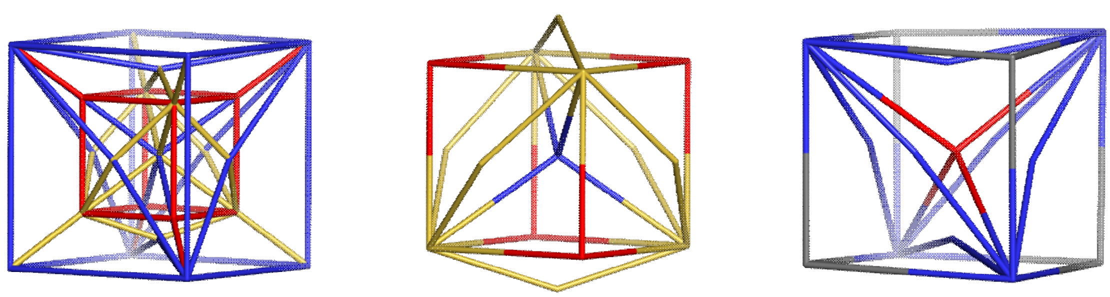
The figure count and topology sequence for $Q_4.8CP^8.24$ are given in Tables 1 and 2, respectively. As can be seen, both CP^8 and $Q_4.8CP^8.24$ have the rank k = 4. There is a single class of vertices in 24-cell, thus a single sequence of connectivity (provided by the layer matrix of connectivity LC) and rings around vertices (in terms of layer of rings LR) will fully describe its topology [15,16]. Omega polynomial [17,18] Ω = 96X^1 shows that there are 96 f_3 (*i.e.*, triangles), counted as non-topologically parallel 96 edges. It means that 24-cell is not a Rhombellane (cf. Proposition).

Table 1. Figure count in Q_4 related structures.

Polytope	v	e	f_3	f_4	f_6	2	$K_{2.3}$	$K_{2.4}$	Ada(Py_4)	3	4	χ	k
CP^8	9	20	12	6	0	18	0	0	(6)	7	-	0	4
$Q_4.8CP^8$	24	96	96	0	0	96	0	0	0	24	-	0	4
CP^4	9	16	0	18	0	18	10	0	0	11	-	0	4
$Q_4.8CP^4$	24	64	0	120	8	128	80	12	2	94	8	2	5

4. A RHOMBELLANIC HYPERCUBE RELATIVE

By deleting, in an alternating manner, four edges incident at each central point in Q_4.8CP^8.24 it results in a new structure, Q_4.8CP^4.24 (Figure 4), which is a rhombellane relative of the hypercube Q_4 (see below). The repeating unit is now CP^4.9, a 4-polytope (k = 4, see Table 1); it consists of ten simplest rhombellanes $K_{2.3}$. There are eight CP^4 facets (of rank k = 4) binding Q_4.8CP^4.24; each pair of CP^4 facets shares a facet of rank k = 3, namely the rhombellane $K_{2.4}$; thus, Q_4.8CP^4.24 is a 5-polytope (k = 5). In the figure count, two adamantine *ada* units (k = 3) and eight hexagons f_6 were considered (Figure 4, middle and right); adamantane is not a polyhedron but a tile [19], similar to rhombellanes, from which it originates. Sequences of Q_4.8CP^4.24 topology are given in Table 2. There are two vertex classes, of degree 4 {16} and 8 {8}, respectively. Omega polynomial consists of a single term, Ω = 1X^64, saying that the edges of Q_4.8CP^4.24 are all topologically parallel and thus the structure is a rhombellane. The vertex classes have all non-connected points (as a bipartite structure), an additional proof supporting the rhombellanic nature of this structure of higher rank. About centrality, counted by our centrality index [15], the 16 points class appears lying more central (C=0.1256396237) than the remaining 8 vertices (C= 0.1203238919). Computations have been done by our Nano-Studio software program [20].



Q_4.8CP^4.24 Ada.CP^4.15 (inside) Ada.CP^4.15 (outside)

Figure 4. A rhombellanic hypercube Q_4 relative (left); details of its inside (middle) and outside (right).

Table 2. Sequence of connectivity (LC) and rings around vertex (LR) in all-centered 8-Cell (Tesseract) Q_4.8CP^n.24.

Polytope	LC	LR	Ω	Degree	Rings
Q_4.8CP^8.24					
24 ×	1 - 8 - 14 - 1	12 - 96 - 168 - 12	96X^1	8	3^12
Q_4.8CP^4.24					
16 ×	1 - 4 - 14 - 4 – 1	18 - 144 - 252 - 144 – 18	1X^64	4	4^18
8 ×	1 - 8 - 6 - 8 - 1	36 - 144 - 216 - 144 - 36		8	4^36

5. CONCLUSION

The smallest rhombellane, [1,1,1]propellane, is a real chemical molecule; its associate graph is the complete bipartite graph, $K_{2.3}$. Generalized rhombellanes are designed by Diudea's rhombellation procedure. Rhombellanes have all the edges topologically parallel, as shown by the single term in Omega polynomial (further involving Hamiltonian circuits visiting their edges). Rhombellanes consist of at least one $K_{2.3}$ subgraph.

A new building way for the 4-polytope, 24-cell, from all-P^8 body centered hypercube Q_4 was proposed. Its P^4 analogue, $Q_4.8CP^4.24$, is a 5-polytope.

Structure representation in terms of small rhombellanes brings more structural insight and may unveil relations among structures apparently not related. Rhombellanes represent a new class of structures, with interesting properties, both in theory and applications.

ACKNOWLEDGMENT. Computer support from Dr. Csaba Nagy is highly acknowledged.

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