

# Hyper-structural Ethers

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**Abstract.** Rhombellanes represent a new structural class, of which functionalized derivatives may be synthesized as real molecules. Several hypothetical structures/molecules were proposed: their topology, energetics, and pharmaceutical properties have been computed. Drug-like properties of some of the proposed molecular structures were compared with existing nano-molecules. Among the designed polymeric networks, the etheric ones represent a promise for the material science and technology.

**Keywords:** *cube, rhombellane, rank, rod-like polymer, triple periodic polymer, ether.*

## 1. Introduction

Crystal engineering and self-assembly processes have recently promoted new classes of finite and/or periodic nanostructures, with promising applications in material science and biosciences [1–7]. Several nano-sized spheroid architectures, based on Platonic and Archimedean solids have been synthesized. A variety of appropriate (as angles and bond length) ligands have been used in such syntheses. As metals to join the ligands, the most used was Pd<sup>2+</sup> [3–6], then Zn<sup>2+</sup> [7] or Cu<sup>2+</sup> [8]. The single-shell spherical structures, possessing large hollows, could be functionalized, both endo- and/or exohedrally. A self-assembled double-shell structure, a sphere-in-sphere, molecular "Russian doll", was also reported [9].

Rhombellanes are structures with all strong rings rhombs/squares, some of them forming local propellane substructures; they have been proposed by Diudea in 2017 [10]. Propellane is an organic molecule, first synthesized in 1982 [11]; by IUPAC nomenclature, it is named tricyclo[1.1.1.0<sup>1,3</sup>]pentane, a hydrocarbon with formula C<sub>5</sub>H<sub>6</sub>. Its reduced form, C<sub>5</sub>H<sub>8</sub>, eventually named bicyclo[1.1.1]pentane, has only rhomb/square rings; it can be represented as K<sub>2,3</sub> - the complete bipartite graph. The two bridge carbon atoms can be functionalized, e.g., by bromine or COOH, or even by repeating the K<sub>2,3</sub> motif, as in the staffane polymer [12,13].

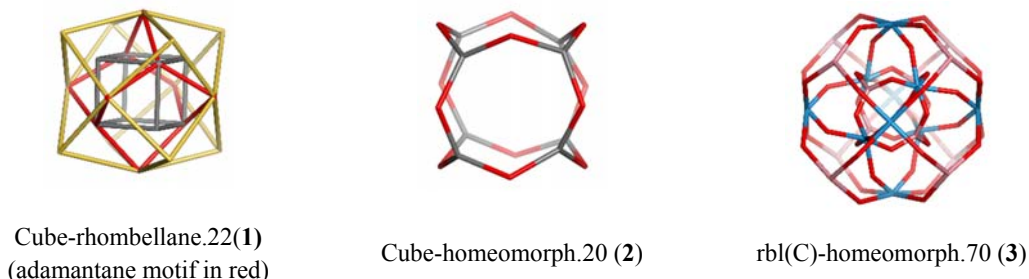
For general surfaces, Euler [14] characteristic  $\chi$  can be calculated as an alternating sum of figures of rank k [15-17]:

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

A structure is a rhombellane if all the five conditions are obeyed [18-22]: (1) All strong rings are squares/rhombs; (2) Vertex classes consist of all non-connected vertices; (3) Omega polynomial has a single term:  $1X^{|E|}$ ; (4) Line graph of the original graph shows a Hamiltonian circuit; (5) Structure contains at least one smallest rhombellane rbl.5.

Omega polynomial  $\Omega(x)$  was defined by Diudea (2006) [23,24] on the ground of opposite edge strips *ops* in the graph:  $\Omega(x) = \sum_s m_s x^s$ . Its first derivative (in  $x = 1$ ) counts the number of edges "e" in a graph:  $\Omega'(1) = \sum_s s m_s = |E(G) = e|$ . There are graphs with a single ops, which is a Hamiltonian circuit of their line-graphs. For such graphs, Omega polynomial has a single term:  $\Omega(x) = 1X^e$ .

The smallest rhombellane, rbl.5, is the complete bipartite  $K_{2,3}$  graph; any  $K_{2,n}$  graph fulfils the five above conditions for rhombellanes. Any  $K_{2,n}$  graph contains  $n(n-1)(n-2)/6$  smallest units  $\text{rbl.5} = K_{2,3}$ . There are graphs with more than two vertex classes obeying the above conditions, namely those designed by the rhombellation operation.



**Figure 1.** Cube-rhombellane and its related homeomorphs.

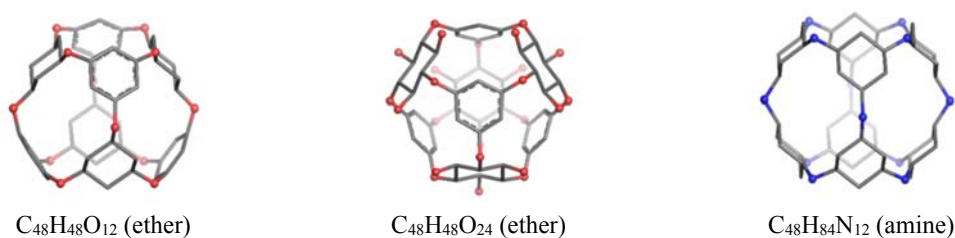
Construction of the cube-rhombellane **1** is illustrated in Fig. 1. Each square face forms a  $K_{2,3}$  rhombellane by joining the opposite corners with homeomorphic diagonals, which join together in an adamantane motif (in red).

A homeomorph of a graph contains on each parent edge one (or more) point(s) of degree two, e.g., the cube homeomorph **2** (Fig. 1, middle). The structure **3** (Fig. 1, right), which is the homeomorph of **1**, has seventy points/atoms; the vertex connectivity in **3** is 6; 3 and 2, respectively.

The paper is a short review of the most important results of the Topo Group Cluj in the new field of rhombellanes.

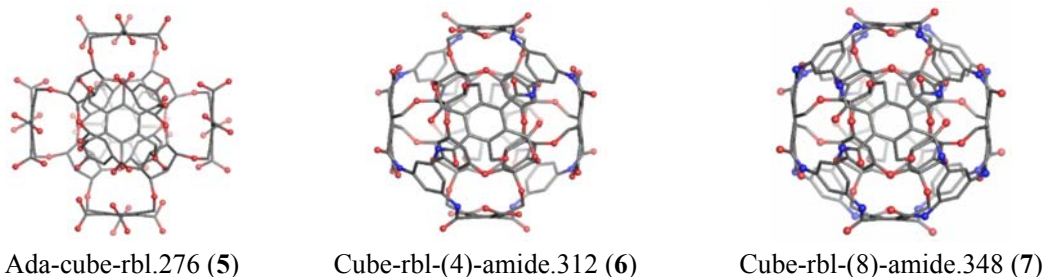
## 2. Cube-rhombellanes

To synthesize **3** as a molecule, we proposed to start from 1,2,3,4,5,6-Hexahydroxy-cyclohexane, that may form an ether **4** (also can be an amine) (Fig. 2), which is a (hyper) homeomorph of the cube **2** and the “core” of rbl(C)-homeomorph **3**; the vertices of connectivity 6 may be the hexahydroxy-cyclohexane while the three-connected points the 1,3,5-trihydroxycyclohexane or its derivatives (e.g., 1,3,5-trihydroxybenzene, etc.) [22,25].



**Figure 2.** Cube-rbl-core (**4**) structures.

Synthesis of Platonic or Archimedean polyhedral clusters by chemical fragments, with metallic ions complexing suitable ligands was already experimented [1-9, 26-28]. For cubane and related structures see refs. [29–31].

**Figure 3.** Cube-rhombellanes.

The structures of interest in this section are listed in Table 1. The cube-rhombellane homeomorphs are named as: Cube-rbl-(a.b.c.d)-amide/ester, where the a.b.c.d bits represent: hexa-connected unit, *tri*-connected unit, connection to the second shell and the *tri*-connected units in the second/external shell, respectively. Structures were designed (and computed by our original Nano Studio software [32]) with the aim of envisaging the plethora of cube-rhombellane substructures, all possible to be functionalized and synthesized.

Cube-rbl-amide,7:(6(6).B(3).Mt(2).8BMt(3)).420, (Table 1, entry 1) is a double shell cluster with eight three-connected units in the second shell; a structure of type “7” is shown in Fig. 3 (right). The other structures represent subgraphs/substructures of the double shell clusters, of type “7”.

Full geometry optimization for some representative structures were performed at B3LYP/6–31G (d, p) level of theory [25,33]. Harmonic vibrational frequencies confirmed that a true stationary point has been obtained. Computational results show for the investigated compounds a good stability, attributed on the rather large HOMO–LUMO energy gaps. The binding energy, expressed as the difference between the total energy of the structure and the energies of the constituent atoms, shows that all the concerned compounds are energetically feasible.

Molecular mechanics (MMFF94, [34]) were utilized in order to explore the internal molecular mobility, accessed in the bioactivity study of these compounds. Among the pharmaceutical important parameters, the following were checked.

**Table 1.** Cube-rhombellanes: structure; n = no. atoms; type.

	Structure	n	C	H	N	O	Type I	Type II
1	C-rbl	420	192	156	24	48	Ether; Amide	7:(6(6).B(3).Mt(2).8BMt(3))
2	Env (420)	288	132	108	24	24	Amide	8:(0.0.0.8BMt(3))
3	Env (420)	336	144	132	24	36	Amide	8:(0.0. Mt(2-OH).8BMt(3))
4	Core	120	48	48	0	24	Ether	4:(6(6).B(3).0.0)
5	Core	108	48	48	0	12	Ether	4:(6(3).B(3).0.0)
6	Core	132	60	60	0	12	Ether	4:(6(3).6(3).0.0)
7	C-rbl (4)	264	132	84	0	48	Ether; Ester	6:((6(6).Mt(2).4B(3))
8	C-rbl (4)	300	144	84	0	72	Ether; Ester	6:((6(6).Mt(2-COOH).4B(3))
9	Ada-C-rbl	276	120	84	0	72	Ether	5:(6(6).B(3).Mt(2).0)
10	C-rbl	348	168	108	24	48	Ether; Amide	7:(6(6).B(3).Mt(2).8B(3))
11	Env (348)	264	120	84	24	36	Amide	8:(0.0.0.8B(3))
12	C-rbl	444	192	180	24	48	Ether; Amide	7:(6(6).6(3).Mt(2).8BMt(3))
13	C-rbl	456	156	192	24	84	Ether; Amide	7:(6(6).6(6).Mt(2).8BMt(3))

Env = envelope; B = benzene; Mt = methylene; (cn) = fragment connectivity.

Globularity (the state of being globular [35]) was computed in comparison with that of fullerene  $C_{70}$ . ADME properties evaluation was performed using QikProp [34] module included in Schrodinger software. A series of descriptors related to bioactivity and drug-ability of these compounds were computed. Retrosynthetic Combinatorial Analysis (RECAP) [36] was performed using a Knime workflow (RetroPath2.0).

An active compound is a collection of molecular fragments according to fragment-based drug design principles. These fragments possess a specific three-dimensional arrangement that defines the whole properties of the compound: geometric, steric, conformational, topological, electronic and physicochemical properties define key aspects of bioactivity. By the medicinal chemistry point of view, these properties define the therapeutic, metabolic and toxic properties.

### 3. Rod-like polymers

By analogy to [1.1.1]propellane [11] and staffanes  $[n]$ stf [12,13,31] (Fig. 4, left), a linear rod-like poly-ether  $[n]$ hhc we designed (Fig. 4, right) [37]. Note that, to make the rod-poly-ether, the 1,2,3,4,5,6-Hexahydro-cyclohexane must be in the conformation all-axial.



**Figure 4.** Rod-like polymers.

This analogy was already exploited [13] in the synthesis of a linear (“zig-zag”) polymer of which building block is 1,3-dehydro-adamantane (Fig. 5, left - named here  $[3]$ dhada).



**Figure 5.** Adamantane derivatives.

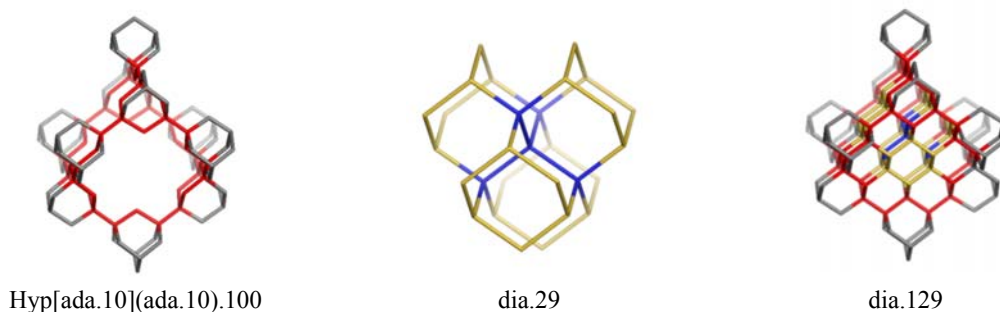
Adamantane ada.10 molecule was discovered by Landa (a Czech chemist) in 1933 in petrol [38]. Dehydro-adamantane dhada.10 (Fig. 5, middle) is obtained by eliminating the two bromine atoms from 1,3-dibromo-adamantane (Fig. 5, right). The number suffixing the structure names counts the heavy atoms in the molecule.

The adamantane ada.10 is named tricyclo[3.3.1.1<sup>3,7</sup>]decane, by IUPAC nomenclature [39]; in hyper-adamantane all atoms are changed by the classical adamantane, ada.10.

### 4. Triple-periodic polymers

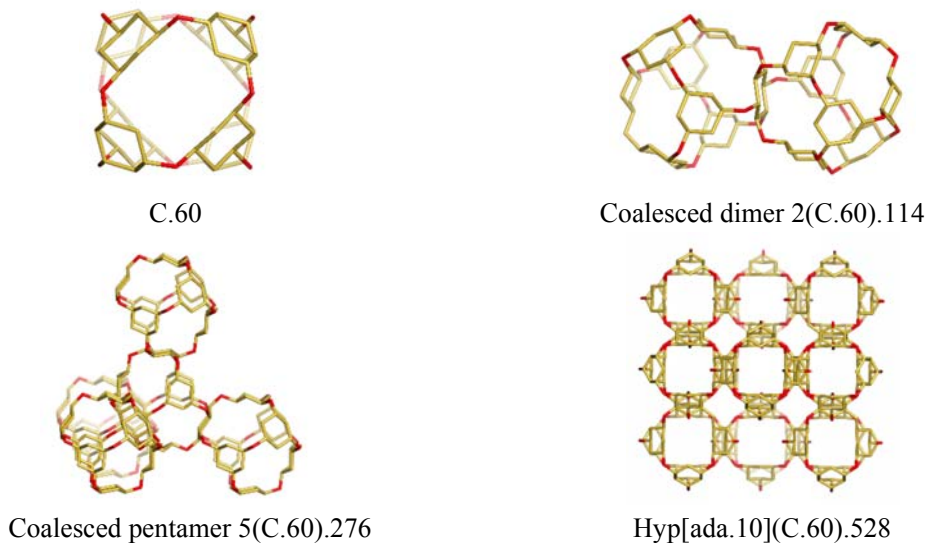
By eliminating the four bromine atoms in tetraboromo-adamantane, is conceivable to undergo a 3D-polymerization, to provide a triple-periodic crystal network [37], named *dia(s)-net*, (space group  $Fd-3m$ ). This “spongy” net has the building block a hyper-adamantane tile, Hyp[ada.10](ada.10).100

and can be embedded in the classical diamond-net (Fig. 6). Topological data for this diamondoid hydrocarbon is given in Table 2.



**Figure 6.** Adamantane derivatives.

When 1,2,3,4,5,6-Hexahydroxy-cyclohexane is in the all-equatorial conformation, it is possible to polymerize along the three Cartesian coordinates [40]; the repeating unit is a hyper-adamantane Hyp[ada.10](C.156).1270 (consisting in etheric cuboids C.156, formally derived from the hexahydroxy-cyclohexane, *hhc*). The suffixing numbers include here both the cyclohexane substituents and hydrogen atoms; for the sake of simplicity, these are further omitted, e.g., Hyp[ada.10](C.156).1270 becomes Hyp[ada.10](C.60).528 (Fig. 7) [40].



**Figure 7.** Etheric hyper-adamantane (right-bottom) and some of its cuboid substructures.

Hyper-adamantanes are structures of rank ( $k$ )/space dimensionality 5 (Table 2); each hyper-hexagonal facet is of rank 4 while the building cells are of rank 3. It is expected that, the network, formed by translating along the  $xyz$ -coordinates, to have the rank  $5+1$ , thus demonstrating the complexity (see ref. [41]) of the surrounding matter, either natural or artificial.

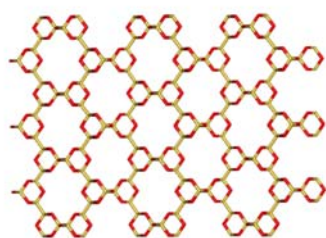
**Table 2.** Topology of hyper-adamantane clusters.

	Hyp[ada.10](0).n	v	e	r <sub>4</sub>	r <sub>6</sub>	r <sub>16</sub>	f <sub>2</sub>	f <sub>3</sub>	f <sub>4</sub>	χ	k
1	ada.10	10	12	0	4	0	4	0	0	2	3
1.1	(ada.10).60	60	78	0	24	0	24	6	0	0	4
1.1	(ada.10).100	100	132	0	40	0	40	10	4	2	5
1.3	(ada.1.10).54	54	72	0	24	0	24	6	0	0	4
1.4	(ada.1.10).88	88	120	0	40	0	40	10	4	2	5
2	C.60	60	72	0	8	6	14	0	0	2	3
2.1	(C.60).324	324	396	0	42	36	78	6	0	0	4
2.2	(C.60).528	528	648	0	68	60	128	10	4	2	5

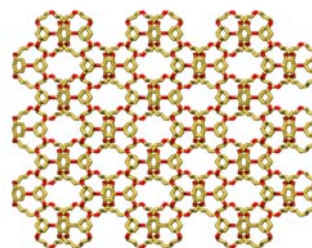
**Table 3.** Triple periodic network: unit/tile; vertex connectivity classes; ring domain; population; degree; point symbol; LM sequence: connectivity (LC) and atom surrounding rings (LR).

Class	Network and vertex classes	LM
1	<b>Hyp[ada.10](ada.10) - net</b>	T <sub>1</sub> : (Hyp[ada.10](ada.10)).100; (v = 100; e = 132; r <sub>6</sub> = 40; r <sub>18</sub> = 4). ada.10 (v = 10; e = 12; r <sub>6</sub> = 4; r <sub>8</sub> = 3)
1.1	(6.6); {60};   deg = 2   6 <sup>2</sup> (6.18); {60};   deg = 2   6 <sup>2</sup> .8 <sup>2</sup> .18 <sup>2</sup>	LC: {60}; 2.6.8.9.18.24.30.54.70.74. LR(4.4); {60}; 2.6.14.18.26.42.54.84.126.158.204. LR(4.12); {60}; 6.24.48.60.102.144.180.324.432.528.780.
1.2	(6.6); {40};   deg = 4   6 <sup>3</sup> (6.18); {40};   deg = 4   6 <sup>3</sup> .8 <sup>3</sup> .18 <sup>6</sup>	LC: {40}; 4.6.9.15.18.27.45.54.75.105. LR(4.4); {40}; 3.9.15.24.33.45.72.99.135.198.231. LR(4.12); {40}; 12.30.54.90.108.162.270.324.486.738.756.
2	<b>Hyp[ada.10](C.60) - net</b>	T <sub>1</sub> : (Hyp[ada.10](C.60)); (v = 528; e = 648; r <sub>6</sub> = 68; r <sub>16</sub> = 60). C.60 (v = 60; e = 72; r <sub>6</sub> = 8; r <sub>16</sub> = 6).
2.1	(6.16); {120}; deg = 2; 16 <sup>2</sup> .	LC: {120}; 2.4.3.5.9.12.18.22.26.22. LR: {120}; 2.6.8.11.18.28.36.44.58.57.69.
2.2	(6.16); {120}; deg = 2; 6.16.	LC: {120}; 2.4.6.8.9.13.20.20.24.28. LR: {120}; 2.7.12.18.20.24.39.52.58.68.82.
2.3	(6.16); {120}; deg = 3; 6.16 <sup>2</sup> .	LC: {120}; 3.3.5.6.9.15.19.24.23.29. LR: {120}; 3.6.10.14.20.30.40.51.54.66.77.
2.4	(6.16); {168}; deg = 3; 6.16 <sup>3</sup> .	LC: {168}; 3.5.7.9.12.14.16.20.23.28. LR: {168}; 4.10.15.18.22.29.36.50.66.70.71.

Topology of the polymeric structures (Fig. 8) is characterized by sequences of connectivity (LC) and rings around vertex (LR) [42-45]. The LR matrix provided different values for different ring domains, e.g., for (r<sub>min</sub>-r<sub>min</sub>) (corresponding to the ring symbol) and (r<sub>min</sub>.r), r-being a chosen value; these values are listed with the LC and LR sequences (Table 3).



*dia(s)*-net (unit: Hyp[ada.10](ada.10).100)



Hyp[ada.10](C.60)-net (unit:  
Hyp[ada.10](C.60).528)

**Figure 8.** Polymeric hyper-diamondoids.

Finding the vertex (subgraph) classes in a graph is related to Topological Symmetry; they are calculated as centrality classes, by using the Centrality index,  $C$ , developed at Topo Group Cluj. It is calculated on layer/shell matrices, as:

$$C(\text{LM} \setminus \text{ShM})_i = \left[ \sum_{k=1}^{\text{ecc}_i} \left( [\text{LM} \setminus \text{ShM}]_{ik}^{2k} \right)^{1/(\text{ecc}_i)^2} \right]^{-1}; \quad C(\text{LM} \setminus \text{ShM}) = \sum_i C(\text{LM} \setminus \text{ShM})_i$$

This index allows to find the graph center and provides an ordering of vertices according to their centrality [41].

All topological data have been computed by Nano Studio software program [32].

## 5. Conclusions

Rhombellanes represent a new class of hypothetical structures, which may be synthesized as real molecules. Cube–rhombellane, in the first step of rhombellation operation, is a double–shell structure showing vertices of degree 3 and 6 respectively, which may be realized by means of cyclohexane (and/or benzene) derivatives. Some suggestions of molecular realization of cube–rhombellane as functionalized structures (ether core, ester or amide envelope) were given. Topology of the discussed structures was detailed. Quantum calculations (at the B3LYP/6-31G (d, p) level of theory) supported the hypothesis: both substructures (at every level of complexity) and the whole double–shell molecules proved to be energetically feasible in the hope of a real synthesis.

Rhombellanes seem to be appropriate and worthwhile molecules for medicinal chemistry. This new class of compounds may be an alternative to classical nano–structures regarding carrier, drug like properties and use for creating bio–nano devices. Drug-like properties of the proposed molecular structures were compared with some existing nano-molecules (fullerenes, nanotubes). Substructures of the proposed molecules, useful in a future synthesis, were provided by retro combinatorial synthesis (RECAP). The results are promising, regarding ADME properties, drug-likeness and nano-properties. In contrast to fullerenes and nanotubules, rhombellanes present a variety of distinct derivatization sites thus making them easier to be chemically manipulated.

With respect to material science and technology, several new crystal-type networks have been designed and their topology detailed. The most important nets are the hydrocarbon “spongy” diamondoid and the etheric hyper-diamondoid nets. The future synthesis of rhombellanes and their networks is of particular interest.

Topology of the polymeric structures was characterized by sequences of connectivity (LC) and rings around vertex (LR), the last one sequence being an original development of our Nano-Studio software program.

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