Rhombellanes and Quasi-Rhombellanes

Mircea V. Diudea

Department of Chemistry, Faculty of Chemistry and Chemical Engineering,
Babes-Bolyai University, Arany Janos Str. 11, 400028 Cluj, Romania
diudea@gmail.com

Abstract. Rhombellanes are mathematical structures, proposed in 2017; they may appear both in periodic crystals or in finite structures. The simplest rhombellane is *rbl*.5 or the $K_{2.3}$ complete bipartite graph. In this paper, rhombellane-like structures are introduced, as an extension of rhombellanic properties. The structural criteria are discussed in terms of molecular topology and examples are given.

Keywords*:* *rhombellane; adamantane; tile, Omega polynomial, 4D structure.*

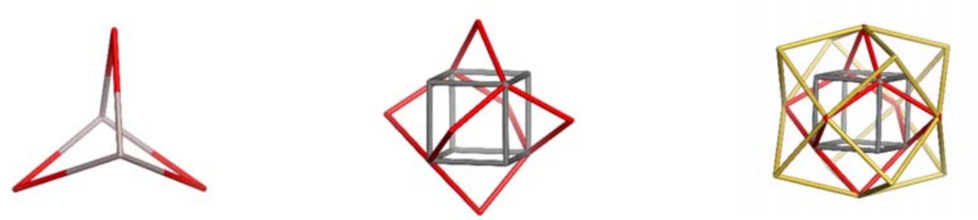
1. Introduction

Rhombellanes are structures consisting of rhomb/square rings, sometimes forming local propellane substructures, introduced by us in 2017 [1].

Propellane is a hydrocarbon with formula C_5H_6, first synthesized in 1982 [2]; its molecule consists of triangle/R_3 rings, realized by inversing the sp^3 carbon atoms of its poles. Propellane reduces to C_5H_8, with only square/R_4 rings; it is the smallest rhombellane, rbl.5 or $K_{2,3}$ - the complete bipartite graph, of which two bridge carbon atoms can be included in the polymer called staffane [3].

A rhombellane was defined by Diudea [4,5] as the structure with: (1) All strong rings being squares/rhombs; (2) Vertex classes consisting of all non-connected vertices; (3) Omega polynomial having a single term: $1X^{|E(G)|}$; (4) Line graph of the parent graph showing a Hamiltonian circuit, HC; (5) At least one rbl.5, the smallest rhombellane.

The design of rhombellanes (Fig. 1) is achieved by the *rhombellation rbl* operation on maps, as shown elsewhere [5-7]. The rhombellane rbl.5/$K_{2,3}$ and its congeners, $K_{2.n}$, may be considered the first step in construction of rhombellanes. Any $K_{2.n}$ graph consists of $n(n-1)(n-2)/6$ $K_{2.3}$/ rbl.5 units. Any $K_{2.n}$ has all rings R_4 and all edges topologically parallel (see below); equivalently, it has Omega polynomial single term: 1X^*e*; *e*=|E(G)|, and, consequently, has a Hamiltonian circuit of its line graph; its vertices are bipartite and non-connected within a class. Thus, $K_{2.n}$ are precisely rhombellanes, fulfilling the above five criteria. The rhombellane of Cube C includes the adamantane ada.10 motif (Fig. 1, middle and right).



$K_{2.3}$= rbl.5 *rbl*(Cube).14 *rbl*(Cube).22

Figure 1. Rhombellane basic structures.

The smallest units, rhombellane rbl.5 and ada.10 hexellane (see below) are not polyhedra, cf. Steinitz theorem [8] but tiles [9]. A tile can be defined, in any rank/dimension, by the following propositions:

i. An n-polytope is bound by facets of rank n-1, f_{n-1}.
ii. The graph of any convex n-polytope is n-connected (Balinski, 1961 [10]).
iii. A subgraph of an n-polytope, having at least one vertex of deg=n-2, is a tile, t_{n-1}.

Thus, a tile is rather a quasi (not entirely) n-polytope; however, in the Euler's alternating sum (see below), a tile t_{n-k} is counted as an f_{n-k} facet.

Omega polynomial [11-13] $\Omega(x)$ was defined by Diudea (2006) on the ground of opposite edge strips *ops* in the graph. Denoting by m, the number of *ops* of length $s=|S|$, then one can write: $\Omega(x) = \Sigma_s m_s X^s$. Its first derivative (in x = 1) counts the number of edges "e" in a graph: $\Omega`(1) = \Sigma_s sm_s = |E(G) = e|$. There are graphs with a single opposite edge stripe, which is a Hamiltonian circuit. For such graphs, Omega polynomial has a single term: $\Omega(x) = 1X^s$; $s = e = |E(G)|$.

Finding vertex (subgraph) classes in a graph is related to Topological Symmetry. The vertex classes in the concerned structures will be calculated as centrality classes, by using the Centrality index, C, developed at Topo Group Cluj [14]. It is calculated on layer/shell matrices [15,16], as:

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

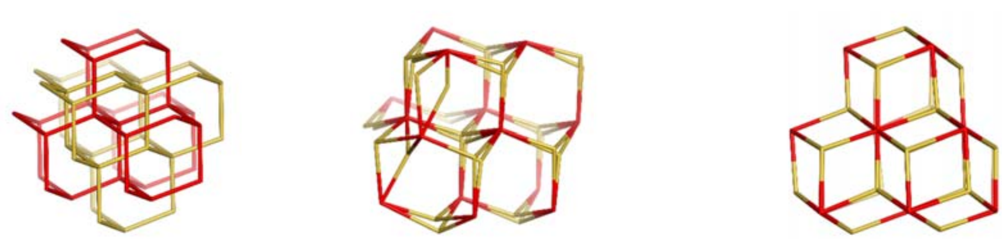
This index allows to find the graph center (*e.g.* the vertex having the largest C_i value) and provides an ordering of graph vertices according to their centrality [17].

2. Results

2.1. Diamondoid crystal networks

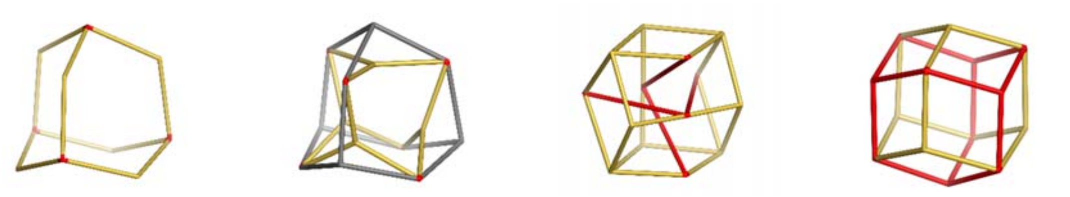
Diamond, *dia*, is the entanglement of *dia* & dual-*dia* (self-dual) within the cubic crystal system. Diamond rhombellane [18], *drb*, has a *dia* & *dia* entanglement, with identification six superposed atoms. Fluorite, CaF_2, *flu*, entangles *dia* & *dia*-(rot 90^o) [5] with identification of six superposed atoms (Fig. 2).

The three above networks are single tile type space filling by: *ada*.10, *arb*.14 and *flu*.14 units/tiles. The first net is uninodal while the last two are binodal; they can be represented as a sequence of vertices v, edges e, faces f, tiles t [19], in a space group: *dia* (1.1.1.**1**; *Fd-3m*), *drb* (2.1.2.**1**; *Fd-3m*) and *flu* (2.1.1.**1**; *Fm-3m*). Adamantane *ada*.10 is named tricyclo[3.3.1.1$^{3.7}$]decane, by IUPAC nomenclature [20]. The relatedness of the three nets is based on the ada.10 unit and construction, that's why are here called diamondoid networks. Fig. 3 illustrates the three corresponding units above.



Diamond dia (*Fd-3m*) *Diamond rhombellane drb* (*Fd-3m*) *Fluorite flu* (*Fm-3m*)

Figure 2. Diamondoids: crystal networks related to *dia*-net.



ada.10 *arb*.14 *arr*(*flu*.14) = *arb*.14 *flu*.14

Figure 3. Adamantoids: units related to ada.10

The unit *arb*.14 resulted by a re-arrangement of the twelve rhombs of *flu*.14 = Rh_{12}.14, (i.e., Rhombic dodecahedron) to: $arr(flu.14) = (2R_6 \|) \perp (2R_6 \|) \& 4R_4 = arb.14$. Two adjacent rhombs will form a hexagon by deleting the common edge; there will be two pairs of hexagons, disposed about orthogonal to each other; in a pair, the two hexagons share two edges; the four remaining rhombs lye in a stripe surrounding the two pairs of hexagons and share a vertex with the subsequent rhomb; the four broken edges are pairwise connected inside, to the opposite 2-connected points shared by the hexagon pairs, that become 4-connected (Fig. 3).

The three above networks are characterized by the sequence of connectivity (LC) (Table 1) and atom ring surrounding (LR) (Table 2); R_m8 counts the rings associated to ada.10 unit.

Table 1. Diamondoids**:** crystal network; unit/tile; connectivity (LC).

Net; tile	Connectivity (LC).
dia; ada.10	
v = 10; deg = 4	4 - 12 - 24 - 42 - 64 - 92 - 124 - 162 - 204 – 252 = 980
drb; arb.14	
v = 8; deg = 4	4 - 25 - 24 - 84 - 64 - 184 - 124 - 324 - 204 - 504 = 1541
v = 6; deg = 8	8 - 12 - 48 - 42 - 128 - 92 - 248 - 162 - 408 - 252 = 1400
flu; flu.14	
v = 8; deg = 4	4 - 22 - 24 - 82 - 64 - 182 - 124 - 322 - 204 – 502 = 1530
v = 6; deg = 8	8 - 12 - 48 - 42 - 128 - 92 - 248 - 162 - 408 – 252 = 1400

Table 2. Diamondoids: crystal network; tile/unit; atom ring surrounding (LR); (Rm= max. ring size counted).

Net; tile (R_m)	Rings (LR).
dia; ada.10 (R_m6)	
v = 10; deg = 4; 6^12	12 - 48 - 144 - 288 - 504 - 768 - 1104 - 1488 - 1944 - 2448 = 8748
ada.10 (R_m8)	
v = 10; deg = 4; 6^12.8^24	36 - 144 - 432 - 864 - 1512 - 2304 - 3312 - 4464 - 5832 - 7344 = 26244
drb; arb.14 (R_m6)	
v = 8; deg = 4; 4^6.6^48	54 - 432 - 1350 - 2592 - 4536 - 6912 - 9936 - 13392 - 17496 - 22032 = 78732
v = 6; deg = 8; 4^12.6^96	108 - 432 - 1296 - 2592 - 4536 - 6912 - 9936 - 13392 - 17496 - 22032 = 78728
arb.14 (R_m8)	
v = 8; deg = 4; 4^6.6^48.8^192	246 - 1968 - 6150 - 11808 - 20664 - 31488 - 45264 - 61008 - 79704 - 100368 = 358668
v = 6; deg = 8; 4^12.6^96.8^384	492 - 1968 - 5904 - 11808 - 20664 - 31488 - 45264 - 61008 - 79704 - 100368 = 358668
flu; flu.14; (R_m4)	
v = 8; deg = 4; 4^6	6 - 48 - 132 - 288 - 492 - 768 - 1092 - 1488 - 1932 – 2448 = 8694
v = 6; deg = 8; 4^12	12 - 48 - 144 - 288 - 504 - 768 - 1104 - 1488 - 1944 – 2448 = 8748

Also, *arb*.14 has its dual *d*(*arb*.14) = $K_{2.4}$ []: each of the four *rbl*.5 of *arb*.14 shares a face with the two ada.10 (sharing six points but no faces); thus, there are two points of deg=4 connected via four points of deg=2, i.e., $K_{2.4}$. Table 3 lists some formulas for the topology of the three diamondoid nets.

Table 3. Topology of three *diamondoid* nets (*n* = no. of units).

#	Subject	Formula
	dia net	$v(n)=2n^3+6n^2+6n$
		$e(n)=4n^3+9n^2+6n-1$
		$R_6(n)=4n^3+3n^2$
		$R_8(n)=12n^2-19n^2+13n-3$
		R_{min}=6; R_{max}=8; $\Omega(6.8)=1X^e$
	drb net	$v(n)=n(n+1)(6n+1)$
		$e(n)=8n^8(2n+1)$
		$R_4(n)=12n^3$
		$R_6(n)=32n(2n^2-2n+1)$
		$R_8(n)=8(88n+2n(n+1)(12n-31)-6)$ $K_{2.3}(n)=4n^2(2n-1)$ R_{min}=4; R_{max}=6; $\Omega(4.6)=1X^e$
	flu net	$v(n)=n(6n^2+7n+1)$ $e(n)=8n^2(2n+1)$ $R_4(n)=2n(6n^2-n+1)$
		$R_8(n)=18(2n^3-2n^2+3n-1)$
		R_{min}=4; R_{max}=8; $\Omega(4.8)=1X^e$

2.2. Adamantoid Hyper-structures

Hyper-structures corresponding to the three above small units are: ada(ada).100, arb(ada).140 and flu(ada).140, respectively (Fig. 4).

ada(ada).100 arb(ada).140 flu(ada).140

Figure 4. Adamantoids corresponding to *dia*, *drb* and *flu* networks, respectively.

Ring structure of the three adamantoids and their paterns is shown in Table 4.

The above adamantoids are structures in the 4-D space, as shown by the alternating sum of facets, of rank *k*, cf. Euler formula [21] for an oriented surface, S: $\chi(S)=f_0-f_1+f_2-f_3+..$); in case $k=3$, $\chi=2$; in case $k=4$, $\chi=0$, and so on (Table 5). Their parents belong to 3-D space, excepting arb.14 which is in 4-D (all its f_3-facets being tiles – see above).

Table 4. Rhombellane-like structures – rings, max rings and the smallest units.

#	Structure	R_4	R_6	R_8	R_{12}	R_{14}	R_{16}	R_{18}	R_{max}	rbl.5	ada.10
1	ada.10	0	4	3	0	0	0	0	**8**	0	1
2	ada(ada).100	0	40	30	0	0	0	4	**20**	0	10
3	arb.14	12	(8)32	48	0	0	0	0	**6**	4	2
4	drb(ada).140	0	56	42	12	96	384	992	**14**	0	14
5	flu.14	12	0	18	0	0	0	0	**8**	0	0
6	flu(ada).140	0	56	42	12	96	384	992	**14**	0	14

Table 5. Rhombellane-like structures – rank / space dimensionality.

Structure	v	e	R_4	R_6	R	rbl.5(ada.10)	M	f_3	χ	k
ada.10	10	12	0	4	4	0	0	0	2	3
arb.14	14	24	12	8	20	4+(2)	4	10	0	4
flu.14	14	24	12	0	12	0	0	0	2	3
Structure	v	e	R_6	$(R_{12})R_{18}$	R	**ada.10**	M	f_3	χ	k
ada(ada).100	100	132	40	4	44	10	2	12	0	4
drb(ada).140	140	192	56	(4)+8	68	14	2	16	0	4
flu(ada).140	140	192	56	(12)	68	14	2	16	0	4

The above results were obtained by numerical analysis of series of structures with increasing number of building blocks.

2.3. Spongy-diamond dia(s) crystal network

A hypothetical tetra-dehydro-adamantane tha.10 molecule (Fig. 5, right), obtainable by eliminating the four bromine atoms in tetrabromo-adamantane, is conceivable to undergo a 3D-polymerization, to provide a triple-periodic crystal network, the spongy-diamond, *dia(s)* [7]). In the real synthesis, a linear polymer, denoted here [*n*]dha.*m* (Fig. 5, left) was obtained from the dehidro-adamantane dha.10 (Fig. 5, middle) [22]. Table 6 lists the topological characterization of the *dia* and *dia*(*s*) networks.

[3]dha.30 oligomer　　dehydro-ada (dha.10)　　tetradehydro-ada (tha.10)

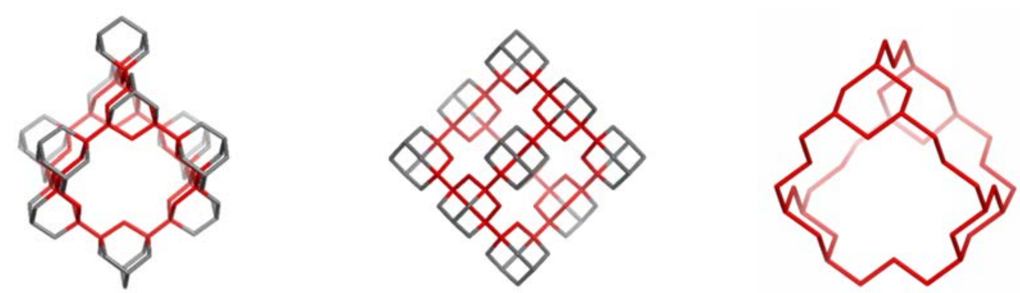
Figure 5. Adamantane derivatives.

Table 6. The *dia* and *dia*(*s*) netsworks: unit/tile; connectivity (LC) and atom surrounding rings (LR).

Net; **tile**	**Connectivity (LC).**
dia; ada.10	
v = 10; deg = 4	4. 12. 24. 42. 64. 92. 124. 162. 204. 252 = 980
dia(s); ada(ada).100	
v = 60; deg = 2	2. 6. 8. 9. 18. 24. 30. 54. 70. 74 = 295
v = 40; deg = 4	4. 6. 9. 15. 18. 27. 45. 54. 75. 105 = 358

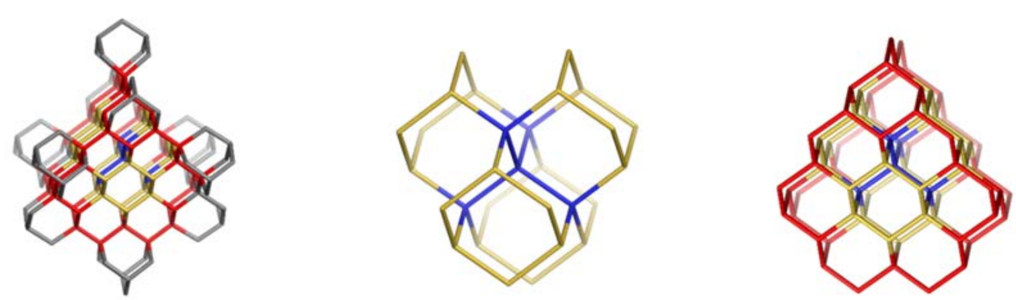
	Atom surrounding rings (LR).
dia; ada.10; (R_m6)	
v = 10; deg = 4; 6^12	12. 48. 144. 288. 504. 768. 1104. 1488. 1944. 2448 = 8748
ada.10 (R_m8)	
v = 10; deg = 4; 6^12.8^24	36. 144. 432. 864. 1512. 2304. 3312. 4464. 5832. 7344 = 26244
dia(s); ada(ada).100; (R_m18)	
v = 60; deg = 2; 6^2.8^2.18^2	6. 24. 48. 60. 102. 144. 180. 324. 432. 528. 780 = 2628
v = 40; deg = 4; 6^3.8^3.18^6	12. 30. 54. 90. 108. 162. 270. 324. 486. 738. 756 = 3138

The triple periodic spongy diamond [7], *dia(s)*, (space group *Fd-3m*), has the unit/building block ada(ada).100 (Fig. 4, left), a hyper-adamantane tile, in which all atoms of ada.10 are changed by ada.10). The unit has a tetrahedral symmetry, as the basic adamantane; *dia(s)*-net and its tiles (ada(ada).100 and its void, Fig. 6) can be perfectly embedded in the *dia*-net (space group *Fd-3m*), as shown in ada(dia).129 (Fig. 7); the missing part of *dia(s)*-net, dia.29 consists of four ada.10 units sharing a common (central) point (Fig. 7, middle, in blue). Thus, the spongy *dia(s)*-net is a kind of *dia*-net, with defects (namely dia.29) repeated at a distance of about 0.7.1 nm (to each-other), as shown in Fig. 8. The filled void(ada(dia).129).71 (Fig. 7, right) is a tetrahedral tile, with faces having six Ada-units (each shared by two faces) around a central ada.10 unit (i.e. dia.29, the core of four ada.10 units) and one ada.10 on each of the four corners, a total of twenty ada.10 units. The filled tile, ada(dia).129 (Fig 7, left) has additional ten ada.10, a total of 30 ada.10 units; by the number of atoms, the *dia(s)*-net has 0.775 = 100/129 of the density of *dia*-net. The Omega polynomial in *dia(s)* network shows $\Omega(6.20)=1X^e$, the net being a quasi-rhombellane.



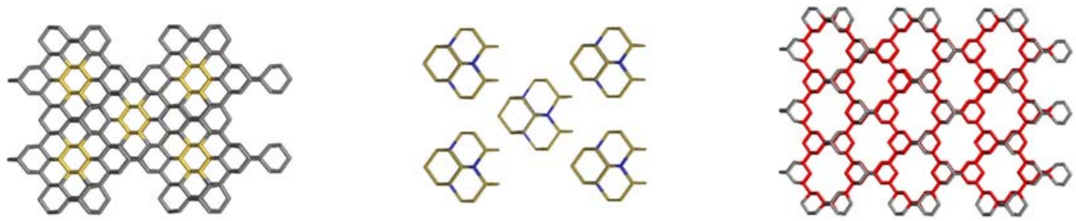
ada(ada).100 | ada(ada).100 (projection) | void(ada(ada).100).42

Figure 6. Unit ada(ada).100 and its void.



ada(dia).129 (#ada.10 = 30) | dia.29 (core) (#ada.10 = 4) | void(ada(dia).129).71 (#ada.10 = 20 = (4×6)/2+4+4)

Figure 7. Filled (by *dia*) ada(ada) unit (left), the missing core (middle) and its void (right).



dia(s) embedding in *dia* net   dia.29 defects in *dia*-net   *dia(s)* - net (empty of dia.29)

Figure 8. Embedding of *dia(s)* in *dia* net.

4. Discussion

Rhombellane criteria can be slightly relaxed to fit to some related structures, called here *quasi*-rhombellanes (Table 7), or rhombellane-like structures.

Table 7. Criteria for rhombellanes and quasi-rhombelanes.

	Rhombellanes	Quasi-rhombellanes
1	All strong rings are R_4	*Rings are R_4 and/or even-sized rings/circuits.*
2	Vertex classes are non-connected inside a class	Vertex classes are non-connected inside a class
3	Omega polynomial has (at $R_{max}4$) a single term: 1x^e	Omega polynomial has (at R_m) a single term: 1x^e
4	Line graph has a Hamiltonian circuit	Line graph has a Hamiltonian circuit
5	There exist smallest units/tiles rbl.5 = $K_{2.3}$	*There are more smallest tiles: rbl.5 = $K_{2.3}$ and/or ada.10, …*

One can see that the R_4-ring condition (1 – Table 7) can be extended to some larger strong rings (e.g., hexagons) or even-sized circuits. This ensures the existence of Omega polynomial single term (3-Table 7) calculated as $\Omega(R_{min}.R_{max})$= 1x^e; rule (3-Table 7) asks for rhombellanes, $\Omega(4.4)$= 1x^e while for quasi-rhombellanes $\Omega(4.R_{max})$= 1x^e. Actually, no rationalization for R_{max} was found but, in even ring/circuit containing structures, always exist a value for R_{max} so that 1x^e be a single term, with the consequence of existing a Hamiltonian circuit (4 – Table 7) for the corresponding line graph of that structure. Condition (2- Table 7) comes from the bipartity of rings/circuits of the smallest structures (that must be tiles not polyhedra), rbl.5 = $K_{2.3}$; ada.10,*..,etc.* (5 – Table 7). Examples of quasi-rhombellanes are given in Table 8, with the corresponding fulfilled criteria.

The three networks: *dia*, *drb* and *flu* show in their units R_{max}: 8;6;8; ada.10 (2 cls: 6(deg2); 4(deg3)); arb.14 (2 cls: 8(deg3); 6(deg4)); flu.14 (2 cls: 8(deg3); 6(deg4)); they have Hamiltonian circuits HC and non-connected classes. The smallest units are rbl.5 and/or ada.10, respectively, thus being quasi-rhombellanes (Table 8). The corresponding hyper-units: ada(ada).100 (9cls); drb(ada).140 (7 cls) and flu(ada).140 (7 cls) also show non-connected classes. The Omega polynomial shows a single term 1x^e, at R_{max}: 20;14;14, respectively, also being quasi-rhombellanes.

In calculating the above criteria (Table 7) Omega polynomial, at $R<R_{max}$ gives no HC; in case one needs to discriminate among structures with the same, this property may be exploited, e.g., arb(ada).140: $\Omega(6.12) = 4x^6+4x^{24}+1x^{72}$; $\Omega(6.14) = 1x^{192}$ and flu(ada).140: $\Omega(6.12) = 4x^6+1x^{72}+1x^{96}$; $\Omega(6.14) = 1x^{192}$), (see Table 8). At $R>R_{max}$, there is no change in 1x^e, since the larger circuits are linear combinations of the smaller rings.

Rhomb-decorated cells, $Rh_{2(n\times3)}$, are rhombellanes for *n*=odd (case (4.4)) while for *n*=even, these structures are quasi-rhombellanes (case (4.8)). These cages have two polar points, of degree n, repeating 3-times between the poles. As shown above, $K_{2.n}$ are all rhombellanes.

Some small graphs, like the hypercube *Qn*; *n*=3, 4 show no R_{max} and no Omega single term 1x^e; however, at $n > 4$, there exists R_{max}=10; also, some small structures have connected (inside) vertex classes, e.g., $Rh_{2(4\times2)}$, $Rh_{2(5\times4)}$, the Cube, etc., simply by the reason there is no room for large circuits

Bipartity appears in even-ring structures. It is not related to the topology of the concerned structures. Rhombellanes are *n*-partite structures, non-connected within a same class; the vertex classes are related to their topology. Vertex classes do not depend of Rmax; they are calculated at the smallest hard rings decorating a given structure.

Table 8. Quasi-rhombellanes – criteria; examples.

#	Structure	R_4 / R_6	Classes	Ω(G,x) (R_{min}.R_{max})	HC	rbl.5	ada.10
1	ada.10	R_6	2(Y)	4X^3 (6.6) 1X^12 (6.8)	N Y	0	1
2	ada(ada).100	R_6	9 (Y)	12X^1+40X^3 (6.6) 12X^1+10X^12 (6.8) 4X^3+1X^120 (6.18) 1X^132 (6.20)	N N N Y	0	10
3	arb.14	R_4 / R_6	2(Y)	4x^6 (4.4) 1X^24 (4.6)	N Y	4	2
4	arb(ada).140	R_6	7 (Y)	24X^1+56X^3 (6.6) 24X^1+14X^12 (6.8) 4X^6+4X^24+1X^72 (6.12) 1X^192 (6.14)	N N N Y	0	14
5	flu.14	R_4	2(Y)	4X^6 (4.4) 1X^24 (4.8)	N Y	0	0
6	flu(ada).140	R_6	7 (Y)	24X^1+56X^3 (6.6) 24X^1+14X^12 (6.8) $4x^6+1x^{72}+1x^{96}$ (6.12) 1X^192 (6.14)	N N N Y	0	14

The crystal networks are characterized by the vertex connectivity (LC) and vertex ring surrounding (LR) sequences, as shown in Tables 1, 2 and 6. LC is the layer matrix of connectivity [14-16] while LR is the corresponding matrix of rings around each vertex in the graph [23]. The characterization of crystal nets by rings, was used in crystallographic characterization as the vertex symbol; however, only in the Topo Group Cluj papers a sequence of all rings surrounding (coming from the layer matrix of rings, of which entries are the sum of all rings around, of the choice length) was described [5,7,17].

In crystal data-bases, there are registered 2-3 hundred of thousands of real crystals and 1-2 million hypothetical networks. It is conceivable that, if a structure is mathematically possible, one may be energetically probable and then its realization in the real world is only a question of time.

In crystals, connectivity is rather a rational fact (see the crystallographic reflexions), since in condensed mater there is no room for the expression of valences (e.g. in gas-phase or liquid-phase), the compactness being the main driving rule. For example, in the cubic *pcu* net, there is environment env=8, rather than valence, based on geometric/topologic space filling [24]. Guest free/full spongy nets (i.e., nets with ordered defects) are possible (see MOFS).

Data for this paper were computed by our original Nano-Studio software [25].

Conclusions

Rhombellanes are structures built on the ground of rbl.5 = $K_{2.3}$ motifs. They may appear both in crystal or quasicrystal networks, also in their homeomorphs, further possible becoming real molecules. The rhombellane-related structure, named here quasi-rhombellanes show mathematical properties very close to rhombellanes, thus enlarging the options for the further development of material science and/or biologically functionalized real compounds.

The considered structures were described in terms of structural molecular topology (substructure figure count – vertices, edges, faces/rings, rbl.5, ada.10); also, topology was described by Omega polynomial.

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