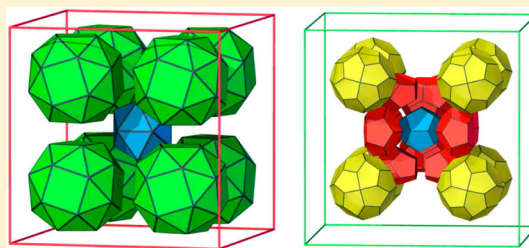


Intermetallic Crystal Structures as Foams. Beyond Frank–Kasper

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S Supporting Information

ABSTRACT: In many intermetallic structures, the atoms and bonds divide space into tilings by tetrahedra. The well-known Frank–Kasper phases are examples. The dual tilings divide space into a tiling by polyhedra that is topologically a foam. The number of faces of the dual polyhedron corresponds to the atom coordination number in the direct structure, and face sharing by adjacent polyhedra corresponds to bonds in the direct structure. A number of commonly occurring intermetallic crystal structures are shown as their duals. A major advantage of this alternative mode of depiction is that coordination of all of the atoms can be seen simultaneously.



1. INTRODUCTION

Intermetallic crystal structures are often of daunting complexity, and their understanding and depiction can be a challenge. Accordingly, they are not well-known and generally ignored in inorganic chemistry texts despite the fact that most of the elements are metals. As a result, there is widespread ignorance among chemists of an extraordinarily rich part of their subject. This is unfortunate because as John Corbett, who gave us so many beautiful intermetallic structures, has remarked, “There is chemistry in intermetallics.”¹ In this paper, we call attention to a way of describing intermetallic structures that has not been used before but which we feel may be useful in better understanding the structures of the most common binary compounds. To complement Corbett’s statement, we add, “There is also geometry in intermetallics.”

What do mean by “foam” in the title? We start with some informal definitions. We are concerned with *tilings* of space in which space is subdivided into generalized polyhedra, which we call *cages*. Our tilings are such that each face of the tile belongs to exactly two tiles; the tilings are *face-to-face*. The set of vertices and edges of the tiling is a periodic graph, often in the context of crystal chemistry called a *net*. A foam is a special kind of tiling.

A polyhedron can be considered as a tiling of the sphere by polygons. Every polyhedron has a dual polyhedron obtained by putting a new vertex in each face and linking each new vertex to those in adjacent faces. A *simple* polyhedron is one in which exactly three faces meet at a vertex. The dual of a simple polyhedron is a *simplicial* polyhedron in which all faces are triangles. A tetrahedron, in which three triangular faces meet at each vertex, is self-dual and is both simple and simplicial.

A *simple tiling* is a filling of space by simple polyhedra in which exactly two polyhedra meet at a common face, three at an edge, and four at a vertex. Every face-to-face tiling has a dual tiling derived by putting new vertices inside the old tiles and connecting them through the faces of adjacent tiles. Noting that

the dual of a dual is the original tiling completes the definition. The dual of a simple tiling is a space filling by tetrahedra sharing faces. The structures of foams are simple tilings. Also here we make the connection to the crystal structures of intermetallic phases because many of them, the topic of this paper, in fact consist of space fillings by tetrahedra.

It is impossible to have a space filling of three-dimensional Euclidean space by tetrahedra in which five tetrahedra meet at an edge. Such a tiling is only possible in a space of positive curvature.² However, there is an important class of intermetallic structures that are known as *tetrahedrally* (or *topologically*) *close-packed* (TCP) or Frank–Kasper phases.³ In these structures, the groups of tetrahedra are those in which either five or six meet at an edge. The structures include the well-known Friauf–Laves phases, the simplest of which, typified by MgCu_2 , is the most common binary structure type in chemistry. Another large group of TCP structures is typified by that of Cr_3Si . The duals of these two structures are simple tilings by polyhedra with 5- and 6-sided faces well-known in crystal chemistry as respectively the type II and I clathrate structures (discussed below). This is not a new observation; Frank and Kasper remarked in 1959, “It is a fascinating matter that there exists a strict correspondence between the structures of such chemically different substances as the gas hydrates and intermetallic compounds...”^{3b} We note that these two gas hydrate structures are also known as the frameworks of silicate minerals melanophlogite and chibaite⁴ and as the frameworks of silicon and germanium clathrates⁵ and, indeed, as a form of elemental Ge.^{5b}

Other frequently occurring intermetallic structures are also space fillings by tetrahedral groups of atoms but in which there

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Table 1. Structure Types Discussed in This Paper^a

structure	<CN>	tiles	DoF	links	dual net	symmetry	foam
CuZn	14	truncated octahedra	1	3	sod	$Im\bar{3}m$	yes
AlB ₂	12.67	N + 2Z	2	4	alb-x-d	$P6/mmm$	yes
ThSi ₂	12.67	M + 2Z	3	6	sgt	$I4_1/amd$	yes
CrB	13.00	O + Z	5	8	cbd	$Cmcm$	yes
FeB	13.00	O + Z	7	10	*	$Pnma$	yes
CuAl ₂	13.33	2Q + Y	3	6	cal-d	$I4/mcm$	yes
MgCu ₂	13.33	P + 2X	1	3	mtn	$Fd\bar{3}m$	yes
MgZn ₂	13.33	P + 2X	4	8	mgz-x-d	$P6_3/mmc$	yes
Cr ₃ Si	13.5	3R + X	1	3	mep	$Pm\bar{3}n$	yes
Zr ₄ Al ₃	13.43	2Q + 2R + 3X	3	7	zra-d	$P6/mmm$	yes
CaCu ₅	13.67	N + 2W + 3X	2	6	doh	$P6/mmm$	yes
NbBe ₃	13.33	N + 2P + 2W + 7X	6	13	*	$R\bar{3}m$	yes
CeNi ₃	13.33	N + 2P + 2W + 7X	5	14	*	$P6_3/mmc$	yes
Ce ₂ Ni ₇	13.33	N + P + 2W + 5X	9	20	*	$P6_3/mmc$	yes
Th ₂ Zn ₁₇	13.37	2N + 2R + 6V + 9X	7	18	*	$R\bar{3}m$	yes
Th ₂ Ni ₁₇	13.37	2N + 2R + 6V + 9X	7	20	*	$P6_3/mmc$	yes
ThMn ₁₂	13.33	L + 4 R + 8X	4	11	tmd	$I4/mmm$	no
BaCd ₁₁	13.00	K + R + 10X	5	14	*	$I4_1/amd$	no
NaZn ₁₃	12.86	J + 13X	3	6	fiv	$Fm\bar{3}c$	no

^aTiles are identified in Figures 2 and 3. <CN> is the average coordination number, and “DoF” is the number of degrees in the structure and “links” the number of distinct interatomic distances. The dual net can be found from the data accompanying 3dt except for cases marked by an asterisk, which are supplied in the Supporting Information.

are also groups of four tetrahedra meeting at an edge. Their duals will be tilings by tiles that include simple polyhedra with quadrilateral faces. In an article by one of us some years ago, it was pointed out that just 12 binary structure types based on tilings by tetrahedra accounted for the structures of more than 5000 compounds.⁶ These were not described as tilings or illustrated at that time. However, the current availability of software for determining and illustrating tilings makes that now possible, and it is done in this paper.⁷

Not all metal structures are based on tilings by tetrahedra. The familiar close-packed structures are tilings by tetrahedra and octahedra. Others can be considered as tilings by tetrahedra and half-octahedra (i.e., square pyramids); we consider three of these also, although their dual structures are not foams in the strict sense.

Why are we interested in the dual structures? One reason is that in the direct structures, particularly those with high coordination, coordination polyhedra intersect, so the full structure showing simultaneously the coordination of all of the atoms cannot be illustrated. In the dual structure, each polyhedron is distinct and associated with just one atom; the number of faces corresponds to the coordination number of that atom, and the sharing of faces between polyhedra corresponds to bonds. We believe that the dual structure gives a much clearer illustration of the role of all of the atoms in the structure for these reasons. In this paper, we discuss explicitly intermetallic structures, but the method is quite general. Applied to ionic crystal structures, one can see simultaneously the coordination of all cations and anions.

We emphasize that the tilings we discuss are primarily combinatorial objects with a defined topology independent of any embedding. We give illustrations using embeddings with edges as nearly equal as possible for convenience. It is important to distinguish the dual tilings of this paper from a dissection of a structure into Voronoi polyhedra. The latter are derived from a specific embedding of the original structure, and the Voronoi polyhedron associated with a given atom is defined

by the surface enclosing all points closer to that atom than to any other. Voronoi polyhedra often have many small faces, and in general the number of faces is greater than the coordination number and depends on the embedding.

Polyhedra are usefully characterized by a *face symbol* of the form $[A^a.B^b...]$, which indicates that it has *a* faces with *A* sides, *b* faces with *B* sides, etc. Nets are often referred to by the RCSR symbol, which consists of three lower-case bold letters such as **abc** or three letters with an extension such as **abc-x**.⁸ Some nets are also those of zeolite frameworks, which have upper-case bold three-letter codes such as **ABC**.⁹ Structure names and crystallographic data all come from *Pearson's Handbook*.¹⁰

In all of the structures that we discuss (Table 1), the number of crystallographically distinct kinds of bonds is greater than the number of degrees of freedom in the structure (unit cell parameters and free internal coordinates). Nevertheless, the actual structures always have the highest possible symmetry for the given topology, which in every case belongs to a holohedral crystal class (point group). This is in contrast to the situation for “ionic” (i.e., metal–nonmetal) compounds, in which, if a topology is realized at all, it is often at lower than maximum possible symmetry to allow optimization of interatomic distances.¹¹

We should mention here a recent quite different approach to intermetallic structures in which large clusters involving several coordination shells and some dozens of atoms are identified in a large variety of intermetallic structures.¹² That work has a different goal, that of finding structural relationships. Our goal is more modest, that of illustrating and understanding basic structures including the roles of all atoms explicitly.

2. RESULTS AND DISCUSSION

2.1. Simplicial Polyhedra and Their Duals. For structures consisting of tilings by tetrahedra of atoms, the coordination figure is a simplicial polyhedron. The corresponding dual tile associated with that atom will be a simple polyhedron. We illustrate this for the coordination of Al in the

crystal structure of AlB_2 in Figure 1. In this structure, there are clearly Al–B and B–B bonds. We also include two kinds of Al–Al bonds of lengths (3.00 and 3.26 Å) comparable to that in the element (3.18 Å).

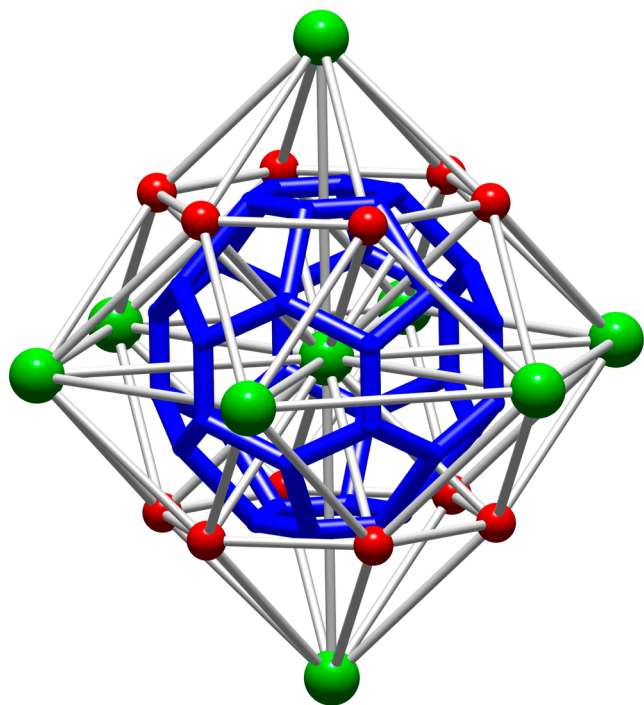


Figure 1. Coordination of Al (green ball) in AlB_2 . The center atom and coordination sphere define the tetrahedra. The blue polyhedron has vertices in the centers of those tetrahedra.

The polyhedra occurring in this paper are shown in Figures 2 and 3 both as coordination polyhedra and as their duals. We

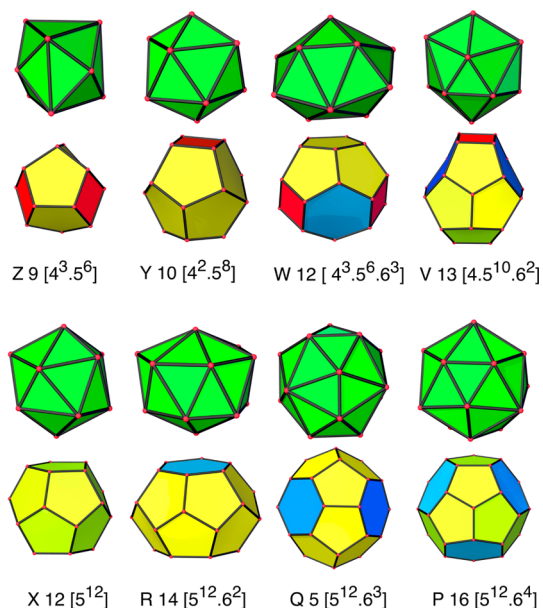


Figure 2. Some simplicial coordination polyhedra (green) and their duals. In the dual, quadrilateral faces are red, pentagonal faces yellow, and hexagonal faces blue. Underneath each pair is a letter code, the coordination number, and the dual face symbol. The bottom four pairs are the Frank–Kasper polyhedra.

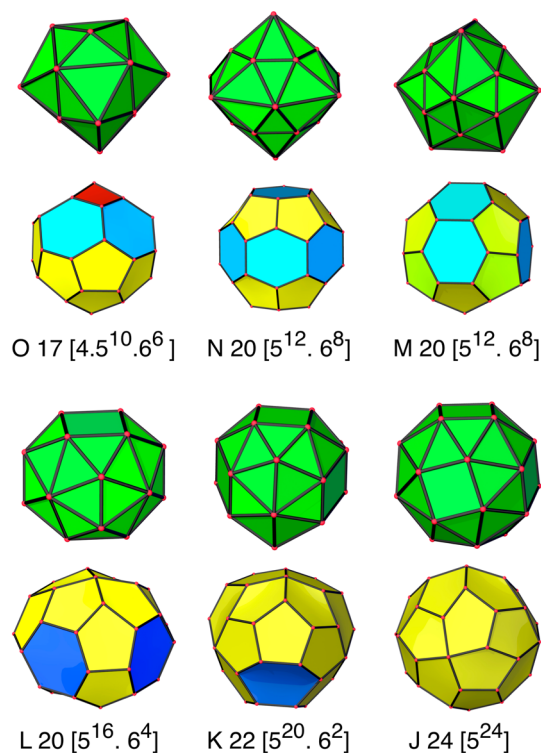


Figure 3. Some larger coordination polyhedra (green) and their duals. Only the top three are simplicial. In the dual, quadrilateral faces are red, pentagonal faces yellow, and hexagonal faces blue. Underneath each pair is a letter code, the coordination number, and the dual face symbol.

include, from important structure types, three polyhedra (J, K, and L) that are not simplicial (some of their faces are squares): their duals are not simple polyhedra (some vertices are 4-coordinated). The letters P, Q, R, and X have long been used to represent the Frank–Kasper coordination polyhedra. Y and Z were identified some years ago;⁶ the other letter designations are new in this paper.

2.2. Some Structures Based on Tilings by Tetrahedra.

In all of the structures considered here, the identification of tetrahedra of atoms in the structure is straightforward. Considering the tetrahedral edges as “bonds” then results in a unique simplicial coordination polyhedron.

2.2.1. Body-Centered-Cubic (bcc) Structure. There are exactly nine topologically distinct ways of filling space by one kind of tetrahedron.¹³ Only one of these structures has just one kind of vertex: this is the bcc structure considered as 14-coordinated (i.e., first and second neighbors).¹⁴ The dual structure is accordingly the only simple tiling with again one kind of vertex and one kind of tile. It is familiar in chemistry as the net of the sodalite framework (RCSR symbol **sod** and zeolite code **SOD**). The structures are illustrated in Figure 4. In this instance, the tile is also the Voronoi polyhedron. It is the truncated octahedron $[4^6.6^8]$. Nearest-neighbor bonds of bcc correspond to sharing of the (larger) hexagonal faces, and second-neighbor links correspond to sharing of the square faces. The binary version of this structure typified by CuZn (β -brass) is, of course, a very large structure family.

2.2.2. AlB_2 and ThSi_2 . The structure of AlB_2 is shared by hundreds of compounds. The conventional description is that Al forms a simple hexagonal lattice with two trigonal-prismatic holes (filled by B) per Al (i.e., a space filling by trigonal prisms).

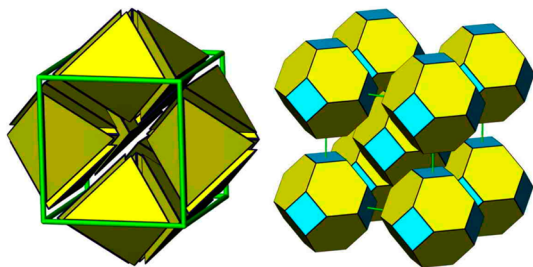


Figure 4. (Left) bcc structure as a tiling by tetrahedra. (Right) Dual structure, a simple tiling by truncated octahedra.

It is shown as a dual structure in Figure 5. The large polyhedron [$5^{12}.6^8$] (N in Figure 3) showing the Al space is

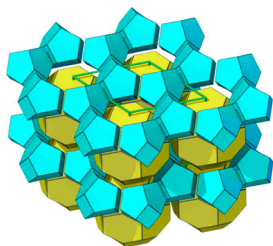


Figure 5. AlB_2 dual structure. The Al polyhedra (hexagonal barrels) are yellow.

often called the *hexagonal barrel*. The B polyhedra are [$4^3.5^6$], Z in Figure 2. In this simple structure, shared square faces correspond to B–B bonds, shared pentagonal faces to Al–B bonds, and shared hexagonal faces to Al–Al bonds. The pattern of B–B bonds is the 3-periodic honeycomb layer, RCSR symbol **hcb**.

The ThSi_2 structure is closely related to that of AlB_2 . The Th packing is the second way (the first was mentioned in the previous paragraph) of filling space with trigonal prisms of just one topological kind, forming a tetragonal sphere packing with RCSR symbol **tsi**. The Si atoms center those prisms. The Th atom polyhedron (M in Figure 3) in the dual structure (Figure 6) again has vertex symbol [$5^{12}.6^8$] but a different topology, with pentagonal faces forming a continuous path like the seam on a tennis ball, and the polyhedron is sometimes called the tennis ball on that account. The Si polyhedra are the same as the B polyhedra in AlB_2 , but the Si–Si bonds now form a 3-periodic net with RCSR symbol **ths**. The tetrahedral (foam) framework is also known as a silicate with zeolite code **SGT**.

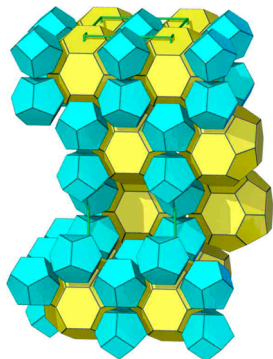


Figure 6. ThSi_2 dual structure. The Th polyhedra (tennis balls) are yellow.

2.2.3. FeB and CrB structures. These two closely related structures (Figure 7) account for more than 300 entries in

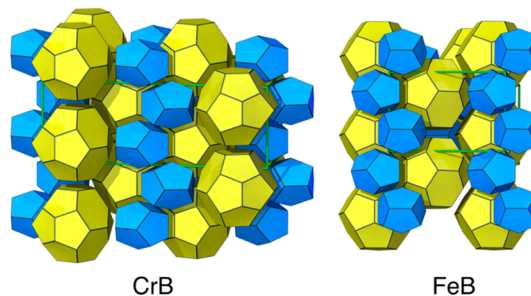


Figure 7. CrB and FeB dual structures. The Cr and Fe polyhedra are yellow.

Pearson's Handbook.¹⁰ As described by Parthé, the larger atom (Cr and Fe) arrangements are periodically twinned hexagonal close packing (FeB) and cubic close packing (CrB).¹⁵ The latter structure type is preferred with the greater disparity in atom sizes, e.g., the CrB type for LaNi and the FeB type for LuNi. The small atom tiles in the dual structure are again the 9-face [$4^3.5^6$] Z polyhedra of the previous structures, but now they share only two quadrangular faces to form Z–Z... rods. The large atom tile is the 17-face O of Figure 3, so that, e.g., Cr is bonded to 10 Cr and 7 B.

2.2.4. CuAl_2 Structure. This simple structure is that of over 100 compounds. Cu is in a square antiprism of Al and further bonded to two Cu atoms through the square faces, forming a bicapped square antiprism, the most symmetrical simplicial polyhedron with 10 vertices, dual polyhedron [$4^2.5^8$], Y in Figure 2. Less obvious is that the Al is 15-coordinated (8 Cu + 7 Al) with dual polyhedron [$5^{12}.6^3$] (one of the Frank–Kasper polyhedra, Q in Figure 2). In the tetragonal structure (Figure 8), the Cu polyhedra form rods parallel to the c axis by sharing square faces (this corresponds to the Cu–Cu bonds).

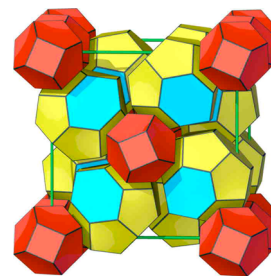


Figure 8. CuAl_2 dual structure viewed almost along the tetragonal c axis. The Al polyhedra are yellow (pentagonal faces) and blue (hexagonal faces).

2.2.5. Frank–Kasper Phases. These are the TCP phases that have been frequently discussed, in part, because their dual structures are of interest in connection with the structures of foams with bubbles that have only 5- and 6-sided faces.¹⁶ The Kelvin problem asks for the lowest energy (lowest surface area) of a monodisperse foam. The best solution known to date is the structure of the type I clathrate (dual of the Cr_3Si structure, also known as A15).¹⁷ This is the only TCP dual structure consisting of 12- and 14-face simple polyhedra (there is no 13-face polyhedron with exclusively 5- and 6-sided faces). All such structures with up to 15 topologically distinct vertices have

been enumerated, and it is known that the Cr_3Si and MgCu_2 structures (each with three kinds of vertices) are the only ones with fewer than five kinds of vertices.¹⁸ We illustrate the two simplest and chemically most important: the duals of the Cr_3Si and MgCu_2 structures in Figures 9 and 10.

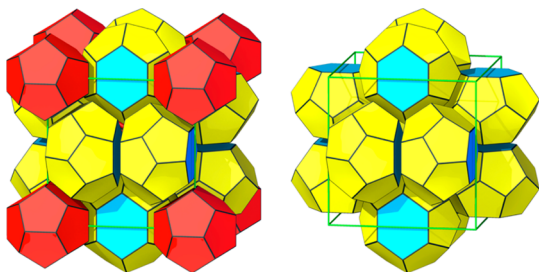


Figure 9. Cr_3Si dual structure (type I clathrate or Weaire–Phelan foam with zeolite code **MEP**). The Co polyhedra are yellow (pentagonal faces) and blue (hexagonal faces). (Right) Excluding the Si dodecahedra (red).

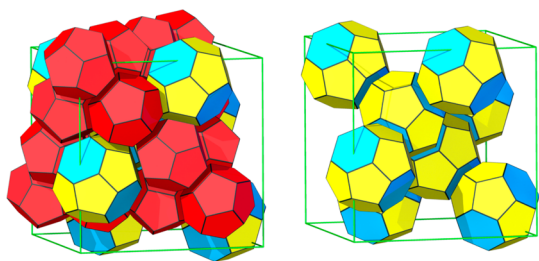


Figure 10. MgCu_2 dual structure. The Mg polyhedra are yellow (pentagonal faces) and blue (hexagonal faces). (Right) Excluding the Cu dodecahedra (red).

Two other TCP phases are listed in Table 1. The MgZn_2 structure (Figure 11) is related to that of MgCu_2 in that, in the

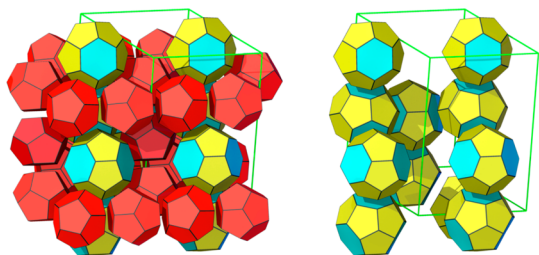


Figure 11. MgZn_2 dual structure. The Mg polyhedra are yellow (pentagonal faces) and blue (hexagonal faces). (Right) Excluding the Zn dodecahedra (red).

latter, the pattern of Mg–Mg bonds is diamond (**dia**) and, in the former, it is that of lonsdaleite (**lon**, “hexagonal diamond”). The structure of Zr_4Al_3 (not shown) is important as the simplest tiling with 12-, 14- and 15-sided faces but has only been identified in Zr_4Al_3 and Hf_4Al_3 .

2.2.6. CaCu_5 . This structure is closely related to the TCP family. Atoms are in 20- and 12-coordination; however, the 12-coordinated atoms have two different coordination figures, the icosahedron, dual $[5^{12}]$, and a simplicial isomer with dual $[4^3.5^6.6^3]$, W in Figure 2. The dual of the 20-coordination polyhedron is again the hexagonal barrel, N in Figure 3. The dual structure (Figure 12) is known as the H clathrate structure and also as the silicate dodecasil 1H, zeolite code **DOH**.

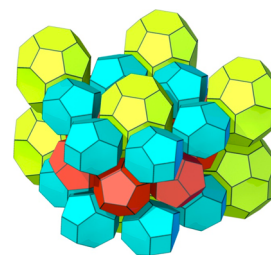


Figure 12. CaCu_5 dual structure (also known as the H hydrate structure with zeolite framework code **DOH**). The Ca polyhedra (barrels) are yellow. The copper polyhedra have 12 faces and are dodecahedra (red) and the W polyhedra (Figure 2).

2.2.7. NbBe_3 , CeNi_3 , and Ce_2Ni_7 . The duals of these three structure types (Figure 13), which serve as the structures of

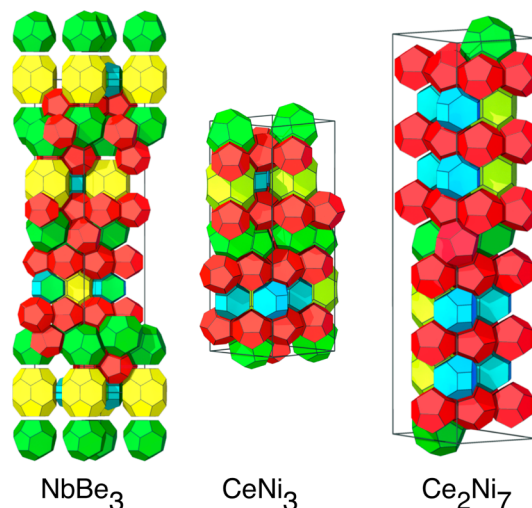


Figure 13. Dual of three related intermetallic structure types. The Nb or Ce polyhedra are N (20-face barrels, yellow) and P (16-face barrels, green). The Be or Ni polyhedra have 12 faces and are dodecahedra (red) and the W polyhedra (Figure 2).

several hundred compounds, use the same tiles as those for CaCu_5 together with the Friauf polyhedron P ($[5^{12}.6^4]$). In NbBe_3 and CeNi_3 , PNP groups, with the P atoms sharing opposite hexagonal faces of N (hexagonal barrel), are arranged in rhombohedral and hexagonal packing, respectively. In Ce_2Ni_7 , there are instead PNP groups, again in rhombohedral packing.

2.2.8. $\text{Th}_2\text{Ni}_{17}$ and $\text{Th}_2\text{Zn}_{17}$. These two structure types are another example of those with the same coordination polyhedra but which have different packings. In $\text{Th}_2\text{Zn}_{17}$ (Figure 14), the large polyhedra, the 20-face hexagonal barrels, N, form rods by sharing opposite hexagonal faces with 14-face R polyhedra $[5^{12}.6^2]$. The sequence is NNRR... in $\text{Th}_2\text{Ni}_{17}$ (Figure 15); there are two types of rods, NN... and NRR..., in the ratio 1:2, so in both structures, there are equal numbers of N and R polyhedra. The remaining atoms are divided between 12-coordination ($[5^{12}]$ in the dual structure) and a new 13-coordinated polyhedron V ($[4.5^{10}.6^2]$ in the dual).

2.3. Structures Based on Tilings of Tetrahedra and Square Pyramids. Normally, upon division of a structure into *natural* tiles, no tile is admitted for which one face is larger than the rest.¹⁹ In particular, octahedra are not split into pairs of square pyramids. However, in some intermetallic structures, the

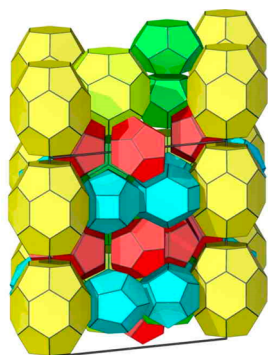


Figure 14. $\text{Th}_2\text{Ni}_{17}$ dual structure. The Th polyhedra (hexagonal barrels) are yellow. The others are V (13 faces, green), R (14 faces, blue), and dodecahedra (red).

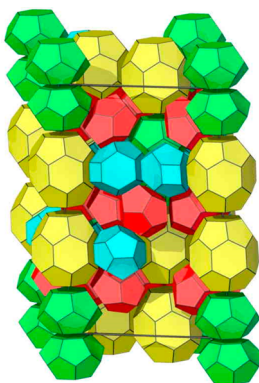


Figure 15. $\text{Th}_2\text{Zn}_{17}$ dual structure. The Th polyhedra (hexagonal barrels) are yellow. The others are V (13 faces, green), R (14 faces, blue), and dodecahedra (red).

octahedra are of the type X_4Y_2 , where Y are large atoms at opposite vertices. It is then convenient for illustration to split the octahedron into two X_4Y square pyramids if this can be done without breaking the symmetry (we always require a tiling to have the intrinsic symmetry of the net of the structure). In the structure of NaZn_{13} , there is a Na_2Zn_4 octahedron with the $\text{Na}\cdots\text{Na}$ diagonal twice as long as the $\text{Zn}\cdots\text{Zn}$ diagonals. The dual structures will have some 5-coordinated vertices and some tiles we consider (J, K, and L in Figure 3) no longer simple polyhedra, so the structure is no longer strictly a foam but closely related.

2.3.1. ThMn_{12} and BaCd_{11} . In these structures (Figures 16 and 17), the large, not simple, polyhedron is accompanied by 14-face (R) polyhedra and pentagonal dodecahedra. In

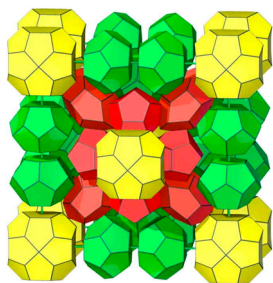


Figure 16. ThMn_{12} dual structure. The Th polyhedra (30 faces, L, yellow) are not simple. The others are R (14 faces, green) and dodecahedra (red).

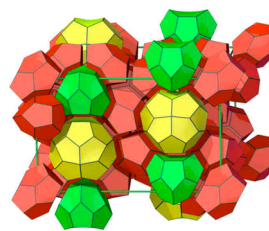


Figure 17. BaCd_{11} dual structure. The Ba polyhedra (22 faces, K, yellow) are not simple. The others are R (15 faces, green) and dodecahedra (red).

ThMn_{12} , the L polyhedra with four hexagonal faces share those faces with those of R polyhedra to form tetragonal layers. In BaCd_{11} , the large K polyhedron, with two hexagon faces, shares those faces with R polyhedra to form rods. Again these are large families of structures.

2.3.2. NaZn_{13} . Our last structure is perhaps the nicest. Na is 24-coordinated by Zn arranged as the vertices of a snub cube $3^4.4$; this is known to be the arrangement of 24 points on the surface of a sphere that maximizes the shortest distance between them (the solution to the Tammes problem).²⁰ Packing such polyhedra sharing square faces produces stoichiometry NaZn_{12} and leaves an icosahedral hole to be filled by a 13th Zn atom (Figure 18). Filling that cavity one

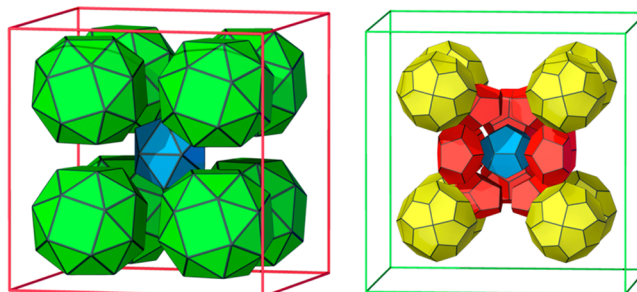


Figure 18. NaZn_{13} structure. Left showing the NaZn_{24} and ZnZn_{12} polyhedra. Right. The dual structure. The Na polyhedron (24-faces, U, yellow) is not simple. The others are dodecahedra (red and blue).

finds, *mirabile dictu*, that all the Zn atoms are in icosahedral coordination. Taking the faces of the snub cube as tile faces, the atoms define tetrahedra and square pyramids. The dual structure (Figure 18) is then a tiling by the dual of the snub cube, (the pentagonal icositetrahedron $[5^{24}]$) and pentagonal dodecahedra ($[5^{12}]$) in the ratio 1:13. Note that in this structure all the rings are 5-rings. It is in this structure type particularly that geometry takes over from chemistry as it is found also in opals formed from silica spheres of two different sizes.²¹

3. EXPERIMENTAL METHODS

All data and structure type designations were taken from *Pearson's Tables*.¹⁰ The program 3dt⁷ accepts tiling data in the form of space group and coordinates of unique faces which were determined by inspection of the crystal structure, although for tilings by tetrahedra and other natural tilings the program TOPOS²² can now be used. 3dt is a Java program that accepts tiling information either as coordinates of the vertices of faces or as a Delaney symbol and draws the tiles as illustrated herein. It converts a tiling to a dual tiling and was used to prepare the illustrations. Delaney symbols are exported by 3dt from data for faces. Systre⁷ was used to determine the intrinsic symmetry and identify degrees of freedom and number of independent

interatomic distances in each structure. For tilings with RCSR symbols in Table 1, the data are included in the 3dt package. Others are listed in the Supporting Information as Delaney symbols readable by 3dt.

■ ASSOCIATED CONTENT

■ Supporting Information

Tiling data for the dual structures of NbBe₃, CeNi₃, Ce₂Ni₇, Th₂Zn₁₇, Th₂Ni₁₇, ThMn₁₂, and BaCd₁₁ are given as Delaney symbols readable by 3dt. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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Notes

The authors declare no competing financial interest.

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