Alternative Descriptions of the *C*23 (PbCl₂), *C*37 (Co₂Si), *B*8ᵦ (Ni₂In) and Related Structure Types

B. G. Hyde,*,a M. O'Keeffe,b W. M. Lyttleb and N. E. Breseb

a Research School of Chemistry, The Australian National University, Canberra, ACT 2601, Australia and b Department of Chemistry, Arizona State University, Tempe, AZ 85287, USA

It is shown that the title structures can be usefully described in a number of different ways which demonstrate their relationships to each other and to other structures. New descriptions include those of filling interstices in eutactic ("close packed") arrays and in terms of two- and three-dimensional nets.

The structure types $C23$ (PbCl₂) and $C37$ (Co₂Si) are well known to be closely related; indeed, sometimes[1] they are not distinguished. They are in fact *isopuntal*, as they have the same symmetry (*Pnma*)[†] and have all atoms in the positions 4*c* of that space group.[1] The structures of the hydrides (*C*29) and the halides etc. (*C*23) differ only in inconsequential details[2] and should really be considered as one structure type (we will call it *C*23), the distinction being made initially on the basis of an erroneous structure being proposed for SrH₂. On the other hand, it has long been recognized[3,4] that this group of related structures can be divided into several subgroups based on lattice parameter ratios. The structure type $B8ᵦ$ (Ni₂In) is also known to be closely related. These, and the related structures to be discussed here, are those of some 1000 compounds (over 400 of type *C*23 alone) involving virtually all (we count 74) of the stable elements, including representatives from every row and column of the periodic table other than the inert gases.

Although, for example, the structure types *C*23 and *C*37 are those of ternaries *ABC*, most discussions focus on the structures of compounds with only two elements, such as PbCl(1)Cl(2) and Co(1)Co(2)Si. The conventional description has been in terms of {Pb}Cl_n and {Si}Co_n coordination polyhedra,[‡] and indeed such a description is very useful: in these terms, for example, the relationship of *C*23 to *C*37 and to structure types such as those of Ni₂In (*B*8ᵦ) and of MoP₂ on the one hand and to that of PbFCl on the other can readily be appreciated.[5,6] (The first three of these structures are shown in Fig. 1.) However, when one finds compounds such as BaCl₂ and YNiSn (to take a pair more or less at random) listed as the same structure type, one is led

to expect that different descriptions of these structures might be appropriate in different circumstances. In this paper we explore several different descriptions that explicitly recognize the ternary nature of the compounds.

Further interest in all these structure types arises because they are also the arrangements of cations in a large group of oxides (oxysalts) such as, in the case of *C*23, sulphates, carbonates, orthosilicates etc.,[7] e.g. β-Ca₂SiO₄, β-K₂SO₄, K₂NbF₇ and K₂ReO₈, as well as[8] the rare-earth rhenium carbides Ln₂ReC₂ etc.

Structural geometry

Anion coordinations and cation arrays in C23 (PbCl₂/SrH₂). It has long been recognized that the cation array in hydrides such as SrH₂ is close to hexagonal eutaxy ("close packing").[9] In this structure[2] H(1) occupies one half of the tetrahedral sites. The pattern of filling is such that {H(1)}Sr₄ tetrahedra sharing edges form chains parallel to *b*, as can be seen from Fig. 2.* H(2) atoms are off-centre in Sr₆ octahedra, so that their coordination is approximately square pyramidal, {H(2)}Sr₅. Such a description applies equally to (other) *C*23s, and in Fig. 3 we show the structure of EuCl₂[10] in these terms.

Thus we are led to suggest that it is useful to reconsider the *C*23 halide and hydride structures in terms of the anion coordination by cations. In addition, this approach reveals relations to other heavy-metal halide and oxide structures, for example those of LaF₃[11] and La₂O₃[7,12] (*D*5₂), in both of which the metal atom arrays are also close to perfect hexagonal eutaxy. The relationship of the *C*23 structure to that of La₂O₃ is particularly suggestive: one half of the tetra-

---

* To whom correspondence should be addressed.
† We will use this standard setting consistently throughout.
‡ {M}X_n indicates that the 'central' atom M is coordinated by *n* X atoms.

---

* This pattern of filling half the tetrahedral sites of an eutactic array of metal atoms does not appear to have been discussed before. (Other, more familiar ways occur in the structures of A-La₂O₃, wurtzite, sphalerite, PtO and tetragonal PbO.)
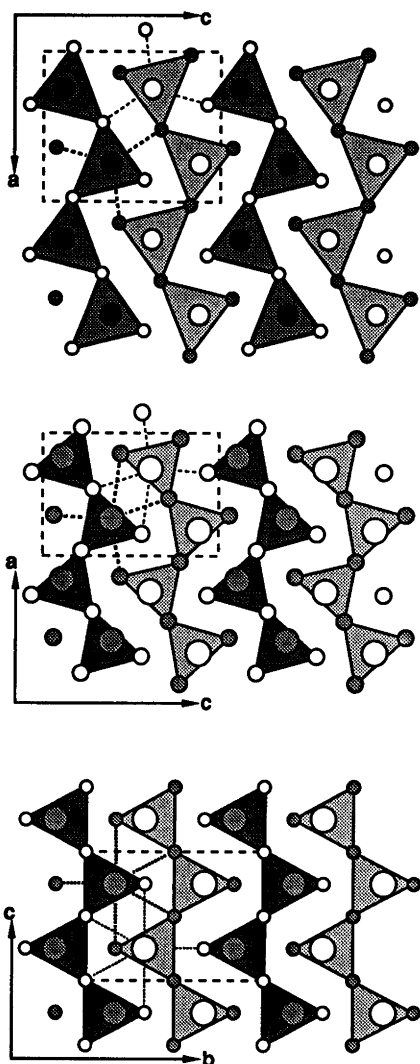
Fig. 1. The structures of (down the page) $EuCl_2$
(*C*23-/$PbCl_2$-type), Co_2Si (*C*37-type) and Ni_2In (*B*8$_b$-type)
depicted as, respectively, Eu-, Si- and In-centred trigonal
prisms, three-, four- and five-capped. (The broken lines outline
orthorhombic unit cells; orthohexagonal in case of Ni_2In.)
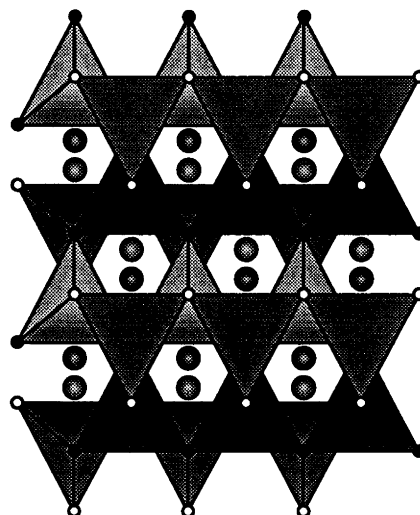Topologically, the 'walls' of prisms are identical.

Fig. 2. Projection of the SrD_2 structure down [100] with *b*
horizontal in the page. Small circles represent Sr: open,
x = 0.25; filled, *x* = 0.75. Larger circles represent D(2): darker,
x = 0.03 or −0.03; lighter, *x* = 0.53 or 0.47. D(1) atoms centre
the tetrahedra.

hedral interstices are filled by anions in both, although the
patterns are different in the two cases. In La_2O_3 the occu-
pied tetrahedral sites are in alternate (001) slabs (unit
{111}layers of CaF_2-type *C*1) and the occupied octahedral
interstices in the intervening slabs (unit {111}layers of
NaCl-type *B*1).

It is also rewarding to analyse the bond lengths in terms
of the Brown–Altermatt[13] bond length – bond valence rela-
tionship, eqn. (1), in which *v* is the bond valence for a bond

$$v = \exp \left[(R - d) / 0.37 \text{ Å} \right] \qquad (1)$$

of length *d*, and *R* is a parameter characteristic of the bond
type. In the present context we are interested in the ap-

parent valence,[12] *V′*, of the H atoms in SrH_2, which is the
sum of *v* [as given by eqn. (1)] for all bonds to a given atom.
The ratio of the apparent valences of H(1) and H(2) should
therefore be given by eqn. (2). This ratio (which should be

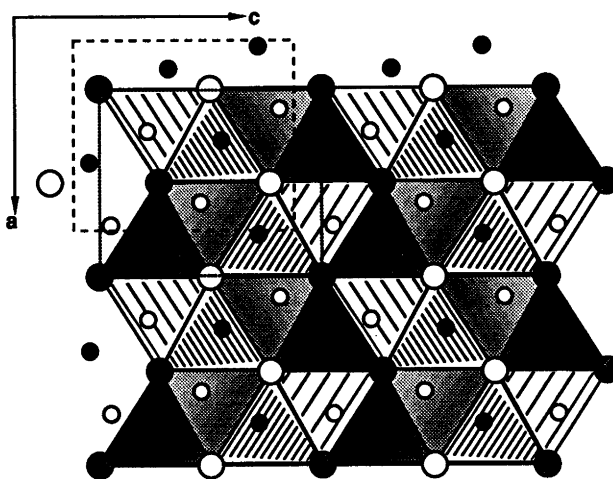$$\frac{V'_1}{V'_2} = \frac{\sum \exp \cdot (-d_{1i} / 0.37)}{\sum \exp (-d_{2i} / 0.37)} \qquad (2)$$

Fig. 3. The structure of $EuCl_2$ projected on (010), and depicted
as {Cl(1)}Eu_4 tetrahedra (dotted) and {Cl(2)}Eu_5 square
pyramids (line shaded): scale, 1 cm = 3 Å. Larger circles are
Eu, smaller ones are Cl (both open for *y/b* = ¾ and shaded for
y/b = ¼). Note the hexagonal eutaxy of Eu.

217

Table 1. Ratios of apparent valences of anions in some *C*23 compounds.

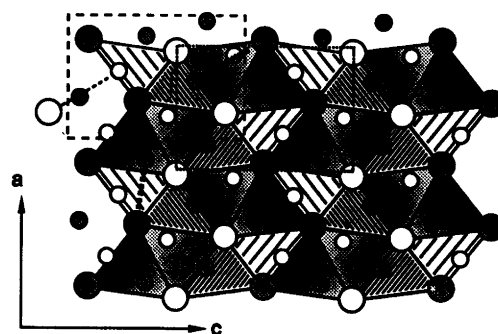| Compound	V_1'/V_2'	Structure ref.
CaD_2	1.65	20
SrD_2	1.65	2
BaD_2	1.81	21
PbF_2	1.62	22
$PbCl_2$	1.25	23
$BaCl_2$	1.66	24
$BaBr_2$	1.44	24
BaI_2	1.33	24
ThS_2	1.58	25

Fig. 4. The structure of *C*37-type Co_2Si projected on (010): scale, 1 cm = 3 Å. Large circles are Si, small ones are Co (open and shaded differ in height by y/b = ½). Note the $\{Co(1)\}Si_5$ half-octahedra and $\{Co(2)\}Si_4$ tetrahedra (both shown, in some instances, with a cap). Cf. Fig. 3.

unity) is, in fact, 1.63, a very marked deviation from the expected value. It is therefore natural to examine the ratio V_1'/V_2' as given by eqn. (2) for other *C*23 compounds. A list of some of these is given in Table 1; in every case the ratio is significantly greater than unity.

Compounds with the La_2O_3 structure provide a similarly striking observation: the apparent valence of the tetrahedral O atom is much greater than that of the octahedral O atom;[12] the ratio is 2.22/1.32 = 1.68, similar to our observation for SrH_2. In this case it has been argued[7,12] that non-bonded metal $\cdots$ metal interactions contribute to stretching of the bonds to the octahedral anion; the same explanation may be extended to *C*23s. In support of this view is the observation (for *C*23s) that, in the barium halides, the apparent-valence ratio becomes closer to unity as the Ba $\cdots$ Ba distances increase, i.e. in the sequence $BaCl_2$, $BaBr_2$, BaI_2.

Relationships between the C23, C37 and B8$_b$ structures. Apart from previously reported,[5,6] conventional relations in terms of e.g. (for $PbCl_2$) $\{Pb\}Cl_6$, coordination polyhedra (cf. Fig. 1), the nature of the close relationships between these structure types is also manifest in projections of the structures analogous to that of *C*23 in Fig. 3. For the other two types these are shown in Figs. 4 and 5.

The difference between *C*23 and *C*37 is that the coordination numbers, clearly 4 and 5 in the former, are tending to increase in the latter (by the addition of the caps): i.e. the coordination polyhedra are tending towards trigonal bipyramids and octahedra. In *B*8$_b$ these tendencies are completed, and the coordination numbers are now, unambiguously, 5 and 6.

It has also been shown that the *C*23 and *C*37 families of structures can be distinguished by the ratios of their lattice parameters.[3,4] Perhaps the most prominent distinction has been between the saline compounds (*C*23 hydrides, halides and chalcides) and the "anti-structure" compounds typified by Co_2Si (*C*37). For the minority atoms (cations in the former) to have perfect hexagonal eutaxy, a/b = $\sqrt{(8/3)}$ = 1.633 and c/b = $\sqrt{3}$ = 1.732 (*Pnma* setting). In Fig. 6 we have plotted these lattice-parameter ratios for all the *C*23

(including *C*29), *C*37 and *B*8$_b$ structures for which we could find data: the continuity of the distribution is remarkable, although *C*23s do tend to cluster near the coordinates for ideal hexagonal eutaxy, while *C*37s have lower values
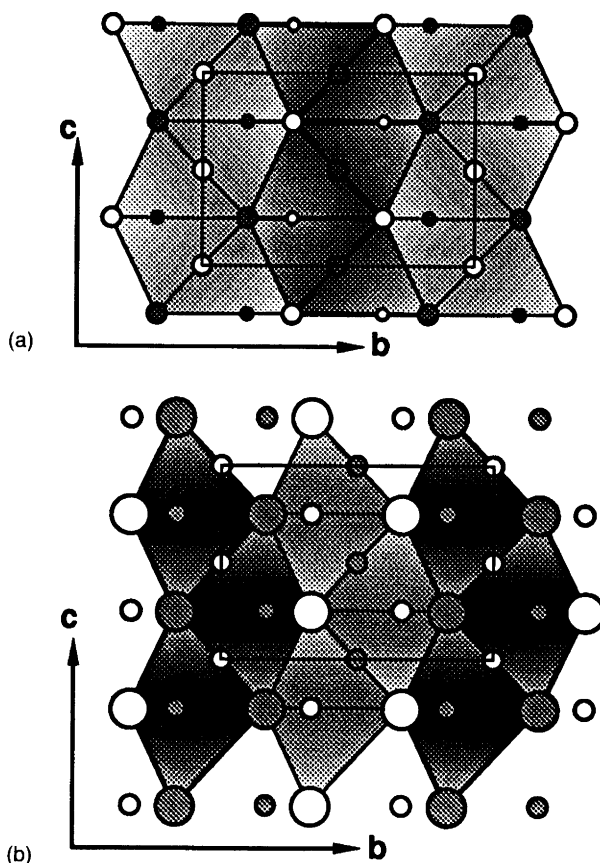

Fig. 5. The *B*8$_b$-type structure of Ni_2In projected on (11$\bar{2}$0) of its hexagonal unit cell: scale, 1 cm = 2 Å. Large circles are In, small ones are Ni (open at 0, filled at ½): (a) the $\{Ni(1)\}In_6$ octahedra, (b) the $\{Ni(2)\}In_5$ trigonal bipyramids. [(a) and (b) interpenetrate to fill space completely.] Note the hexagonally eutactic array of In, and cf. Figs. 3 and 4.

of *a/b*, close to those of the *B8*_bs.* The transitions *C23→C37→B8*_b appear to be virtually continuous, as suggested above on the basis of their structural geometry.

*Relationships between C23, C37, B8*_b *and the C32 (AlB₂) structures.* The first three are really ternary structures, although typified by $PbCl_2/SrH_2$, Co_2Si and Ni_2In. The last of the three (not detailed above) is Ni(1)Ni(2)In, with space group $P6_3/mmc$ and all atoms in fixed positions: Ni(1) in 2(*a*), Ni(2) in 2(*d*) and In in 2(*c*). Their relations in terms of walls of $\{Pb\}Cl_6$ [or $\{Sr\}H_6$], $\{Co\}Si_6$ or $\{In\}Ni_6$ trigonal prisms (Fig. 1) is well documented, the prisms being tricapped (so that Pb/Sr is 9-coordinated), tetra-capped (Si 10-coordinated) and penta-capped (Ni 11-coordinated), respectively.[6] (However, as already mentioned, in spite of this difference the first two are not always distinguished.) A number of compounds such as MnCoSi have both *C37* and *B8*_b structures (the latter being the higher-temperature polymorph).

As we have seen, it is also revealing to consider the Ni_2In structure in terms of the In atom array, which again approximates to hexagonal eutaxy (cf. Fig. 6). However, in
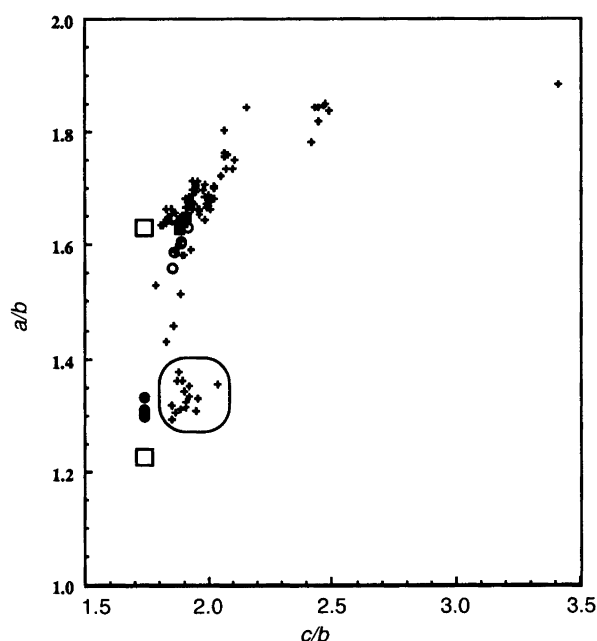

Fig. 6. Lattice parameter ratios for *C23*-, *C29*-, *C37*- and *B8*_b-type structures. Open squares are for perfect hexagonal eutactic cations (above; 1.732, 1.633) and for the *B8*_b-type Ni_2In (below; 1.732, 1.228); the 'box' encloses all *C37*-type M_2X structures such as Co_2Si; small black squares are the *C29* alkaline-earth dihydrides. The circles represent dimorphic substances MnAB (A = Co or Ni, B = Si or Ge) which are *C23*-type at lower temperature (open) and *B8*_b-type at higher temperature (filled).

contrast to *C23* and *C37*,[†] Ni(1) is now in the centre of the In_6 octahedra (rather than off-centre in five coordination), and Ni(2) is in a face shared between two tetrahedral sites so that its coordination is now five-fold (a trigonal bipyramid). In order for the bipyramidal coordination of Ni(2) to be reasonably regular [the observed bond lengths are 2.41 (3×) and 2.57 (2×) Å], the axial ratio *c/a* for $NiIn_2$ is reduced from the ideal value of 1.63 (for perfect eutaxy, 'close packing') to 1.23.

Both Ni(2) and In lie on layers perpendicular to *c*, forming composite [Ni(2)+In] honeycomb (6^3) layers. If all the atoms within these layers were chemically identical, the *c* axis of the structure would be halved and the symmetry would become *P6/mmm*. Formally, the structure would then be the *C32* type of AlB_2 (Fig. 7). [It has Al in 1(*a*) and B in 2(*d*).] However, to correspond to Ni_2In, the axial ratio would have to be about *c/a* = 0.6: an example[1] is afforded by $NbAu_2$ (*c/a* = 0.59). In contrast, AlB_2 itself has *c/a* = 1.08.

However, it transpires that the division between the two types is neither sharp nor very obvious; and compounds have been[1] rather arbitrarily classified as *C32* or *B8*_b. [The confusion is not helped by the fact that the binary AlB_2 has a *Structurbericht* symbol for a ternary structure (*C32*), while the ternary Ni_2In has one for a binary structure (*B8*_b).] Fig. 8 shows the distribution of axial ratios for compounds assigned to these two structure types: clearly their domains overlap. While there is perhaps a preponderance of *B8*_b types at lower axial ratios and of *C32* types at higher values, these are not mutually exclusive domains. In addition, although one could divide them into two groups (around the two maxima), this would require the reclassification of very many compounds, and would still not be completely unambiguous.

The *B8*_a (NiAs) family of structures also has a wide range of axial ratios, and is related to the present family by removing the 'tetrahedrally' coordinated atom: cf. Fig. 9 with Fig. 5. As these and *C32/B8*_b compounds are also
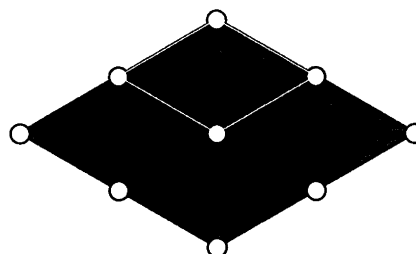

Fig. 7. The structure of AlB_2 projected on (0001); scale 1 cm = 2 Å. Large circles are Al at height *z/c* = 0, small ones are B at *z/c* = ½. $\{B\}Al_6$ trigonal prisms are shown, and the hexagonal unit cell is outlined in white.

---

*The reason for the lower value of *a/b* is, of course, that the tetrahedral atoms are moving into the bases of the tetrahedra, thus causing them to expand.

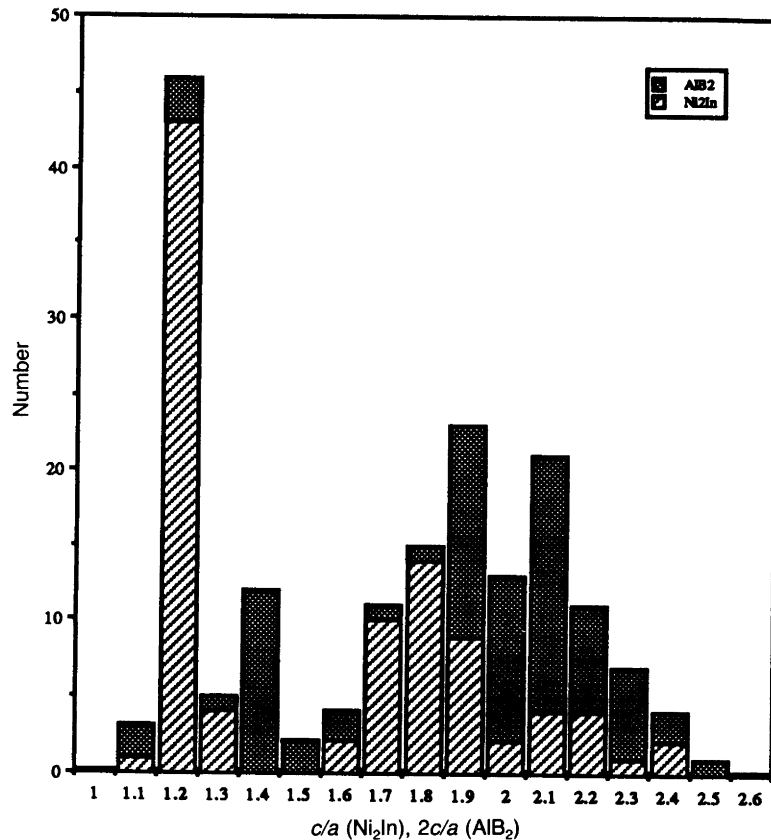[†]There is some distortion from hexagonal eutaxy in *C37* (Fig. 4).

Fig. 8. Frequency distribution of *c/a* values for both 'Ni$_2$In' and 'AlB$_2$' types. (Intervals are 0.05 for the former and 0.025 for the latter.)

reported to have variable stoichiometry, the possibility that they are all one family should be, and indeed has been, considered.

But we are still not done. The structure of ω-Ti [$=$Ti(1)Ti(2)$_2$] is also in this family (space group *P6/mmm* with *c/a* $=$ 0.61), so that it too belongs to the Ni$_2$In/AlB$_2$ branch. The relationship of this structure to *bcc* is well known.[14,15] (The transition between them involves only

Fig. 9. The *B8$_a$*-type structure of NiAs projected on (11$\bar{2}$0) of the hexagonal unit cell [$\equiv$(100) of the orthohexagonal cell]; scale 1 cm $=$ 1 Å. Larger circles are Ni, smaller are As: open at *x* $=$ 0, filled at *x* $=$ ½. Cf. Fig. 5.

small atomic displacements.) Thus we can consider as ultimate parent ('ancestor') structures the binary AlB$_2$ for large *c/a* and elemental *bcc* for small *c/a*.

Net descriptions

Relationship between three-dimensional nets in the C32, C23/29 and the CeCu$_2$ structure types. If we consider MgB$_2$ (*c/a* $=$ 1.14) to be a type compound for *C*32, we note that it could formally be written Mg^{2+}(B$^-$)$_2$, with B$^-$ (isoelectronic with C) forming graphite-like (6^3) layers stacked prismatically ($\cdots aaa \cdots$). Thus MgB$_2$ could be considered as a Zintl compound.

Puckering these 6^3 layers [so that fourth bonds (either 'up' or 'down') are formed between them] can convert this 'graphite' part into four-connected, three-dimensional nets. One such conversion is (rather obviously) into the lonsdaleite ('hexagonal diamond') net, in which, around a hexagon, the new bond sequence is ...up down up down up down... This transforms the net in MgB$_2$ to that in the CaIn$_2$-type structure: yet another large family. [CaIn$_2$ can likewise be written Ca^{2+}(In$^-$)$_2$, and we note that In$^-$ is isoelectronic with Sn (which has a cubic diamond form).] As we will show later, a different pattern of connecting the honeycomb layers produces the SrAl$_2$ structure type.
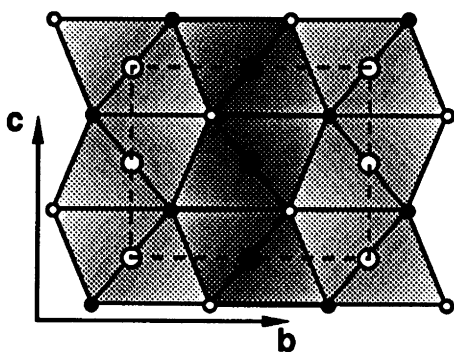
In the structure of SrH_2, Sr and H(1) form a four-connected net in which all nodes are topologically the same: in fact, the net is identical to one described by Smith[16] as deriving from interconnected plane 6^3 nets, and identified by him as occurring in framework aluminosilicates such as $RbAlSiO_4$ (and given his catalogue number 4). In its most symmetrical form the symmetry of this net is *Imma*, and it has also been recognized[17] as occurring in a large family of
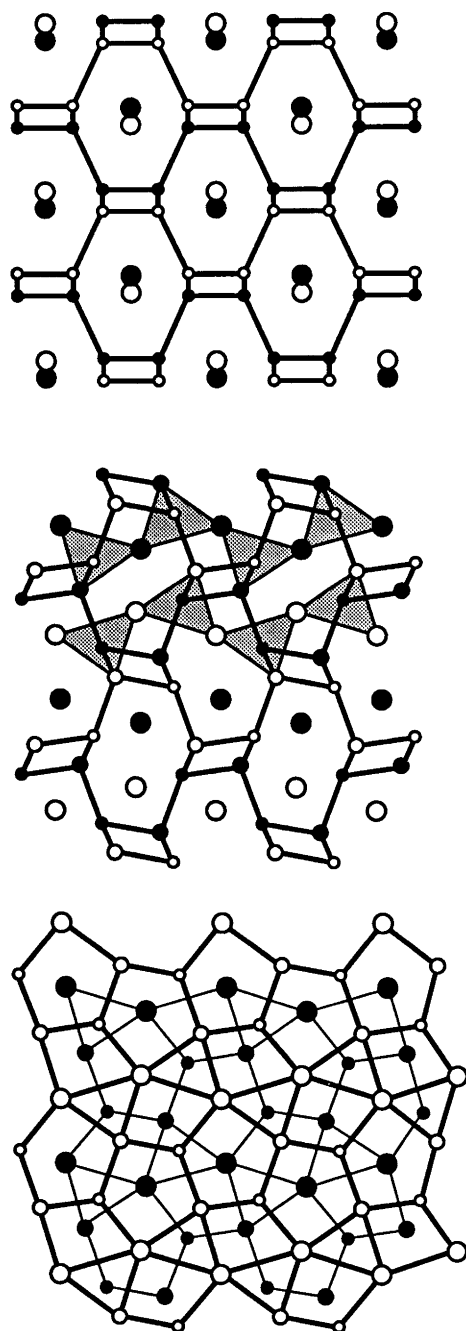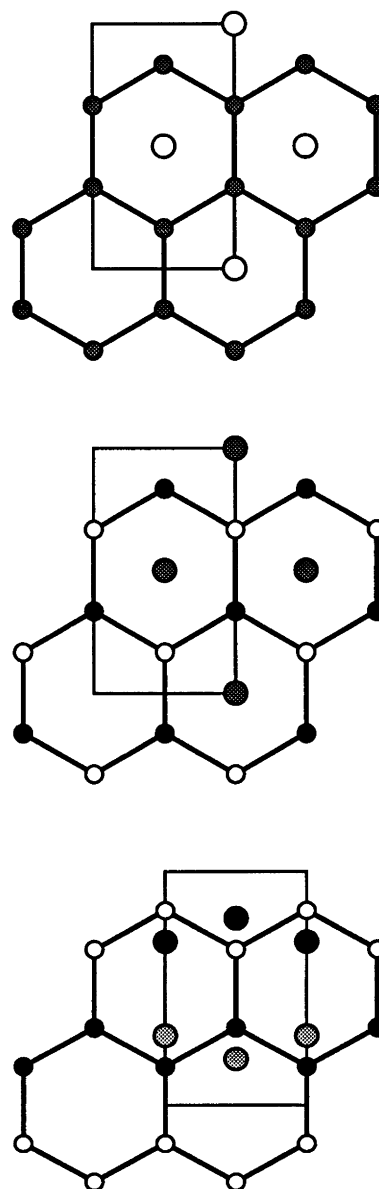

Fig. 10. Top: the structure of $SrAl_2$ projected on (100) with *b* horizontal and *c* vertical on the page. Large circles represent Sr atoms and small circles represent Al atoms. Filled and empty circles differ in elevation by *a*/2 = 2.42 Å. The heavy lines indicate the Al net defined by the four shortest Al⋯Al distances. This would appear as a honeycomb (6^3) net if projected down *a*. Middle: the structure of SrMgSi drawn on the same scale projected on (010) with *a* horizontal and *c* vertical on the page. Large circles represent Sr atoms, intermediate circles represent Mg atoms and small circles represent Si atoms. Filled and empty circles differ in elevation by *b*/2 = 2.28 Å. The heavy lines indicate the Mg/Si net defined by the four shortest Mg⋯Si distances. The lightly outlined triangles in the top half represent triangular faces of (Mg,Sr) prisms surrounding Si. Bottom: The same atoms as in the middle drawing but now with the nets at $y = \frac{1}{4}$ and $y = \frac{3}{4}$ emphasized.

Fig. 11. 'Basal plane' projections of the MgB_2, $CaIn_2$ and $SrAl_2$ structures showing the 6^3 nets and 'stuffing' atoms (large), and using a common, orthorhombic or (for the top two) orthohexagonal unit cell. Top: MgB_2 [Mg at 0 and ½ (open), B at ±¼ (shaded)]; centre: $CaIn_2$ [Ca at ±¼ (shaded), In at ¼ ± 0.045 (open; bonds 'down'), ¾ ± 0.045 (filled; bonds 'up']; bottom: $SrAl_2$ [Sr at 0.3 (light), 0.7 (dark); Al at ¼ ± 0.16 (open; bonds 'down'), ¾ ± 0.16 (filled; bonds 'up')]. Note the different sequences of up/down bonds linking the layers in the latter two.

structures of the same symmetry, of which the prototypical compound[1] is $CeCu_2$. We therefore expect that there will be a simple relationship between the $CeCu_2$ structure (of which there are more than 100 examples known)[1] and the $C23$ structure. To illustrate this point we give examples of each structure type chosen for their chemical similarity, *viz.* $SrAl_2$ ($CeCu_2$ type) and SrMgSi ($C23$). These two compounds have unit cells of similar size: $SrAl_2$ (*Imma*) is $4.84 \times 7.99 \times 7.92$ Å and SrMgSi (*Pnma*) is $7.78 \times 4.56 \times 8.49$ Å. Fig. 10 shows how the two structures are related and depicts analogous nets in both.

In Fig. 11 we show, in plan, the nets (and other atoms) in the three structures MgB_2, $CaIn_2$ and $SrAl_2$. It is worth noting that, for $SrAl_2$, the axial ratio equivalent to $(c/a)_{hex}$ is $(b/a)_{Imma} = 1.65$, i.e. midway between the values of 1.23 for Ni_2In and 2.17 (for the equivalent doubled cell) for AlB_2 (cf. Fig. 8). (The values are 2.28 for MgB_2 and 1.58 for $CaIn_2$.)

This description of the structure of $SrAl_2$ emphasizes its nature as a 'Zintl' compound; formally it may be written as $Sr^{2+}(Al^-)_2$ with the Al^- forming a four-connected net in a manner analogous to Al^- forming a diamond net in LiAl ($= Li^+Al^-$). SrMgSi is isoelectronic with $SrAl_2$, but its symmetry is lowered by ordering of Mg and Si. Thus the $SrAl_2$ structure (high-symmetry, $CeCu_2$ type) may be considered the binary parent of $C23$ compounds, for which the stuffed four-connected net description is also appropriate.

The C23 structure in terms of plane nets. In many compounds with the $C23$ structure, the difference in electronegativity is quite small (YNiSn is an example), so one is led to look for a description that treats all atoms on an equal footing. An obvious such description is in terms of the nets of atoms at $y = ¼$ and $¾$.* Fig. 10 also illustrates this description, again using coordinates for SrMgSi for convenience in comparison. This planar net is remarkable in that it is its own dual, so that atoms above and below the centres of polygons in a layer form the same net. (In the structure the two layers are related by a 2_1 axis.) For a net to be self-dual it is necessary for the number of N-gons to be equal to the number of N-connected nodes. The $C23$ net contains equal numbers of triangles, quadrangles and pentagons, and the nodes (also occurring in equal numbers) are 4.5^2, $3.4.5^2$ and $3.4.3.4.5$. In this connection it might be noted that of the approximately 100 plane nets occurring in crystal structures previously described and discussed by O'Keeffe and Hyde,[19] only one (4^4) was self-dual. According to this net description Sr is in capped pentagonal prisms, Mg in capped quadrangular prisms, and Si in capped triangular prisms.

The description in terms of nets is still essentially ternary, as there are three topologically distinct nodes in the net. However, if the triangles and pentagons were con-

Table 2. Correspondence between atoms in the *ABC* structures discussed in this paper.

Compound	A	B	C
$PbCl_2$	Pb	Cl	Cl
Co_2Si	Si	Co	Co
Ni_2In	In	Ni	Ni
$SrAl_2^a$	Al	Al	Sr
SrMgSi	Si	Mg	Sr
AlB_2^a	B	B	Al
NiAs	As	–	Ni

[a]In the $SrAl_2$ and AlB_2 structures, A and B are crystallographically the same.

verted into squares one would recover the self-dual net 4^4. The analogous stacking of such nets could correspond to either the *bbc* or *fcc* lattice packings according to the inter-layer spacing, so that the parent structure in this instance is an elemental structure. The *bcc* structure also occurred as a parent structure above.

Conclusions

The several relationships between the remarkable families of structures we have been discussing show dramatically how the same or similar structure types can adjust to the presence of different elements. In particular there is a gradual change along lines joining typical metallic compounds, ionic compounds and those compounds (Zintl compounds) in which more than one type of bonding might be recognized. It is important therefore not to draw conclusions about the nature of bonding in crystals from the occurrence of a given crystal structure. Perhaps more importantly, the existence of so many compounds with closely related structures emphasizes the underlying unity of chemical bonding and warns us not to force crystals into procrustean beds labelled 'ionic', 'covalent', 'metallic' etc.

In these generally ternary structures ABC one can identify three kinds of atom. A is often approximately in hexagonal eutaxy, B in 'octahedral' sites and C in 'tetrahedral' sites. Table 2 identifies the atoms in the various sites for the compounds discussed and can serve as a summary of the structural relationships.

References

1. Villars, P. and Calvert, L. D. *Pearson's Handbook of Crystallographic Data for Intermetallic Phases,* American Society of Metals, Metals Park, Ohio 1985.

---

* A comparison of analogous nets in $C23$, $C37$ and $B8_b$ has been given by Shoemaker and Shoemaker.[18]

2. Brese, N. E., O'Keeffe, M. and Von Dreele, R. B. *J. Solid State Chem.* **88** (1990) 571.
3. Jeitschko, W. *Acta Crystallogr., Sect. B 24* (1968) 930.
4. Flahaut, J. and Thévet, F. *J. Solid State Chem. 32* (1979) 365.
5. Hyde, B. G., Andersson, S., Bakker, M., Plug, C. M. and O'Keeffe, M. *Progr. Solid State Chem. 12* (1979) 273.
6. Hyde, B. G. and Andersson, S. *Inorganic Crystal Structures*, Wiley, New York 1989.
7. O'Keeffe, M. and Hyde, B. G. *Struct. Bonding 61* (1985) 77.
8. Jeitschko, W., Block, G., Kahnert, G. E. and Behrens, R. K. *J. Solid State Chem. 89* (1990) 191.
9. Wyckoff, R. W. G. *Crystal Structures*, Wiley, New York 1963, Vol. 1, p. 303.
10. Bärnighausen, H. *Inorg. Chem. 24* (1985) 408.
11. O'Keeffe, M. and Hyde, B. G. *J. Solid State Chem. 13* (1975) 172.
12. O'Keeffe, M. *Struct. Bonding 71* (1989) 161.
13. Brown, I. D. and Altermatt, D. *Acta Crystallogr., Sect. B 41* (1985) 244.
14. Andersson, S. *Arkiv. Kem. 15* (1960) 247.
15. O'Keeffe, M. and Andersson, S. *Acta Crystallogr., Sect. A 33* (1977) 914.
16. Smith, J. V. *Am. Miner. 62* (1977) 703.
17. Lyttle, W. H. *M. S. Thesis*, Arizona State University 1982.
18. Shoemaker, C. B. and Shoemaker, D. P. *Acta Crystallogr. 18* (1965) 900.
19. O'Keeffe, M. and Hyde, B. G. *Philos. Trans R. Soc. (London), Ser. A 295* (1980) 553.
20. Andresen, A. F., Maeland, A. J. and Slotfeld-Ellingsen, D. *J. Solid State Chem. 20* (1977) 93.
21. Bronger, W., Chi-Chien, S. and Müller, P. Z. *Anorg. Allg. Chem. 545* (1987) 69.
22. Byström, A. *Arkiv. Kem. Miner. Geol., Ser. A 24*, No. 33 (1947); see *Struct. Rep. 11* (1947–48) 265.
23. Nozik, Ju. Z., Fykin, L. E. and Muradjan, L. A. *Sov. Phys. Crystallogr. 21* (1976) 38.
24. Brackett, E. B., Brackett, T. E. and Sears, R. L. *J. Phys. Chem. 67* (1963) 2132.
25. Graham, J. and McTaggart, F. K. *Austr. J. Chem. 13* (1960) 67.