Supplementary material:
Structural building principles of complex face-centered cubic intermetallics

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1. Atomic sites – Superstructure description

Table 1
Symmetry relations between basic and modulated structures.

$F\bar{4}3m$	$cF16$	→ maximal non-isomorphic subgroup	$\vec{a}' = 3\vec{a}$	index 27	→ $F\bar{4}3m$	$cF464$
$Fd\bar{3}m$	$cF16$	→ maximal non-isomorphic subgroup (& origin shift $-(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ with origin choice 1)	$\vec{a}' = 3\vec{a}$	index 27	→ $Fd\bar{3}m$	$cF464$
$P\bar{4}3m$	$cP16$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}' = 2\vec{a}$	index 2	→ $F\bar{4}3m$	$cF128$
$F\bar{4}3m$	$cF128$	→ maximal isomorphic subgroup (loss of centering)	-	index 4	→ $P\bar{4}3m$	$cP128$
$P\bar{4}3m$	$cP128$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}'' = 2\vec{a}'$	index 2	→ $F\bar{4}3m$	$cF1024$
$Pm\bar{3}m$	$cP16$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}' = 2\vec{a}$	index 2	→ $Fm\bar{3}m$	$cF128$
$Fm\bar{3}m$	$cF128$	→ maximal isomorphic subgroup (loss of centering)	-	index 4	→ $Pn\bar{3}m$	$cP128$
$Pn\bar{3}m$	$cP128$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}'' = 2\vec{a}'$	index 2	→ $Fd\bar{3}m$	$cF1024$
$Pm\bar{3}m$	$cP16$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}' = 2\vec{a}$	index 2	→ $Fm\bar{3}m$	$cF128$
$Fm\bar{3}m$	$cF128$	→ maximal isomorphic subgroup (loss of centering)	-	index 4	→ $Pm\bar{3}m$	$cP128$
$Pm\bar{3}m$	$cP128$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}'' = 2\vec{a}'$	index 2	→ $Fm\bar{3}m$	$cF1024$
$Pm\bar{3}m$	$cP16$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}' = 2\vec{a}$	index 2	→ $Fm\bar{3}m$	$cF128$
$Fm\bar{3}m$	$cF128$	→ maximal isomorphic subgroup (loss of centering)	-	index 4	→ $Pm\bar{3}m$	$cP128$
$Pm\bar{3}m$	$cP128$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}'' = 2\vec{a}'$	index 2	→ $Fm\bar{3}c$	$cF1024$
$Pm\bar{3}$	$cP16$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}' = 2\vec{a}$	index 2	→ $Fm\bar{3}$	$cF128$
$Fm\bar{3}$	$cF128$	→ maximal isomorphic subgroup (loss of centering)	-	index 4	→ $Pn\bar{3}$	$cP128$
$Pn\bar{3}$	$cP128$	→ maximal non-isomorphic subgroup (*klassengleich*)	$\vec{a}'' = 2\vec{a}'$	index 2	→ $Fd\bar{3}$	$cF1024$

The basic structures of all cubic compounds discussed in this work correspond to a $cF16$-NaTl structure ($Fd\bar{3}m$, ab) or to derivatives of it, which exhibit lower symmetry.

The average structure of the $cF464$-structures in $F\bar{4}3m$ preserve the space group symmetry the basic structure contains four Wyckoff positions, each one resulting from six Wyckoff positions of the original structure:

- site 1 – $4a$ $0,0,0 \Leftarrow 4a$, $16e3$, $16e6$, $24f2$, $48h1$, $48h6$;
- site 2 – $4c$ $\frac{1}{4},\frac{1}{4},\frac{1}{4} \Leftarrow 4d$, $16e2$, $16e5$, $24g1$, $48h4$, $48h5$;
- site 3 – $4b$ $\frac{1}{2},\frac{1}{2},\frac{1}{2} \Leftarrow 4b$, $16e1$, $16e8$, $24f1$, $48h3$, $48h8$;
- site 4 – $4d$ $\frac{3}{4},\frac{3}{4},\frac{3}{4} \Leftarrow 4c$, $16e4$, $16e7$, $24g2$, $48h2$, $48h7$.

The average structure of the $cF464$-structures in $Fd\bar{3}m$ also exhibit the same symmetry as the original structures. The Wyckoff positions of the basic structure and the corresponding ones in the original unit cell are the following[1]:

- site 1 – $8a$ $0,0,0 \Leftarrow 8b$, $32e1$, $32e2$, $96g2$, $96g3$;
- site 2 – $8b$ $\frac{1}{2},\frac{1}{2},\frac{1}{2} \Leftarrow 8a$, $96g1$, $96g4$.

The average structure of $cF1124$-$Cu_{56.9}Cd_{43.1}$ ($F\bar{4}3m$) has space group symmetry $P\bar{4}3m$. The atomic sites of the basic structure are: $1a$ $0,0,0$; $1b$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $3c$ $0,\frac{1}{2},\frac{1}{2}$; $3d$ $\frac{1}{2},0,0$; $4e$ x,x,x ($x=\frac{1}{4}$); $4e$ x,x,x ($x=\frac{3}{4}$).

The average structures of $cF(1192-40)$-$Cd_{66.7}Na_{33.3}$ and $cF(1192-23)$-$Al_{53.6}Mg_{46.4}$ ($Fd\bar{3}m$) has space group symmetry $Pm\bar{3}m$. The atomic sites of the basic structure are: $1a$ $0,0,0$; $1b$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $3c$ $0,\frac{1}{2},\frac{1}{2}$; $3d$ $\frac{1}{2},0,0$; $8g$ x,x,x ($x=\frac{1}{4}$). The symmetry and sites are the same for the $(4\times4\times4)$-fold superstructures in space groups $Fm\bar{3}m$ and $Fm\bar{3}c$.

The average structure of the $(4\times4\times4)$-fold superstructure in space group $Fd\bar{3}$ has space group symmetry $Pm\bar{3}$. The atomic sites of the basic structure are: $1a$ $0,0,0$; $1b$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$; $3c$ $0,\frac{1}{2},\frac{1}{2}$; $3d$ $\frac{1}{2},0,0$; $8g$ x,x,x ($x=\frac{1}{4}$)[2].

[1] The classification of sites $96g2$ and $96g4$ is slightly ambiguous, since they have similar distances to both, sites 1 and 2 of the basic structure.
[2] The coordinates of the Wyckoff positions are the same as in space group $Pm\bar{3}m$ (see above), but their site symmetry is lower.

2. Symmetry relations

Table 2
Details on the structure types between *cI*2-W and the investigated complex intermetallic structures. Space groups in parentheses belong to the same lattice complex / exhibit the same Wyckoff coordinates.

Structure type	Pearson symbol	Space group	Wyckoff sequence	Represented structures	Comments
W	$cI2$	$Im\bar{3}m$	a	$Im\bar{3}m - cI2$, $(Pn\bar{3}m - cP2)$	
CsCl	$cP2$	$Pm\bar{3}m$	ab	$Pm\bar{3}m - cP2$, $(P\bar{4}3m - cP2)$	
$Fe_{13}Ge_3$ †	$cP16$	$Pm\bar{3}m$	$abcdg$	$Pm\bar{3}m - cP16$, $(Pm\bar{3} - cP16)$	
$CuHg_2Ti$	$cF16$	$F\bar{4}3m$	$abcd$	$F\bar{4}3m - cF16$	
NaTl	$cF16$	$Fd\bar{3}m$	ab	$Fd\bar{3}m - cF16$	
Ir_4Sc_{11}	$cF120$	$Fm\bar{3}m$	$abdef^2$	$Fm\bar{3}m - cF128$, $(Fm\bar{3} - cF128)$	+ site c
$Ti_6Co_7Al_{17}$	$cF120$	$F\bar{4}3m$	abe^4fg	$F\bar{4}3m - cF128$	+ sites cd
Tl_7Sb_2	$cI54$	$Im\bar{3}m$	$aefh$	$Im\bar{3}m - cI54$	
Al_4Cu_9	$cP52$	$P\bar{4}3m$	e^4fgi^2	$P\bar{4}3m - cP54$	+ sites ab
Cu_5Zn_8	$cI52$	$I\bar{4}3m$	(e^2gk) ‡	$(Pn\bar{3}m - cP52)$	+ site a

† $Fe_{15}Co$ and Fe_9Co_7 exhibit the same Wyckoff sequence with different occupations due to a differing composition.
‡ These sites refer to space group $Pn\bar{3}m$. The Wyckoff sequence in space group $I\bar{4}3m$ is c^2eg.

Table 3
Wyckoff sites in space group $Im\bar{3}m$ of the Bärnighausen tree, *cI*2, *cI*16, *cI*432.

Site	Site symmetry	x	y	z	Generating site
	$Im\bar{3}m$, (229), $cI2$, $a \times a \times a - a$				
$2a$	$\bar{m}3m$	0	0	0	
	$Im\bar{3}m$, (229), $cI16$, $2a \times 2a \times 2a - abc$				
$2a$	$m\bar{3}m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP2$)
$6b$	$4/m\bar{m}.m$	0	1/2	1/2	$1a$ ($Pm\bar{3}m$, $cP2$)
$8c$	$\bar{.}3m$	1/4	1/4	1/4	$1b$ ($Pm\bar{3}m$, $cP2$)
	$Im\bar{3}m$, (229), $cI432$, $6a \times 6a \times 6a - abce^2f^2gh^2ijk^4$				
$2a$	$m\bar{3}m$	0	0	0	$2a$ ($Im\bar{3}m$, $cI16$)
$6b$	$4/m\bar{m}.m$	0	1/2	1/2	$6b$ ($Im\bar{3}m$, $cI16$)
$8c$	$.3m$	1/4	1/4	1/4	$8c$ ($Im\bar{3}m$, $cI16$)
$12e$	$4m.m$	1/3	0	0	$2a$ ($Im\bar{3}m$, $cI16$)
$12e$	$4m.m$	1/6	0	0	$6b$ ($Im\bar{3}m$, $cI16$)
$16f$	$.3m$	1/3	1/3	1/3	$2a$ ($Im\bar{3}m$, $cI16$)
$16f$	$.3m$	1/12	1/12	1/12	$8c$ ($Im\bar{3}m$, $cI16$)
$24g$	$mm2..$	1/6	0	1/2	$6b$ ($Im\bar{3}m$, $cI16$)
$24h$	$m.m2$	1/3	0	0	$2a$ ($Im\bar{3}m$, $cI16$)
$24h$	$m.m2$	0	1/6	1/6	$6b$ ($Im\bar{3}m$, $cI16$)
$48i$	$..2$	1/4	1/12	5/12	$8c$ ($Im\bar{3}m$, $cI16$)
$48j$	$m..$	0	1/6	1/3	$6b$ ($Im\bar{3}m$, $cI16$)
$48k$	$..m$	1/4	1/4	1/12	$8c$ ($Im\bar{3}m$, $cI16$)
$48k$	$..m$	1/6	1/6	1/3	$6b$ ($Im\bar{3}m$, $cI16$)
$48k$	$..m$	1/12	1/12	1/4	$8c$ ($Im\bar{3}m$, $cI16$)
$48k$	$..m$	5/12	5/12	1/12	$8c$ ($Im\bar{3}m$, $cI16$)

Table 4
Wyckoff sites in space group $Pm\bar{3}m$ of the Bärnighausen tree, *cP*2, *cP*16, *cP*128.

Site	Site symmetry	x	y	z	Generating site
	$Pm\bar{3}m$, (221), $cP2$, $a \times a \times a - ab$				
$1a$	$m\bar{3}m$	0	0	0	$2a$ ($Im\bar{3}m$, $cI2$)
$1b$	$\bar{m}3m$	1/2	1/2	1/2	$2a$ ($Im\bar{3}m$, $cI2$)
	$Pm\bar{3}m$, (221), $cP16$, $2a \times 2a \times 2a - abcdg$				
$1a$	$m\bar{3}m$	0	0	0	$2a$ ($Im\bar{3}m$, $cI16$)
$1b$	$m\bar{3}m$	1/2	1/2	1/2	$2a$ ($Im\bar{3}m$, $cI16$)
$3c$	$4/mm.m$	0	1/2	1/2	$6b$ ($Im\bar{3}m$, $cI16$)
$3d$	$4/mm.m$	1/2	0	0	$6b$ ($Im\bar{3}m$, $cI16$)
$8g$	$\bar{.}3m$	1/4	1/4	1/4	$8c$ ($Im\bar{3}m$, $cI16$)
	$Pm\bar{3}m$, (221), $cP128$, $4a \times 4a \times 4a - abcdefg^3hijm^2$				
$1a$	$m\bar{3}m$	0	0	0	$4a$ ($Fm\bar{3}m$, $cF128$)
$1b$	$m\bar{3}m$	1/2	1/2	1/2	$4b$ ($Fm\bar{3}m$, $cF128$)
$3c$	$4/mm.m$	0	1/2	1/2	$4a$ ($Fm\bar{3}m$, $cF128$)
$3d$	$4/mm.m$	1/2	0	0	$4b$ ($Fm\bar{3}m$, $cF128$)
$6e$	$4m.m$	1/4	0	0	$24e$ ($Fm\bar{3}m$, $cF128$)
$6f$	$4m.m$	1/4	1/2	1/2	$24e$ ($Fm\bar{3}m$, $cF128$)
$8g$	$.3m$	1/4	1/4	1/4	$8c$ ($Fm\bar{3}m$, $cF128$)
$8g$	$.3m$	1/8	1/8	1/8	$32f$ ($Fm\bar{3}m$, $cF128$)
$8g$	$.3m$	3/8	3/8	3/8	$32f$ ($Fm\bar{3}m$, $cF128$)
$12h$	$mm2..$	1/4	1/2	0	$24e$ ($Fm\bar{3}m$, $cF128$)
$12i$	$m.m2$	0	1/4	1/4	$24d$ ($Fm\bar{3}m$, $cF128$)
$12j$	$m.m2$	1/2	1/4	1/4	$24d$ ($Fm\bar{3}m$, $cF128$)
$24m$	$..m$	5/8	5/8	1/8	$32f$ ($Fm\bar{3}m$, $cF128$)
$24m$	$..m$	7/8	7/8	3/8	$32f$ ($Fm\bar{3}m$, $cF128$)

Table 5
Wyckoff sites in space group $P\bar{4}3m$ of the Bärnighausen tree, $cP2$, $cP16$, $cP128$.

Site	Site symmetry	x	y	z	Generating site
	$P\bar{4}3m$, (215), $cP2$, $a \times a \times a - ab$				
$1a$	$\bar{4}3m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP2$)
$1b$	$\bar{4}3m$	1/2	1/2	1/2	$1b$ ($Pm\bar{3}m$, $cP2$)
	$P\bar{4}3m$, (215), $cP16$, $2a \times 2a \times 2a - abcde^2$				
$1a$	$\bar{4}3m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP16$)
$1b$	$\bar{4}3m$	1/2	1/2	1/2	$1b$ ($Pm\bar{3}m$, $cP16$)
$3c$	$\bar{4}2.m$	0	1/2	1/2	$3c$ ($Pm\bar{3}m$, $cP16$)
$3d$	$\bar{4}2.m$	1/2	0	0	$3d$ ($Pm\bar{3}m$, $cP16$)
$4e$	$.3m$	1/4	1/4	1/4	$8g$ ($Pm\bar{3}m$, $cP16$)
$4e$	$.3m$	3/4	3/4	3/4	$8g$ ($Pm\bar{3}m$, $cP16$)
	$P\bar{4}3m$, (215), $cP128$, $4a \times 4a \times 4a - abcde^6fghi^6$				
$1a$	$\bar{4}3m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP128$)
$1b$	$\bar{4}3m$	1/2	1/2	1/2	$1b$ ($Pm\bar{3}m$, $cP128$)
$3c$	$\bar{4}2.m$	0	1/2	1/2	$3c$ ($Pm\bar{3}m$, $cP128$)
$3d$	$\bar{4}2.m$	1/2	0	0	$3d$ ($Pm\bar{3}m$, $cP128$)
$4e$	$.3m$	1/4	1/4	1/4	$8g$ ($Pm\bar{3}m$, $cP128$)
$4e$	$.3m$	3/4	3/4	3/4	$8g$ ($Pm\bar{3}m$, $cP128$)
$4e$	$.3m$	1/8	1/8	1/8	$8g$ ($Pm\bar{3}m$, $cP128$)
$4e$	$.3m$	3/8	3/8	3/8	$8g$ ($Pm\bar{3}m$, $cP128$)
$4e$	$.3m$	5/8	5/8	5/8	$8g$ ($Pm\bar{3}m$, $cP128$)
$4e$	$.3m$	7/8	7/8	7/8	$8g$ ($Pm\bar{3}m$, $cP128$)
$6f$	$2.mm$	1/4	0	0	$6e$ ($Pm\bar{3}m$, $cP128$)
$6g$	$2.mm$	1/4	1/2	1/2	$6f$ ($Pm\bar{3}m$, $cP128$)
$12h$	$2..$	1/4	1/2	0	$12h$ ($Pm\bar{3}m$, $cP128$)
$12i$	$..m$	1/4	1/4	0	$12i$ ($Pm\bar{3}m$, $cP128$)
$12i$	$..m$	1/4	1/4	1/2	$12j$ ($Pm\bar{3}m$, $cP128$)
$12i$	$..m$	5/8	5/8	1/8	$24m$ ($Pm\bar{3}m$, $cP128$)
$12i$	$..m$	7/8	7/8	3/8	$24m$ ($Pm\bar{3}m$, $cP128$)
$12i$	$..m$	1/8	1/8	5/8	$24m$ ($Pm\bar{3}m$, $cP128$)
$12i$	$..m$	3/8	3/8	7/8	$24m$ ($Pm\bar{3}m$, $cP128$)

Table 6
Wyckoff sites in space group $Pn\bar{3}m$ of the Bärnighausen tree, $cP2$, $cP16$, $cP128$.

Site	Site symmetry	x	y	z	Generating site
	$Pn\bar{3}m$, (224), $cP2$, $a \times a \times a - a$				
$2a$	$\bar{4}3m$	0	0	0	$2a$ ($Im\bar{3}m$, $cI2$)
	$Pn\bar{3}m$, (224), $cP16$, $2a \times 2a \times 2a - abcd$				
$2a$	$\bar{4}3m$	0	0	0	$2a$ ($Im\bar{3}m$, $cI16$)
$4b$	$.\bar{3}m$	1/4	1/4	1/4	$8c$ ($Im\bar{3}m$, $cI16$)
$4c$	$.\bar{3}m$	3/4	3/4	3/4	$8c$ ($Im\bar{3}m$, $cI16$)
$6d$	$\bar{4}2.m$	0	1/2	1/2	$6b$ ($Im\bar{3}m$, $cI16$)
	$Pn\bar{3}m$, (224), $cP128$, $4a \times 4a \times 4a - abcde^2fgk^3$				
$2a$	$\bar{4}3m$	0	0	0	$8c$ ($Fm\bar{3}m$, $cF128$)
$4b$	$.\bar{3}m$	1/4	1/4	1/4	$4a$ ($Fm\bar{3}m$, $cF128$)
$4c$	$.\bar{3}m$	3/4	3/4	3/4	$4b$ ($Fm\bar{3}m$, $cF128$)
$6d$	$\bar{4}2.m$	0	1/2	1/2	$8c$ ($Fm\bar{3}m$, $cF128$)
$8e$	$.3m$	3/8	3/8	3/8	$32f$ ($Fm\bar{3}m$, $cF128$)
$8e$	$.3m$	5/8	5/8	5/8	$32f$ ($Fm\bar{3}m$, $cF128$)
$12f$	2.22	1/4	0	1/2	$24d$ ($Fm\bar{3}m$, $cF128$)
$12g$	$2.mm$	1/4	0	0	$24d$ ($Fm\bar{3}m$, $cF128$)
$24k$	$..m$	1/4	1/4	1/2	$24e$ ($Fm\bar{3}m$, $cF128$)
$24k$	$..m$	7/8	7/8	3/8	$32f$ ($Fm\bar{3}m$, $cF128$)
$24k$	$..m$	1/8	1/8	5/8	$32f$ ($Fm\bar{3}m$, $cF128$)

Table 7
Wyckoff sites in space group $Pm\bar{3}$ of the Bärnighausen tree, $cP16$.

Site	Site symmetry	x	y	z	Generating site
	$Pm\bar{3}$, (200), $cP16$, $2a \times 2a \times 2a - abcdi$				
$1a$	$m\bar{3}.$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP16$)
$1b$	$m\bar{3}.$	1/2	1/2	1/2	$1b$ ($Pm\bar{3}m$, $cP16$)
$3c$	$mmm..$	0	1/2	1/2	$3c$ ($Pm\bar{3}m$, $cP16$)
$3d$	$mmm..$	1/2	0	0	$3d$ ($Pm\bar{3}m$, $cP16$)
$8i$	$.3.$	1/4	1/4	1/4	$8g$ ($Pm\bar{3}m$, $cP16$)

Table 8
Wyckoff sites in space group $Pn\bar{3}$ of the Bärnighausen tree, $cP128$.

Site	Site symmetry	x	y	z	Generating site
	$Pn\bar{3}$, (201), $cP128$, $4a \times 4a \times 4a - abcde^2fgh^3$				
$2a$	$2\bar{3}.$	0	0	0	$8c$ ($Fm\bar{3}$, $cF128$)
$4b$	$.\bar{3}.$	1/4	1/4	1/4	$4a$ ($Fm\bar{3}$, $cF128$)
$4c$	$.\bar{3}.$	3/4	3/4	3/4	$4b$ ($Fm\bar{3}$, $cF128$)
$6d$	$222..$	0	1/2	1/2	$8c$ ($Fm\bar{3}$, $cF128$)
$8e$	$.3.$	3/8	3/8	3/8	$32f$ ($Fm\bar{3}$, $cF128$)
$8e$	$.3.$	5/8	5/8	5/8	$32f$ ($Fm\bar{3}$, $cF128$)
$12f$	$2..$	1/4	0	0	$24d$ ($Fm\bar{3}$, $cF128$)
$12g$	$2..$	1/4	1/2	0	$24d$ ($Fm\bar{3}$, $cF128$)
$24h$	$2..$	1/2	1/4	1/4	$24e$ ($Fm\bar{3}$, $cF128$)
$24h$	$2..$	3/8	7/8	7/8	$32f$ ($Fm\bar{3}$, $cF128$)
$24h$	$2..$	5/8	1/8	1/8	$32f$ ($Fm\bar{3}$, $cF128$)

Table 9
Wyckoff sites in space group $Fm\bar{3}m$ of the Bärnighausen tree, $cF128$, $cF1024$.

Site	Site symm.	x	y	z	Generating site
	$Fm\bar{3}m$, (225), $cF128$, $4a \times 4a \times 4a - abcdef^2$				
$4a$	$m\bar{3}m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP16$)
$4b$	$m\bar{3}m$	1/2	1/2	1/2	$1a$ ($Pm\bar{3}m$, $cP16$)
$8c$	$\bar{4}3m$	1/4	1/4	1/4	$1b$ ($Pm\bar{3}m$, $cP16$)
$24d$	$m.mm$	0	1/4	1/4	$3c$ ($Pm\bar{3}m$, $cP16$)
$24e$	$4m.m$	1/4	0	0	$3d$ ($Pm\bar{3}m$, $cP16$)
$32f$	$.3m$	1/8	1/8	1/8	$8g$ ($Pm\bar{3}m$, $cP16$)
$32f$	$.3m$	3/8	3/8	3/8	$8g$ ($Pm\bar{3}m$, $cP16$)
	$Fm\bar{3}m$, (225), $cF1024$, $8a \times 8a \times 8a - abcde^3f^6hi^2jk^5$				
$4a$	$m\bar{3}m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP128$)
$4b$	$m\bar{3}m$	1/2	1/2	1/2	$1a$ ($Pm\bar{3}m$, $cP128$)
$8c$	$\bar{4}3m$	1/4	1/4	1/4	$1b$ ($Pm\bar{3}m$, $cP128$)
$24d$	$m.mm$	0	1/4	1/4	$3c$ ($Pm\bar{3}m$, $cP128$)
$24e$	$4m.m$	1/4	0	0	$3d$ ($Pm\bar{3}m$, $cP128$)
$24e$	$4m.m$	1/8	0	0	$6e$ ($Pm\bar{3}m$, $cP128$)
$24e$	$4m.m$	3/8	0	0	$6e$ ($Pm\bar{3}m$, $cP128$)
$32f$	$.3m$	1/8	1/8	1/8	$8g$ ($Pm\bar{3}m$, $cP128$)
$32f$	$.3m$	3/8	3/8	3/8	$8g$ ($Pm\bar{3}m$, $cP128$)
$32f$	$.3m$	1/16	1/16	1/16	$8g$ ($Pm\bar{3}m$, $cP128$)
$32f$	$.3m$	3/16	3/16	3/16	$8g$ ($Pm\bar{3}m$, $cP128$)
$32f$	$.3m$	9/16	9/16	9/16	$8g$ ($Pm\bar{3}m$, $cP128$)
$32f$	$.3m$	11/16	11/16	11/16	$8g$ ($Pm\bar{3}m$, $cP128$)
$48h$	$m.m2$	0	1/8	1/8	$12i$ ($Pm\bar{3}m$, $cP128$)
$48i$	$m.m2$	1/2	1/8	1/8	$12i$ ($Pm\bar{3}m$, $cP128$)
$48i$	$m.m2$	1/8	1/4	1/4	$6f$ ($Pm\bar{3}m$, $cP128$)
$96j$	$m..$	0	1/8	1/4	$12h$ ($Pm\bar{3}m$, $cP128$)
$96k$	$..m$	1/4	1/8	1/8	$12j$ ($Pm\bar{3}m$, $cP128$)
$96k$	$..m$	5/16	5/16	1/16	$24m$ ($Pm\bar{3}m$, $cP128$)
$96k$	$..m$	7/16	7/16	3/16	$24m$ ($Pm\bar{3}m$, $cP128$)
$96k$	$..m$	13/16	13/16	9/16	$24m$ ($Pm\bar{3}m$, $cP128$)
$96k$	$..m$	15/16	15/16	11/16	$24m$ ($Pm\bar{3}m$, $cP128$)

Table 10
Wyckoff sites in space group $Fm\bar{3}c$ of the Bärnighausen tree, $cF1024$.

Site	Site symmetry	x	y	z	Generating site
	$Fm\bar{3}c$, (226), $cF1024$, $8a \times 8a \times 8a - abcdefg^3hi^2j^2$				
$8a$	432	1/4	1/4	1/4	$1b$ ($Pm\bar{3}m$, $cP128$)
$8b$	$m3.$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP128$)
$24c$	$4m.2$	1/4	0	0	$3d$ ($Pm\bar{3}m$, $cP128$)
$24d$	$4/m..$	0	1/4	1/4	$3c$ ($Pm\bar{3}m$, $cP128$)
$48e$	$mm2..$	1/8	0	0	$6e$ ($Pm\bar{3}m$, $cP128$)
$48f$	$4..$	1/8	1/2	1/2	$6f$ ($Pm\bar{3}m$, $cP128$)
$64g$	$.3.$	1/8	1/8	1/8	$8g$ ($Pm\bar{3}m$, $cP128$)
$64g$	$.3.$	1/16	1/16	1/16	$8g$ ($Pm\bar{3}m$, $cP128$)
$64g$	$.3.$	3/16	3/16	3/16	$8g$ ($Pm\bar{3}m$, $cP128$)
$96h$	$..2$	1/4	1/8	1/8	$12j$ ($Pm\bar{3}m$, $cP128$)
$96i$	$m..$	0	1/8	1/4	$12h$ ($Pm\bar{3}m$, $cP128$)
$96i$	$m..$	0	1/8	1/8	$12i$ ($Pm\bar{3}m$, $cP128$)
$192j$	1	5/16	5/16	1/16	$24m$ ($Pm\bar{3}m$, $cP128$)
$192j$	1	7/16	7/16	3/16	$24m$ ($Pm\bar{3}m$, $cP128$)

Table 11
Wyckoff sites in space group $F\bar{4}3m$ of the Bärnighausen tree, $cF16$, $cF128$, $cF432$.

Site	Site symmetry	x	y	z	Generating site
	$F\bar{4}3m$, (216), $cF16$, $2a \times 2a \times 2a - abcd$				
$4a$	$\bar{4}3m$	0	0	0	$8a$ ($Fd\bar{3}m$, $cF16$)
$4b$	$\bar{4}3m$	1/2	1/2	1/2	$8b$ ($Fd\bar{3}m$, $cF16$)
$4c$	$\bar{4}3m$	1/4	1/4	1/4	$8a$ ($Fd\bar{3}m$, $cF16$)
$4d$	$\bar{4}3m$	3/4	3/4	3/4	$8b$ ($Fd\bar{3}m$, $cF16$)
	$F\bar{4}3m$, (216), $cF128$, $4a \times 4a \times 4a - abcde^4fg$				
$4a$	$\bar{4}3m$	0	0	0	$1a$ ($P\bar{4}3m$, $cP16$)
$4b$	$\bar{4}3m$	1/2	1/2	1/2	$1a$ ($P\bar{4}3m$, $cP16$)
$4c$	$\bar{4}3m$	1/4	1/4	1/4	$1b$ ($P\bar{4}3m$, $cP16$)
$4d$	$\bar{4}3m$	3/4	3/4	3/4	$1b$ ($P\bar{4}3m$, $cP16$)
$16e$	$.3m$	1/8	1/8	1/8	$4e$ ($P\bar{4}3m$, $cP16$)
$16e$	$.3m$	3/8	3/8	3/8	$4e$ ($P\bar{4}3m$, $cP16$)
$16e$	$.3m$	5/8	5/8	5/8	$4e$ ($P\bar{4}3m$, $cP16$)
$16e$	$.3m$	7/8	7/8	7/8	$4e$ ($P\bar{4}3m$, $cP16$)
$24f$	$2.mm$	1/4	0	0	$3d$ ($P\bar{4}3m$, $cP16$)
$24g$	$2.mm$	0	1/4	1/4	$3c$ ($P\bar{4}3m$, $cP16$)
	$F\bar{4}3m$, (216), $cF432$, $6a \times 6a \times 6a - abcde^8f^2g^2h^4$				
$4a$	$\bar{4}3m$	0	0	0	$4a$ ($F\bar{4}3m$, $cF16$)
$4b$	$\bar{4}3m$	1/2	1/2	1/2	$4b$ ($F\bar{4}3m$, $cF16$)
$4c$	$\bar{4}3m$	1/4	1/4	1/4	$4c$ ($F\bar{4}3m$, $cF16$)
$4d$	$\bar{4}3m$	3/4	3/4	3/4	$4d$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	1/3	1/3	1/3	$4a$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	2/3	2/3	2/3	$4a$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	1/6	1/6	1/6	$4b$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	5/6	5/6	5/6	$4b$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	1/12	1/12	1/12	$4d$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	5/12	5/12	5/12	$4d$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	7/12	7/12	7/12	$4c$ ($F\bar{4}3m$, $cF16$)
$16e$	$.3m$	11/12	11/12	11/12	$4c$ ($F\bar{4}3m$, $cF16$)
$24f$	$2.mm$	1/3	0	0	$4a$ ($F\bar{4}3m$, $cF16$)
$24f$	$2.mm$	1/6	0	0	$4b$ ($F\bar{4}3m$, $cF16$)
$24g$	$2.mm$	1/12	1/4	1/4	$4d$ ($F\bar{4}3m$, $cF16$)
$24g$	$2.mm$	7/12	1/4	1/4	$4c$ ($F\bar{4}3m$, $cF16$)
$48h$	$..m$	1/3	1/3	0	$4a$ ($F\bar{4}3m$, $cF16$)
$48h$	$..m$	1/6	1/6	1/2	$4b$ ($F\bar{4}3m$, $cF16$)
$48h$	$..m$	5/12	5/12	1/4	$4c$ ($F\bar{4}3m$, $cF16$)
$48h$	$..m$	1/12	1/12	3/4	$4d$ ($F\bar{4}3m$, $cF16$)

Table 12
Wyckoff sites in space group $F\bar{4}3m$ of the Bärnighausen tree, $cF1024$.

Site	Site symm.	x	y	z	Generating site
	$F\bar{4}3m$, (216), $cF1024$, $8a \times 8a \times 8a - abcde^{12}f^3g^3h^{12}i$				
$4a$	$\bar{4}3m$	0	0	0	$1a$ ($P\bar{4}3m$, $cF128$)
$4b$	$\bar{4}3m$	1/2	1/2	1/2	$1a$ ($P\bar{4}3m$, $cP128$)
$4c$	$\bar{4}3m$	1/4	1/4	1/4	$1b$ ($P\bar{4}3m$, $cP128$)
$4d$	$\bar{4}3m$	3/4	3/4	3/4	$1b$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	1/8	1/8	1/8	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	3/8	3/8	3/8	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	5/8	5/8	5/8	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	7/8	7/8	7/8	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	1/16	1/16	1/16	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	3/16	3/16	3/16	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	5/16	5/16	5/16	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	7/16	7/16	7/16	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	9/16	9/16	9/16	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	11/16	11/16	11/16	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	13/16	13/16	13/16	$4e$ ($P\bar{4}3m$, $cP128$)
$16e$	$.3m$	15/16	15/16	15/16	$4e$ ($P\bar{4}3m$, $cP128$)
$24f$	$2.mm$	1/4	0	0	$3d$ ($P\bar{4}3m$, $cP128$)
$24f$	$2.mm$	1/8	0	0	$6f$ ($P\bar{4}3m$, $cP128$)
$24f$	$2.mm$	5/8	0	0	$6f$ ($P\bar{4}3m$, $cP128$)
$24g$	$2.mm$	0	1/4	1/4	$3c$ ($P\bar{4}3m$, $cP128$)
$24g$	$2.mm$	1/8	1/4	1/4	$6g$ ($P\bar{4}3m$, $cP128$)
$24g$	$2.mm$	5/8	1/4	1/4	$6g$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	1/8	1/8	0	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	5/8	5/8	1/2	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	1/8	1/8	1/4	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	5/8	5/8	3/4	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	5/16	5/16	1/16	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	7/16	7/16	3/16	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	1/16	1/16	5/16	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	3/16	3/16	7/16	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	13/16	13/16	9/16	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	15/16	15/16	11/16	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	9/16	9/16	13/16	$12i$ ($P\bar{4}3m$, $cP128$)
$48h$	$..m$	11/16	11/16	15/16	$12i$ ($P\bar{4}3m$, $cP128$)
$96i$	1	1/8	1/4	0	$12h$ ($P\bar{4}3m$, $cP128$)

Table 13
Wyckoff sites in space group $Fd\bar{3}m$ of the Bärnighausen tree, $cF16$, $cF432$.

Site	Site symmetry	x	y	z	Generating site
	$Fd\bar{3}m$, (227), $cF16$, $2a \times 2a \times 2a - ab$				
$8a$	$\bar{4}3m$	0	0	0	$2a$ ($Pn\bar{3}m$, $cP2$)
$8b$	$\bar{4}3m$	1/2	1/2	1/2	$2a$ ($Pn\bar{3}m$, $cP2$)
	$Fd\bar{3}m$, (227), $cF432$, $6a \times 6a \times 6a - abe^4f^2g^2$				
$8a$	$\bar{4}3m$	0	0	0	$8a$ ($Fd\bar{3}m$, $cF16$)
$8b$	$\bar{4}3m$	1/2	1/2	1/2	$8b$ ($Fd\bar{3}m$, $cF16$)
$32e$	$.3m$	1/3	1/3	1/3	$8a$ ($Fd\bar{3}m$, $cF16$)
$32e$	$.3m$	1/12	1/12	1/12	$8b$ ($Fd\bar{3}m$, $cF16$)
$32e$	$.3m$	5/12	5/12	5/12	$8b$ ($Fd\bar{3}m$, $cF16$)
$32e$	$.3m$	7/12	7/12	7/12	$8a$ ($Fd\bar{3}m$, $cF16$)
$48f$	$2.mm$	1/3	0	0	$8a$ ($Fd\bar{3}m$, $cF16$)
$48f$	$2.mm$	5/6	0	0	$8b$ ($Fd\bar{3}m$, $cF16$)
$96g$	$..2$	7/12	7/12	1/4	$8a$ ($Fd\bar{3}m$, $cF16$)
$96g$	$..2$	1/12	1/12	3/4	$8b$ ($Fd\bar{3}m$, $cF16$)

Table 14
Wyckoff sites in space group $Fd\bar{3}m$ of the Bärnighausen tree, $cF1024$.

Site	Site symm.	x	y	z	Generating site
	$Fd\bar{3}m$, (227), $cF1024$, $8a \times 8a \times 8a - abcde^5f^3g^6h$				
$8a$	$\bar{4}3m$	0	0	0	$2a$ ($Pn\bar{3}m$, $cP128$)
$8b$	$\bar{4}3m$	1/2	1/2	1/2	$2a$ ($Pn\bar{3}m$, $cP128$)
$16c$	$.\bar{3}m$	1/8	1/8	1/8	$4b$ ($Pn\bar{3}m$, $cP128$)
$16d$	$.\bar{3}m$	5/8	5/8	5/8	$4b$ ($Pn\bar{3}m$, $cP128$)
$32e$	$.3m$	3/8	3/8	3/8	$4c$ ($Pn\bar{3}m$, $cP128$)
$32e$	$.3m$	3/16	3/16	3/16	$8e$ ($Pn\bar{3}m$, $cP128$)
$32e$	$.3m$	5/16	5/16	5/16	$8e$ ($Pn\bar{3}m$, $cP128$)
$32e$	$.3m$	11/16	11/16	11/16	$8e$ ($Pn\bar{3}m$, $cP128$)
$32e$	$.3m$	13/16	13/16	13/16	$8e$ ($Pn\bar{3}m$, $cP128$)
$48f$	$2.mm$	1/4	0	0	$6d$ ($Pn\bar{3}m$, $cP128$)
$48f$	$2.mm$	1/8	0	0	$12g$ ($Pn\bar{3}m$, $cP128$)
$48f$	$2.mm$	5/8	0	0	$12g$ ($Pn\bar{3}m$, $cP128$)
$96g$	$..m$	1/8	1/8	1/4	$24k$ ($Pn\bar{3}m$, $cP128$)
$96g$	$..m$	5/8	5/8	3/4	$24k$ ($Pn\bar{3}m$, $cP128$)
$96g$	$..m$	7/16	7/16	3/16	$24k$ ($Pn\bar{3}m$, $cP128$)
$96g$	$..m$	1/16	1/16	5/16	$24k$ ($Pn\bar{3}m$, $cP128$)
$96g$	$..m$	15/16	15/16	11/16	$24k$ ($Pn\bar{3}m$, $cP128$)
$96g$	$..m$	9/16	9/16	13/16	$24k$ ($Pn\bar{3}m$, $cP128$)
$96h$	$..2$	1/8	0	1/4	$12f$ ($Pn\bar{3}m$, $cP128$)

Table 15
Wyckoff sites in space group $Fm\bar{3}$ of the Bärnighausen tree, $cF128$.

Site	Site symmetry	x	y	z	Generating site
	$Fm\bar{3}$, ($\bar{2}02$), $cF128$, $4a \times 4a \times 4a - abcdef^2$				
$4a$	$m\bar{3}.$	0	0	0	$1a$ ($Pm\bar{3}$, $cP16$)
$4b$	$m\bar{3}.$	1/2	1/2	1/2	$1a$ ($Pm\bar{3}$, $cP16$)
$8c$	$23.$	1/4	1/4	1/4	$1b$ ($Pm\bar{3}$, $cP16$)
$24d$	$2/m..$	0	1/4	1/4	$3c$ ($Pm\bar{3}$, $cP16$)
$24e$	$mm2..$	1/4	0	0	$3d$ ($Pm\bar{3}$, $cP16$)
$32f$	$.3.$	1/8	1/8	1/8	$8i$ ($Pm\bar{3}$, $cP16$)
$32f$	$.3.$	3/8	3/8	3/8	$8i$ ($Pm3$, $cP16$)

Table 16
Wyckoff sites in space group $Fd\bar{3}$ of the Bärnighausen tree, $cF1024$.

Site	Site symm.	x	y	z	Generating site
	$Fd\bar{3}$, (203), $cF1024$, $4a \times 4a \times 4a - abcde^5f^3g^7$				
$8a$	$23.$	0	0	0	$2a$ ($Pn\bar{3}$, $cP128$)
$8b$	$2\bar{3}.$	1/2	1/2	1/2	$2a$ ($Pn\bar{3}$, $cP128$)
$16c$	$.\bar{3}.$	1/8	1/8	1/8	$4b$ ($Pn\bar{3}$, $cP128$)
$16d$	$.\bar{3}.$	5/8	5/8	5/8	$4b$ ($Pn\bar{3}$, $cP128$)
$32e$	$.3.$	3/8	3/8	3/8	$4c$ ($Pn\bar{3}$, $cP128$)
$32e$	$.3.$	3/16	3/16	3/16	$8e$ ($Pn\bar{3}$, $cP128$)
$32e$	$.3.$	5/16	5/16	5/16	$8e$ ($Pn\bar{3}$, $cP128$)
$32e$	$.3.$	11/16	11/16	11/16	$8e$ ($Pn\bar{3}$, $cP128$)
$32e$	$.3.$	13/16	13/16	13/16	$8e$ ($Pn\bar{3}$, $cP128$)
$48f$	$2..$	1/4	0	0	$6d$ ($Pn\bar{3}$, $cP128$)
$48f$	$2..$	1/8	0	0	$12f$ ($Pn\bar{3}$, $cP128$)
$48f$	$2..$	5/8	0	0	$12f$ ($Pn\bar{3}$, $cP128$)
$96g$	1	1/8	1/4	0	$12g$ ($Pn\bar{3}$, $cP128$)
$96g$	1	1/4	1/8	1/8	$24h$ ($Pn\bar{3}$, $cP128$)
$96g$	1	3/4	5/8	5/8	$24h$ ($Pn\bar{3}$, $cP128$)
$96g$	1	3/16	7/16	7/16	$32f$ ($Pn\bar{3}$, $cP128$)
$96g$	1	5/16	1/16	1/16	$32f$ ($Pn\bar{3}$, $cP128$)
$96g$	1	11/16	15/16	15/16	$32f$ ($Pn\bar{3}$, $cP128$)
$96g$	1	13/16	9/16	9/16	$32f$ ($Pn3$, $cP128$)

Table 17
Wyckoff sites in the additional space groups of the inset to the Bärnighausen tree, $Im\bar{3}m - cI54$, $Pm\bar{3}m - cP54$, $P\bar{4}3m - cP54$, $Pn\bar{3}m - cP54$.

Site	Site symmetry	x	y	z	Generating site
	$Im\bar{3}m$, (229), $cI54$, $3a \times 3a \times 3a - aefh$				
$2a$	$m\bar{3}m$	0	0	0	$2a$ ($Im\bar{3}m$, $cI2$)
$12e$	$4m.m$	1/3	0	0	$2a$ ($Im\bar{3}m$, $cI2$)
$16f$	$.3m$	1/3	1/3	1/3	$2a$ ($Im\bar{3}m$, $cI2$)
$24h$	$m.m2$	0	1/3	1/3	$2a$ ($Im\bar{3}m$, $cI2$)
	$Pm\bar{3}m$, (221), $cP54$, $3a \times 3a \times 3a - abefg^2ij$				
$1a$	$m\bar{3}m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP2$)
$1b$	$m\bar{3}m$	1/2	1/2	1/2	$1b$ ($Pm\bar{3}m$, $cP2$)
$6e$	$4m.m$	1/3	0	0	$1a$ ($Pm\bar{3}m$, $cP2$)
$6f$	$4m.m$	1/6	1/2	1/2	$1b$ ($Pm\bar{3}m$, $cP2$)
$8g$	$.3m$	1/3	1/3	1/3	$1a$ ($Pm\bar{3}m$, $cP2$)
$8g$	$.3m$	1/6	1/6	1/6	$1b$ ($Pm\bar{3}m$, $cP2$)
$12i$	$m.m2$	0	1/3	1/3	$1a$ ($Pm\bar{3}m$, $cP2$)
$12j$	$m.m2$	1/2	1/6	1/6	$1b$ ($Pm\bar{3}m$, $cP2$)
	$P\bar{4}3m$, (215), $cP54$, $3a \times 3a \times 3a - abe^4fgi^2$				
$1a$	$\bar{4}3m$	0	0	0	$1a$ ($Pm\bar{3}m$, $cP54$)
$1b$	$\bar{4}3m$	1/2	1/2	1/2	$1b$ ($Pm\bar{3}m$, $cP54$)
$4e$	$.3m$	1/3	1/3	1/3	$8g$ ($Pm\bar{3}m$, $cP54$)
$4e$	$.3m$	2/3	2/3	2/3	$8g$ ($Pm\bar{3}m$, $cP54$)
$4e$	$.3m$	1/6	1/6	1/6	$8g$ ($Pm\bar{3}m$, $cP54$)
$4e$	$.3m$	5/6	5/6	5/6	$8g$ ($Pm\bar{3}m$, $cP54$)
$6f$	$2.mm$	1/3	0	0	$6e$ ($Pm\bar{3}m$, $cP54$)
$6g$	$2.mm$	1/6	1/2	1/2	$6f$ ($Pm\bar{3}m$, $cP54$)
$12i$	$..m$	1/3	1/3	0	$12i$ ($Pm\bar{3}m$, $cP54$)
$12i$	$..m$	1/6	1/6	1/2	$12j$ ($Pm\bar{3}m$, $cP54$)
	$Pn\bar{3}m$, (224), $cP54$, $3a \times 3a \times 3a - ae^2gk$				
$2a$	$\bar{4}3m$	0	0	0	$2a$ ($Pn\bar{3}m$, $cP2$)
$8e$	$.3m$	1/3	1/3	1/3	$2a$ ($Pn\bar{3}m$, $cP2$)
$8e$	$.3m$	2/3	2/3	2/3	$2a$ ($Pn\bar{3}m$, $cP2$)
$12g$	$2.mm$	1/3	0	0	$2a$ ($Pn\bar{3}m$, $cP2$)
$24k$	$..m$	1/3	1/3	0	$2a$ ($Pn\bar{3}m$, $cP2$)

The Wyckoff sites of the two largest structures in space group $F\bar{4}3m$, also shown in the Bärnighausen tree as $cF5488$ and $cF21\,296$, are not given. They may be derived using the *International Tables for Crystallography - Volume A1: Symmetry Relations Between Space Group* (Ed.s Hans Wondratschek and Ulrich Müller, 2006).

3. Atomic sites – Coordinates

The sites belonging to the different clusters in cubic complex intermetallic structures in space group $F\bar{4}3m$ are given in Table 18. The ones of the hypothetic subtype V are given in Table 19.

Table 18

Main cluster found in the structure of cubic complex intermetallics of space group $F\bar{4}3m$. Given are the sites belonging to a certain cluster (shell), the number of atoms, and the polyhedron built up by them. The following shells correspond to special clusters: 1st shell, 1st variant – (14 atoms) rhombic dodecahedron, 1st shell, 2nd variant – FK_{16}^{28} / Friauf polyhedron, 2nd shell – FK_{40}^{76} / Frank-Kasper polyhedron with 76 faces and 40 vertices, 3rd shell, 6th variant –F_{76}^{40} / fullerene polyhedron with 40 faces and 76 vertices. The subtypes I..IV in which the respective clusters occur are indicated in columns *ST*.

Nr. of atoms	Sites around cluster center $(0,0,0)$		$\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)$		$\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$		$\left(\frac{3}{4},\frac{3}{4},\frac{3}{4}\right)$	
Cluster center								
1	4*a*	*ST*	4*c*	*ST*	4*b*	*ST*	4*d*	*ST*
First cluster shell								
14	16*e*4/5, 24*f*1	I..IV	16*e*1/6, 24*g*1	I..III	16*e*2/7, 24*f*2	I	16*e*3/8, 24*g*2	I,II
16	-	-	16*e*1, 48*h*5	IV	16*e*2, 48*h*6	II..IV	16*e*3, 48*h*7	III,IV
Second cluster shell								
40	16*e*1, 48*h*1/2/4	I..IV	16*e*2, 48*h*1/2/3	I..IV	16*e*3, 48*h*2/3/4	I..IV	16*e*4, 48*h*1/3/4	I..IV
Third cluster shell								
58	16*e*6/8, 24*f*2/*g*2, 48*h*3	I	16*e*5/7, 24*f*1/*g*2, 48*h*4	I	16*e*6/8, 24*f*1/*g*1, 48*h*1	I, II	16*e*5/7, 24*f*2/*g*1, 48*h*2	I
64	16*e*6/8, 24*g*2, 48*h*3/6	II						
70			16*e*5, 24*f*1/*g*2, 48*h*4/6	II				
54							16*e*5, 24*g*1, 48*h*2/6	II,III
60	16*e*6, 48*h*3/6/7	III					16*e*5, 48*h*2/5/6	IV
76			16*e*5, 24*f*1, 48*h*4/6/7	III,IV				
70					16*e*6, 24*f*1/*g*1, 48*h*1/7	III,IV		
72	48*h*3/5/6/7	IV						
66					24*f*1, 48*h*1/5/7	IV		

Table 19

Main cluster found in the hypothetical structure of subtype V of cubic complex intermetallics in space group $F\bar{4}3m$. The clusters which do not occur in the above-discussed other subtypes are highlighted by bold letters. Given are the sites belonging to a certain cluster (shell), the number of atoms, and the polyhedron built up by them.

Cluster shell	Polyhedron	Nr. of atoms	Sites around cluster center $(0,0,0)$	$\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)$	$\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$	$\left(\frac{3}{4},\frac{3}{4},\frac{3}{4}\right)$
Center	-	1	4*a*	4*c*	4*b*	4*d*
1st	FK_{16}^{28}	16	**16e4**, **48h8**	16*e*1, 48*h*5	16*e*2, 48*h*6	16*e*3, 48*h*7
2nd	FK_{40}^{76}	40	16*e*1, 48*h*1, 2, 4	16*e*2, 48*h*1, 2, 3	16*e*3, 48*h*2, 3, 4	16*e*4, 48*h*1, 3, 4
3rd		72	48*h*3, 5, 6, 7	**48h4**, **6**, **7**, **8**	**48h1**, **5**, **7**, **8**	**48h2**, **5**, **6**, **8**

Table 20

Development of the third cluster shells throughout the subtypes I$\cdots$V (*ST*) with number of vertices and different faces (*t* triangular, *q* quadrangular, *p* pentagonal, *h* hexagon) for the sites of highest symmetry $4a\cdots d$ (000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, $\frac{1}{4}\frac{1}{4}\frac{1}{4}$, and $\frac{3}{4}\frac{3}{4}\frac{3}{4}$, respectively).

	No. of vertices				No. of different faces			
ST	4*a*	4*c*	4*b*	4*d*	4*a*	4*c*	4*b*	4*d*
I	58	58	58	58	$t^4q^{12}p^{12}h^{12}$	$t^4q^{12}p^{12}h^{12}$	$t^4q^{12}p^{12}h^{12}$	$t^4q^{12}p^{12}h^{12}$
II	64	70	58	54	$t^4p^{24}h^{12}$	$p^{24}h^{16}$	$t^4q^{12}p^{12}h^{12}$	$t^8q^{12}p^{24}$
III	60	76	70	54	t^8p^{36}	$p^{12}h^{28}$	$p^{24}h^{16}$	$t^8q^{12}p^{24}$
IV	72	76	66	60	$t^4p^{24}h^{16}$	$p^{12}h^{28}$	$t^4p^{36}h^4$	t^8p^{36}
V	72	72	72	72	$t^4p^{24}h^{16}$	$t^4p^{24}h^{16}$	$t^4p^{24}h^{16}$	$t^4p^{24}h^{16}$

The sites of the clusters in structures in space group $Fd\bar{3}m$ are listed in Table 21. The sites of the one-shell clusters used in the modular explanation of the $cF464$-structures in space group $Fd\bar{3}m$ are given in Table 22.

Table 21

Clusters found in the structure of cubic complex intermetallics of space group $Fd\bar{3}m$. Given are the sites belonging to a certain cluster (shell), the number of atoms, and the polyhedron built up by them.

Cluster shell	Polyhedron Shape	Atoms	Sites	Capped polyhedron Shape	Add. atoms	Additional sites	Atoms
Center	-	1	8*a*				1
1st	*tt*	12	12 × 96*g*2	FK_{16}^{28}	+4	+ 4 × 32*e*1	16
2nd	F_{28}^{16}	28	4 × 32*e*2, 24 × 96*g*1	FK_{44}^{84}	+16	+ 4 × 32*e*1, 12 × 96*g*3	40
3rd	F_{84}^{44}	84	24 × 96*g*2, 24 × 96*g*3, 36 × 96*g*4				
Center	-	0	16*d*				0
1st				icosahedron	12	6 × 96*g*3, 6 × 96*g*4	
2nd	dodecahedron	20	2 × 8*b*, 6 × 32*e*2, 12 × 96*g*1				

Table 22
Atomic sites of one-shell clusters used in the modular explanation of cubic complex intermetallics of space group $Fd\bar{3}m$. Given are the sites belonging to the cluster around a specified cluster center, the number of atoms, and the polyhedron built up by them.

Center	Polyhedron	Atoms		Sites
8*a*	truncated tetrahedron	12		$12 \times 96g2$
	Friauf polyhedron	16	+	$4 \times 32e1$
32*e*2	truncated tetrahedron	12		$3 \times 96g2$, $3 \times 96g3$, $6 \times 96g4$
	Friauf polyhedron	16	+	$3 \times 96g1$, $1 \times 8b$
96*g*1	truncated tetrahedron	12		$2 \times 32e1$, $4 \times 96g2$, $4 \times 96g3$, $2 \times 96g4$
	Friauf polyhedron	16	+	$3 \times 96g1$, $1 \times 32e1$
16*d*	icosahedron	12		$6 \times 96g3$, $6 \times 96g4$
8*b*	truncated tetrahedron	12		$12 \times 96g4$
	Friauf polyhedron	16	+	$4 \times 32e2$

The sites of both structure types can be directly related to one another as shown in Table 23. The site symmetry is preserved except for 32*e*/16*e* sites, which have symmetry $.\bar{3}m$ in space group $Fd\bar{3}m$ and $.3m$ in $F\bar{4}3m$. Not listed are the 24*f* and 24*g* sites, which contribute to rhombic dodecahedra around $\bar{4}3m$ sites, which do not occur in the $Fd\bar{3}m$ structures. Correspondingly, only half of the 16*e* sites are related to the 32*e* sites of space group $Fd\bar{3}m$. Of sites 96*g*3 and 96*g*4, only half of the positions could be related to sites in $F\bar{4}3m$ structures: 48*h*5 is part of site 96*g*2, as 48*h*6 relates directly to 96*g*4. When we investigate the relationship between the structures it becomes clear that the inner cluster shells, which have the shape of Friauf polyhedra, should contain sites 16*e*3 and 16*e*4 instead of 16*e*5 and 16*e*8. They can be regarded as being oriented conversely and accordingly, not sites 48*h*7 and 48*h*8 are occupied but their counterparts, corresponding to half of the positions described by sites 96*g*3 and 96*g*4 in space group $Fd\bar{3}m$. Therein, one half of the polyhedra have an opposite orientation with respect to the other half, whereas in the $F\bar{4}3m$ structures, all sub-units are oriented similarly.

Table 23
Relations of the atomic sites in cubic complex intermetallics of space groups $Fd\bar{3}m$ and $F\bar{4}3m$.

	$Fd\bar{3}m$		$F\bar{4}3m$	
	Site	Site symmetry	Site	Site symmetry
	8*a*	$\bar{4}3m$	4*a*, 4*c*	$\bar{4}3m$
	8*b*	$\bar{4}3m$	4*b*, 4*d*	$\bar{4}3m$
	32*e*1	$.\bar{3}m$	16*e*1, 16*e*5	$.3m$
	32*e*2	$.\bar{3}m$	16*e*2, 16*e*8	$.3m$
	96*g*1	$..m$	48*h*1, 48*h*2	$..m$
	96*g*2	$..m$	48*h*3, 48*h*4	$..m$
	96*g*3	$..m$	48*h*5 & ..	$..m$
	96*g*4	$..m$	48*h*6 & ..	$..m$

4. Atomic sites – Occupations

Table 24
Site occupations of all discussed complex intermetallic structures in space group $F\bar{4}3m$. A + denotes that a site is occupied, a - that it is empty. Sites labelled with different letters are occupied the following modifications: m - mixed occupation, d - deficient occupation, s - split site. The $In_{54.5}Pd_{29.3}Ce_{16.3}$ structure is subject to two specific features: the 16*e*1 site (marked with a 2) is replaced by two sites 16*e* whose average corresponds to the 16*e*1 position. The 48*h*3 site is not occupied but instead a (split) site 96*i*.

	4				16e								24*f*		24*g*		48*h*						
Structure	*a*	*b*	*c*	*d*	1	2	3	4	5	6	7	8	1	2	1	2	1	2	3	4	5	6	7
Subtype I (10 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	-	-	-
$Li_{64.3}In_{26.5}Ag_{9.2}$	+	m	+	m	+	+	+	+	m	+	+	m	+	+	m	+	+	+	m	m	-	-	-
$Li_{81.0}Pb_{19.0}$	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	-	-	-
$Li_{81.0}Sn_{19.0}$	+	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	-	-	-
$Li_{81.0}Ge_{19.0}$	d	-	-	-	+	+	+	+	s	+	+	+	+	+	+	+	+	+	+	+	-	-	-
$Zn_{80.9}Pd_{14.5}Al_{4.6}$	-	-	-	-	+	+	s	+	m	+	+	m	+	+	+	m	+	+	+	m	-	-	-
$Zn_{82.7}Pt_{17.3}$	-	-	-	-	ms	+	+	m	+	ds	+	+	m	d	m	d	+	d	+	+	-	-	-
$Zn_{81.6}Pt_{18.4}$	-	-	-	-	s	+	+	m	+	ds	+	+	m	+	m	+	+	d	+	+	-	-	-
$Zn_{78.7}Pd_{16.0}Al_{5.3}$	-	-	-	-	+	+	ds	+	m	+	+	d	+	+	+	m	+	+	+	m	-	-	-
$Zn_{77.0}Pt_{23.0}$	-	-	-	-	md	+	+	+	+	md	+	+	m	m	m	-	+	+	+	+	-	-	-
$Zn_{80.0}Pt_{20.0}$	-	-	-	-	+	+	m	+	d	+	+	+	+	+	+	+	ms	+	+	+	-	-	-
$Zn_{78.5}Pd_{14.0}Al_{7.5}$	-	-	-	-	+	+	+	+	m	+	+	-	+	+	+	+	+	+	+	m	-	-	-
$Cu_{73.9}Sn_{23.2}Ni_{2.9}$	-	-	-	-	+	+	+	+	+	+	d	+	+	+	+	+	d	+	+	+	-	-	-
$Cu_{78.6}Sn_{21.4}$	-	-	-	-	+	+	+	+	+	+	d	+	+	+	+	+	+	+	+	+	-	-	-
$Cu_{79.8}Sn_{20.2}$	-	-	-	-	+	+	+	+	+	+	+	m	m	+	+	+	+	+	+	m	-	-	-
Subtype I/II (3 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	d	+	+	d	+	+	+	+	+	+	-	d	-
$Zn_{89.1}Ir_{10.9}$	-	d	-	-	m	+	+	+	+	+	d	-	+	d	m	+	+	+	+	+	-	d	-
$Zn_{90.5}Ir_{9.5}$	-	d	d	-	m	+	+	+	+	ds	d	-	+	d	m	+	+	+	s	+	-	d	-
$Zn_{91.1}Ir_{8.9}$	-	d	d	-	m	+	+	+	+	ds	d	-	+	d	m	+	+	+	+	+	-	d	-
Subtype II (12 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	-	+	+	-	+	+	+	+	+	+	-	+	-
$Na_{86.3}Tl_{13.7}$	-	-	-	-	+	+	+	+	+	+	-	-	d	-	+	+	+	+	+	+	-	+	-
$Sc_{86.3}Os_{13.7}$	-	-	-	-	+	+	+	+	+	+	-	-	+	-	+	+	+	+	+	+	-	+	-
$Mg_{87.3}Ru_{12.7}$	-	-	-	-	+	+	+	m	+	m	-	-	+	-	+	+	+	+	+	+	-	+	-
$Mg_{86.3}Rh_{13.7}$	-	-	-	-	+	+	+	+	+	+	-	-	+	-	+	+	+	+	+	+	-	+	-
$Mg_{87.9}Ir_{12.1}$	-	+	-	-	+	+	+	+	+	-	-	-	+	-	+	+	+	+	+	+	-	+	-
$Mg_{85.9}Pd_{14.1}$	-	d	-	-	+	m	+	+	+	-	-	-	+	-	+	+	+	+	+	+	-	+	-
$Mg_{86.3}Ir_{13.7}$	-	-	-	-	+	+	+	+	+	+	-	-	+	-	+	+	+	+	+	+	-	+	-
$Zn_{95.3}Mo_{4.7}$	d	+	m	-	+	+	+	+	d	d	-	-	+	-	d	+	+	+	+	+	-	+	-
$Al_{65.3}Cu_{18.1}Cr_{16.6}$	-	d	-	-	+	+	+	m	m	+	-	-	+	-	+	m	+	+	+	m	-	d	-
$Zn_{86.6}Fe_{6.7}Ni_{6.7}$	-	+	d	-	+	+	m	+	+	mds	-	-	+	-	m	+	+	+	+	+	-	+	-
$Zn_{78.4}Fe_{21.6}$	-	-	-	-	m	+	+	m	m	+	-	-	+	-	+	+	+	+	+	+	-	+	-
$In_{54.5}Pd_{29.3}Ce_{16.3}$	-	+	-	-	2	+	+	+	+	+	-	+	+	-	+	+	+	+	96*i*	+	-	s	-
$Zn_{67.5}Ce_{16.7}Mg_{15.8}$	-	+	+	-	+	+	+	+	+	+	-	+	+	-	+	+	+	+	96*i*	+	-	+	-
Subtype III (3 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	-	-	+	-	+	-	+	+	+	+	-	+	+
$Mg_{83.6}Gd_{16.4}$	+	+	+	+	+	+	+	+	+	d	-	-	+	-	d	-	+	m	+	+	-	+	+
$Cd_{80.4}Sm_{19.6}$	+	+	+	+	+	+	+	+	+	+	-	-	+	-	+	-	+	+	+	+	-	+	+
$Al_{63.6}Ta_{36.4}$	-	+	+	+	+	+	+	+	+	s	-	-	+	-	s	-	+	s	s	sm	-	s	+
$Mg_{82.4}Y_{9.0}Ce_{8.6}$	+	m	m	+	+	+	+	m	+	d	-	-	+	-	d	-	+	m	+	+	-	+	+
$Na_{49.2}Ba_{28.8}Li_{22.0}$	-	+	-	+	+	+	+	+	+	+	-	-	+	-	+	-	+	2	+	+	-	+	+
Subtype IV (1 structure)																							
theoretical	+	+	+	+	+	+	+	+	+	-	-	-	+	-	-	-	+	+	+	+	+	+	+
$Na_{49.1}Sn_{26.3}In_{24.6}$	+	+	+	+	+	+	+	+	+	-	-	-	+	-	-	-	+	+	+	+	+	m	+
Subtype V (0 structures)																							
theoretical and site 48*h*8	+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-	+	+	+	+	+	+	+

Table 25
Site occupations of all discussed complex intermetallic structures in space group $F\bar{4}3m$. The atomic sorts, occupying the respective sites, are given. In the case of mixed occupations, the first letters of all featured elements are given (alternatively the second letters in case of ambiguities).

	4				16e								24*f*		24*g*		48*h*						
Structure	*a*	*b*	*c*	*d*	1	2	3	4	5	6	7	8	1	2	1	2	1	2	3	4	5	6	7
Subtype I (10 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	-	-	-
$Li_{64.3}In_{26.5}Ag_{9.2}$	Li	L/A	Li	A/L	Ag	In	Li	Li	L/A	Li	Li	I/L	In	Li	A/L	Li	Li	Li	I/L	I/L	-	-	-
$Li_{81.0}Pb_{19.0}$	Li	-	-	-	Pb	Li	Li	Pb	Li	Li	Li	Li	Li	Pb	Li	Pb	Li	Li	Li	Li	-	-	-
$Li_{81.0}Sn_{19.0}$	Li	-	-	-	Sn	Li	Li	Sn	Li	Li	Li	Li	Li	Sn	Li	Sn	Li	Li	Li	Li	-	-	-
$Li_{81.0}Ge_{19.0}$	Li	-	-	-	Ge	Li	Li	Ge	Li	Li	Li	Li	Li	Ge	Li	Ge	Li	Li	Li	Li	-	-	-
$Zn_{80.9}Pd_{14.5}Al_{4.6}$	-	-	-	-	Pd	Pd	Zn	Pd	Z/A	Zn	Zn	A/Z	Zn	Zn	Zn	P/Z	Zn	Zn	Zn	Z/A	-	-	-
$Zn_{82.7}Pt_{17.3}$	-	-	-	-	Z/P	Pt	Pt	Z/P	Zn	Zn	Zn	Zn	P/Z	Zn	Z/P	Zn	Zn	Zn	Zn	Zn	-	-	-
$Zn_{81.6}Pt_{18.4}$	-	-	-	-	Zn	Pt	Pt	Z/P	Zn	Zn	Zn	Zn	P/Z	Zn	Z/P	Zn	Zn	Zn	Zn	Zn	-	-	-
$Zn_{78.7}Pd_{16.0}Al_{5.3}$	-	-	-	-	Pd	Pd	Zn	Pd	Z/A	Zn	Zn	Al	Zn	Zn	Zn	P/Z	Zn	Zn	Zn	Z/A	-	-	-
$Zn_{77.0}Pt_{23.0}$	-	-	-	-	Z/P	Pt	Pt	Pt	Zn	Z/P	Zn	Zn	P/Z	Z/P	P/Z	-	Zn	Zn	Zn	Zn	-	-	-
$Zn_{80.0}Pt_{20.0}$	-	-	-	-	Pt	Pt	Z/P	Zn	Zn	Zn	Zn	Zn	Pt	Zn	Zn	Pt	Zn	Zn	Zn	Zn	-	-	-
$Zn_{78.5}Pd_{14.0}Al_{7.5}$	-	-	-	-	Zn	Pd	Al	Pd	Z/A	Zn	Zn	-	Zn	Zn	Zn	Pd	Zn	Zn	Zn	Z/A	-	-	-
$Cu_{73.9}Sn_{23.2}Ni_{2.9}$	-	-	-	-	Cu	Sn	Cu	Cu	Cu	Cu	Cu	Cu	Cu	Cu	Sn	Cu	Cu	Cu	Cu	Sn	-	-	-
$Cu_{78.6}Sn_{21.4}$	-	-	-	-	Cu	Sn	Cu	Cu	Cu	Cu	Cu	Cu	Cu	Cu	Sn	Cu	Cu	Cu	Cu	Sn	-	-	-
$Cu_{79.8}Sn_{20.2}$	-	-	-	-	Cu	Sn	Cu	Cu	Cu	Cu	Cu	C/S	C/S	Cu	Sn	Cu	Cu	Cu	Cu	C/S	-	-	-
Subtype I/II (3 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	d	+	+	d	+	+	+	+	+	+	-	d	-
$Zn_{89.1}Ir_{10.9}$	-	Zn	-	-	Z/I	Zn	Ir	Ir	Zn	Zn	Zn	-	Zn	Zn	Z/I	Zn	Zn	Zn	Zn	Zn	-	Zn	-
$Zn_{90.5}Ir_{9.5}$	-	Zn	Ir	-	Z/I	Zn	Ir	Ir	Zn	Zn	Zn	-	Zn	Zn	Z/I	Zn	Zn	Zn	Zn	Zn	-	Zn	-
$Zn_{91.1}Ir_{8.9}$	-	Zn	Ir	-	Z/I	Zn	Ir	Ir	Zn	Zn	Zn	-	Zn	Zn	Z/I	Zn	Zn	Zn	Zn	Zn	-	Zn	-
Subtype II (12 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	-	+	+	-	+	+	+	+	+	+	-	+	-
$Na_{86.3}Tl_{13.7}$	-	-	-	-	Na	Na	Tl	Tl	Na	Na	-	-	Na	-	Tl	Na	Na	Na	Na	Na	-	Na	-
$Sc_{86.3}Os_{13.7}$	-	-	-	-	Sc	Sc	Os	Os	Sc	Sc	-	-	Sc	-	Os	Sc	Sc	Sc	Sc	Sc	-	Sc	-
$Mg_{87.3}Ru_{12.7}$	-	-	-	-	Mg	Mg	Ru	R/M	Mg	M/R	-	-	Mg	-	Ru	Mg	Mg	Mg	Mg	Mg	-	Mg	-
$Mg_{86.3}Rh_{13.7}$	-	-	-	-	Mg	Mg	Rh	Rh	Mg	Mg	-	-	Mg	-	Rh	Mg	Mg	Mg	Mg	Mg	-	Mg	-
$Mg_{87.9}Ir_{12.1}$	-	Mg	-	-	Ir	Mg	Ir	Ir	Mg	-	-	-	Mg	-	Mg	Mg	Mg	Mg	Mg	Mg	-	Mg	-
$Mg_{85.9}Pd_{14.1}$	-	Mg	-	-	Pd	M/P	Pd	Pd	Mg	-	-	-	Mg	-	Mg	Mg	Mg	Mg	Mg	Mg	-	Mg	-
$Mg_{86.3}Ir_{13.7}$	-	-	-	-	Mg	Mg	Ir	Ir	Mg	Mg	-	-	Mg	-	Ir	Mg	Mg	Mg	Mg	Mg	-	Mg	-
$Zn_{95.3}Mo_{4.7}$	Zn	Zn	M/Z	-	Zn	Zn	Mo	Zn	Zn	Zn	-	-	Zn	-	Zn	Zn	Zn	Zn	Zn	Zn	-	Zn	-
$Al_{65.3}Cu_{18.1}Cr_{16.6}$	-	Cu	-	-	Cr	Al	Cr	r/u	A/u	Al	-	-	Al	-	Cr	A/u	Al	Al	Al	A/u	-	Cu	-
$Zn_{86.6}Fe_{6.7}Ni_{6.7}$	-	Zn	F/N	-	Zn	Zn	F/N	Zn	Zn	F/N	-	-	Zn	-	F/N	Zn	Zn	Zn	Zn	Zn	-	Zn	-
$Zn_{78.4}Fe_{21.6}$	-	-	-	-	F/Z	Zn	Fe	F/Z	F/Z	Fe	-	-	Zn	-	Fe	Zn	Zn	Zn	Zn	Zn	-	Zn	-
$In_{54.5}Pd_{29.3}Ce_{16.3}$	-	In	-	-	*P+I*	Ce	Ce	Pd	In	Pd	-	In	Ce	-	Ce	In	In	In	*Pd*	In	-	In	-
$Zn_{67.5}Ce_{16.7}Mg_{15.8}$	-	Mg	Zn	-	Zn	Ce	Ce	Zn	Zn	Zn	-	Zn	Ce	-	Ce	Mg	Mg	Zn	*Zn*	Zn	-	Zn	-
Subtype III (3 structures)																							
theoretical	+	+	+	+	+	+	+	+	+	+	-	-	+	-	+	-	+	+	+	+	-	+	+
$Mg_{83.6}Gd_{16.4}$	Mg	Gd	Gd	Mg	Mg	Mg	Gd	Gd	Mg	Mg	-	-	Mg	-	Mg	-	Mg	G/M	Mg	Mg	-	Mg	Mg
$Cd_{80.4}Sm_{19.6}$	Cd	Sm	Sm	Cd	Cd	Cd	Sm	Sm	Cd	Cd	-	-	Cd	-	Cd	-	Cd	Sm	Cd	Cd	-	Cd	Cd
$Al_{63.6}Ta_{36.4}$	-	Ta	Ta	Ta	Al	Ta	Ta	Ta	Al	Al	-	-	Al	-	Al	-	Ta	Al	Ta	A/T	-	Al	Al
$Mg_{82.4}Y_{9.0}Ce_{8.6}$	Mg	C/Y	C/Y	Mg	Mg	Mg	Y	C/Y	Mg	Mg	-	-	Mg	-	Mg	-	Mg	*CYM*	Mg	Mg	-	Mg	Mg
$Na_{49.2}Ba_{28.8}Li_{22.0}$	-	Ba	-	Ba	Li	Ba	Ba	Ba	Na	Li	-	-	Na	-	Li	-	Ba	*N+L*	Ba	Na	-	Na	Na
Subtype IV (1 structure)																							
theoretical	+	+	+	+	+	+	+	+	+	-	-	-	+	-	-	-	+	+	+	+	+	+	+
$Na_{49.1}Sn_{26.3}In_{24.6}$	Na	Na	Na	Na	Na	Na	Na	Na	Sn	-	-	-	In	-	-	-	Na	Na	Na	Sn	Sn	I/S	In

Table 26
Site occupations of all discussed complex intermetallic structures in space group $Fd\bar{3}m$. A + denotes that a site is occupied, a - that it is empty. Sites labelled with different letters are occupied the following modifications: m - mixed occupation, d - deficient occupation. Also given are – in the right half of the table - the atomic sorts, occupying the respective sites. The additional site found in $Zn_{61.0}Ca_{35.6}Ni_{3.4}$ – 16*d* – is fully occupied by Ni.

	8		32e		96*g*				8		32e		96*g*			
Structure	*a*	*b*	1	2	1	2	3	4	*a*	*b*	1	2	1	2	3	4
$In_{70.7}K_{29.3}$	+	+	+	+	+	+	+	+	In	K	In	K	K	In	In	In
$Ga_{50.0}Na_{29.3}In_{20.7}$	+	+	+	+	+	+	+	+	Ga	Na	Ga	Na	Na	In	Ga	Ga
$Ga_{48.9}Na_{30.4}Cd_{20.7}$	+	d	m	+	+	m	+	+	Na	Na	Cd/Ga	Na	Na	Cd/Ga	Ga	Ga
$Ga_{63.0}Na_{31.0}Ag_{6.0}$	+	+	m	+	+	m	+	+	Na	Na	Ag/Ga	Na	Na	Ag/Ga	Ga	Ga
$Ga_{53.4}Li_{31.0}Cu_{8.6}In_{6.9}$	+	+	+	+	+	+	+	m	Li	Li	In	Li	Li	Ga	Ga	Ga/Cu
$Ga_{47.5}Mg_{31.2}Cu_{21.3}$	d	+	d	+	+	+	+	+	Mg	Mg	Ga	Mg	Mg	Ga	Cu	Ga
$Zn_{61.0}Ca_{35.6}Ni_{3.4}$	-	+	+	+	+	+	+	+	-	Ca	Ca	Ca	Ca	Zn	Zn	Zn

5. Coordination shells around low-symmetry sites in $Al_{63.6}Ta_{36.4}$

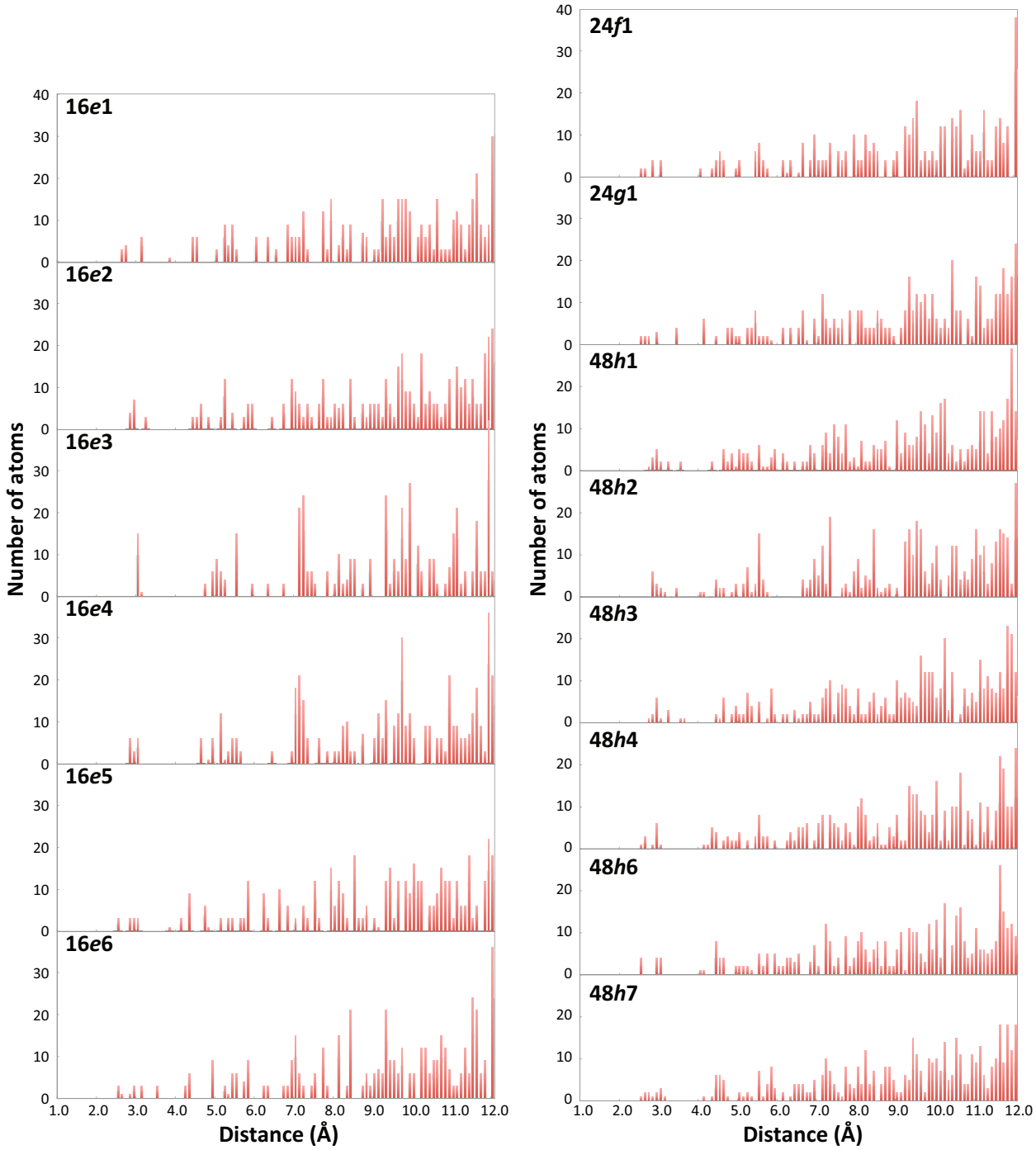

Figure 1
Frequency of interatomic distances of atoms in the environment of the lower-symmetry atomic sites in $Al_{63.6}Ta_{36.4}$.

6. (110) layers

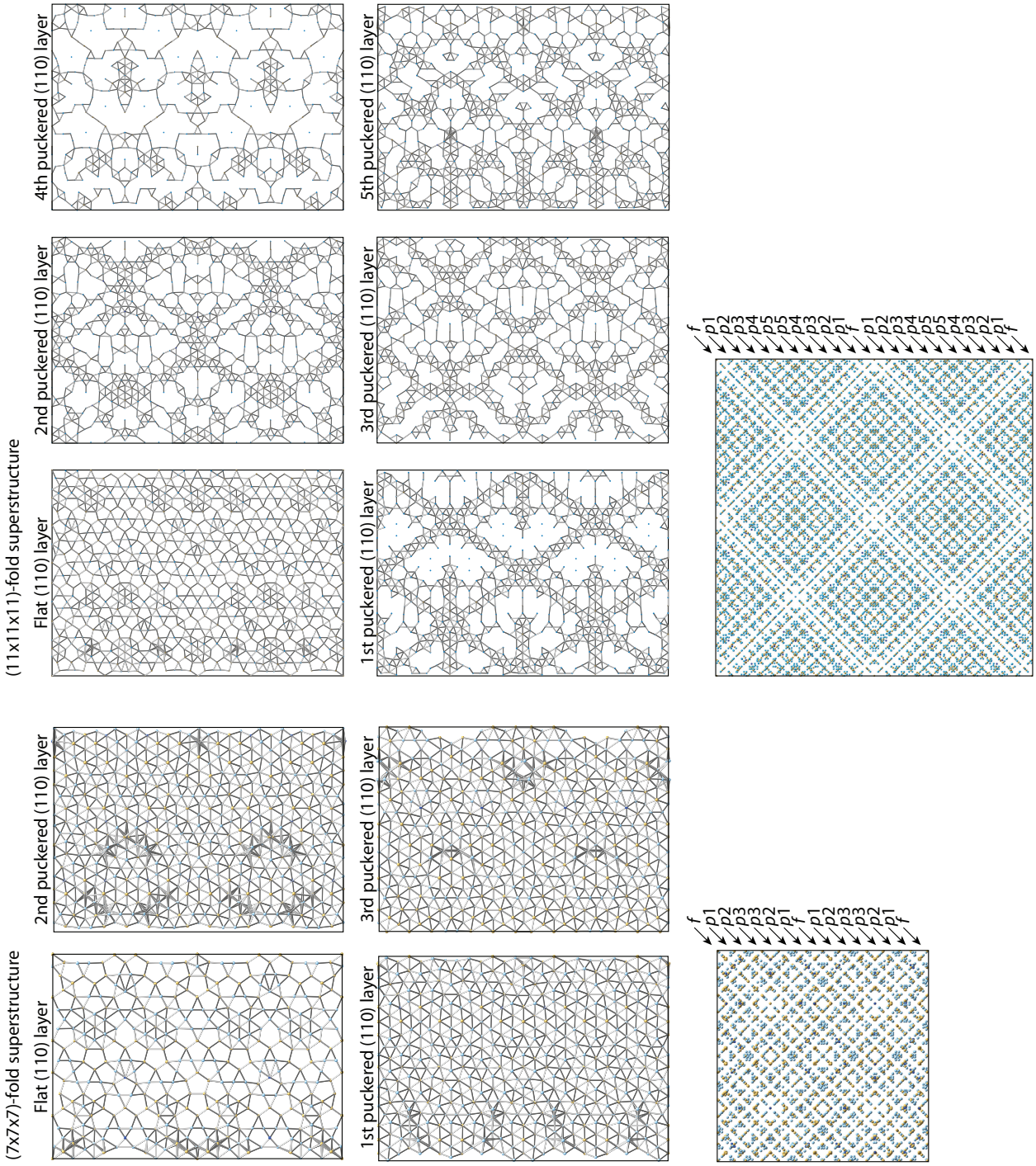

Figure 2
(110) layers of the two giant-unit-cell Al-Cu-Ta compounds (with $p = 7$ and $p = 11$), as well as their arrangement.

7. First-principles calculations

Table 27

Details on the performed *ab initio* calculations for structures of space group $F\bar{4}3m$. Given are the number of calculated electrons per atom (*e*/atom) and the number of atoms in the calculated unit cell (atoms/u.c.), both values given for each atomic sort in the order of content in the unit cell, as well as the idealization steps applied to partly disordered structures. The structures $Cu_{73.9}Sn_{23.2}Ni_{2.9}$ and $Zn_{86.6}Fe_{6.7}Ni_{6.7}$ had to be calculated in the variants $Cu_{76.8}Sn_{23.2}$ and $Zn_{86.6}Fe_{13.4}$, as well as $Zn_{86.6}Ni_{13.4}$, respectively, because the Ni sites had not been specified on structure determination.

Structure	*e*/atom	atoms/u.c.	Applied idealization steps
Subtype I (14 structures)			
$Li_{64.3}In_{26.5}Ag_{9.2}$	3, 13, 11	59, 38, 11	4*b*: 0.8 Li, 0.2 Ag → 1 Li; 4*d*: 0.82 Ag, 0.18 Li → 1 Ag; 16*e*5: 0.57 Li, 0.43 Ag → 1 Li; 16*e*8: 0.77 In, 0.23 Li → 1 In; 24*g*1: 0.54 Ag, 0.46 Li → 1 Ag; 48*h*3: 0.54 In, 0.46 Li → 1 In; 48*h*4: 0.75 In, 0.25 Li → 1 In
$Li_{81.0}Pb_{19.0}$	3, 14	85, 20	-
$Li_{81.0}Sn_{19.0}$	3, 14	85, 20	-
$Li_{81.0}Ge_{19.0}$	3, 14	85, 20	4*a*: 0.75 → 1 Li; 16*e*5: 0.75/0.25 → 1 Li
$Zn_{80.9}Pd_{14.5}Al_{4.6}$	12, 16, 3	82, 18, 4	16*e*3: 0.83/0.19 Zn → 1 Zn; 16*e*5: 0.94 Zn, 0.05 Al → 1 Zn; 16*e*8: 0.78 Al, 0.22 Zn → 1 Al; 24*g*2: 0.52 Pd, 0.48 Zn → 1 Pd; 48*h*4: 0.88 Zn, 0.12 Al → 1 Zn
$Zn_{82.7}Pt_{17.3}$	12, 10	86, 18	16*e*1: 0.24/0.39 Zn, 0.34 Pt → 1 Zn; 16*e*4: 0.61 Zn, 0.39 Pt → 1 Zn; 16*e*6: 0.5/0.27 → 1 Zn; 24*f*1: 0.51 Pt, 0.49 Zn → 1 Pt; 24*f*2: 0.71 → 1 Zn; 24*g*1: 0.53 Zn, 0.47 Pt → 1 Zn; 24*g*2: 0.69 → 1 Zn; 48*h*2: 0.91 → 1 Zn
$Zn_{81.6}Pt_{18.4}$	12, 10	90, 14	16*e*1: 0.70/0.31 → 1 Zn; 16*e*4: 0.86/0.14 → 1 Zn; 16*e*6: 0.68/0.17 → 1 Zn; 24*f*1: 0.85 Pt, 0.15 Zn → 1 Pt; 24*g*1: 0.86 Pt, 0.14 Zn → 1 Pt; 48*h*2: 0.90 → 1 Zn
$Zn_{78.7}Pd_{16.0}Al_{5.3}$	12, 16, 3	82, 18, 4	16*e*3: 0.51/0.21 → 1 Zn; 16*e*5: 0.78 Zn, 0.22 Al → 1 Zn; 16*e*8: 0.74 → 1 Al; 24*g*2: 0.71 Pd, 0.29 Zn → 1 Pd; 48*h*4: 0.87 Zn, 0.13 Al → 1 Zn
$Zn_{77.0}Pt_{23.0}$	12, 10	70, 24	16*e*1: 0.5 Zn, 0.5 Pt → 1 Zn; 16*e*6: 0.92 Zn, 0.18 Pt → 1 Zn; 24*f*1: 0.67 Pt, 0.33 Zn → 1 Pt; 24*f*2: 0.92 Zn, 0.18 Pt → 1 Zn; 24*g*1: 0.67 Pt, 0.33 Zn → 1 Pt
$Zn_{80.0}Pt_{20.0}$	12, 10	84, 20	16*e*3: 0.88 Zn, 0.12 Pt → 1 Zn; 16*e*5: 0.62 → 1 Zn; 48*h*1: 0.87/0.12 → 1 Zn
$Zn_{78.5}Pd_{14.0}Al_{7.5}$	12, 16, 3	82, 14, 4	16*e*5: 0.81 Zn, 0.19 Al → 1 Zn; 48*h*4: 0.77 Zn, 0.23 Al → 1 Zn
$Cu_{73.9}Sn_{26.1}$	11, 4	82, 22	16*e*7: 0.75 → 1 Cu; 48*h*1: 0.75 → 1 Cu (Ni sites unspecified)
$Cu_{78.6}Sn_{21.4}$	11, 4	82, 22	16*e*7: 0.75 → 1 Cu
$Cu_{79.8}Sn_{20.2}$	11, 4	82, 22	16*e*8: 0.83 Cu, 0.17 Sn → 1 Cu; 24*f*1: 0.81 Cu, 0.19 Sn → 1 Cu; 48*h*4: 0.86 Sn, 0.14 Cu → 1 Sn
Subtype I/II (3 structures)			
$Zn_{89.1}Ir_{10.9}$	12, 9	93, 8	4*b*: 0.51 → 1 Zn; 16*e*1: 0.82 Zn, 0.18 Ir → 1 Zn; 16*e*7: 0.64 → 1 Zn; 24*f*2: 0.62 → 1 Zn; 24*g*1: 0.62 Zn, 0.38 Ir → 1 Zn; 48*h*6: 0.33 Zn → 0
$Zn_{90.5}Ir_{9.5}$	12, 9	95, 8	4*b*: 0.63 → 1 Zn; 4*c*: 0.25 Ir → 0; 16*e*1: 0.91 Zn, 0.09 Ir → 1 Zn; 16*e*6: 0.62/0.25 → 1 Zn; 16*e*7: 0.45 Zn → 0; 24*f*2: 0.36 Zn → 0; 24*g*1: 0.84 Zn, 0.16 Ir → 1 Zn; 48*h*3: 0.62/0.40 → 1 Zn; 48*h*6: 0.57 → 1 Zn
$Zn_{91.1}Ir_{8.9}$	12, 9	95, 8	4*b*: 0.70 → 1 Zn; 4*c*: 0.41 Ir → 0; 16*e*1: 0.98 Zn, 0.02 Ir → 1 Zn; 16*e*6: 0.60/0.30 → 1 Zn; 16*e*7: 0.42 Zn → 0; 24*f*2: 0.29 Zn → 0; 24*g*1: 0.90 Zn, 0.10 Ir → 1 Zn; 48*h*6: 0.62 → 1 Zn
Subtype II (14 structures)			
$Na_{86.3}Tl_{13.7}$	9, 13	88, 14	24*f*1: 0.94 → 1 Na
$Sc_{86.3}Os_{13.7}$	11, 14	88, 14	-
$Mg_{87.3}Ru_{12.7}$	8, 14	88, 14	16*e*4: 0.75 Ru, 0.25 Mg → 1 Ru; 16*e*6: 0.67 Mg, 0.33 Ru → 1 Mg
$Mg_{86.3}Rh_{13.7}$	8, 15	88, 14	-
$Mg_{87.9}Ir_{12.1}$	8, 9	87, 12	-
$Mg_{85.9}Pd_{14.1}$	8, 16	87, 12	4*b*: 0.97 → 1 Mg; 16*e*2: 0.51 Mg, 0.49 Pd → 1 Mg
$Mg_{86.3}Ir_{13.7}$	8, 9	88, 14	-
$Zn_{95.3}Mo_{4.7}$	12, 12	100, 5	4*a*: 0.65 → 1 Mo; 4*c*: 0.57 Mo, 0.43 Zn → 1 Mo; 16*e*5: 0.35 → 1 Zn; 16*e*6: 0.44 → 1 Zn; 24*g*1: 0.70 → 1 Zn
$Al_{65.3}Cu_{18.1}Cr_{16.6}$	3, 12, 17	72, 18, 12	4*b*: 0.28 Cu → 0; 16*e*4: 0.74 Cr, 0.26 Cu → 1 Cr; 16*e*5: 0.79 Al, 0.21 Cu → 1 Al; 24*g*2: 0.58 Al, 0.42 Cu → 1 Al; 48*h*4: 0.85 Al, 0.15 Cu → 1 Al; 48*h*6: 0.5 → 1 Cu
$Zn_{86.6}Fe_{13.4}$	12, 14	89, 15	4*c*: 0.68 Fe/Ni → 1 Fe; 16*e*3: 1 Fe/Ni → 1 Fe; 16*e*6: 0.53 Fe/Ni, 0.25 Fe/Ni → 1 Fe; 24*g*1: 1 Fe/Ni → 1 Fe
$Zn_{86.6}Ni_{13.4}$	12, 16	89, 15	4*c*: 0.68 Fe/Ni → 1 Ni; 16*e*3: 1 Fe/Ni → 1 Ni; 16*e*6: 0.53 Fe/Ni, 0.25 Fe/Ni → 1 Ni; 24*g*1: 1 Fe/Ni → 1 Ni
$Zn_{78.4}Fe_{21.6}$	14, 12	76, 26	16*e*1: 1 Fe/Zn → 1 Fe; 16*e*4: 1 Fe/Zn → 1 Fe; 16*e*5: 1 Fe/Zn → 1 Fe
$In_{54.5}Pd_{29.3}Ce_{16.3}$	13, 16, 12	67, 36, 20	48*h*3: 0.66/0.34 → 1 Pd; 48*h*6: 0.68/0.32 → 1 In
$Zn_{67.5}Ce_{16.7}Mg_{15.8}$	12, 12, 8	81, 20, 19	-
Subtype III (5 structures)			
$Mg_{83.6}Gd_{16.4}$	8, 9	90, 22	16*e*6: 0.70 → 1 Mg; 24*g*2: 0.86 → 1 Mg; 48*h*2: 0.68 Gd, 0.32 Mg → 1 Gd
$Cd_{80.4}Sm_{19.6}$	12, 11	90, 22	-
$Al_{63.6}Ta_{36.4}$	3, 11	72, 39	16*e*6: 0.33/0.33/0.33 → 1 Al; 24*g*1: 0.5/0.5 → 1 Al; 48*h*2: 0.79/0.21 → 1 Al; 48*h*3: 0.82/0.18 → 1 Ta; 48*h*4: 0.71/0.14/0.14 → 1 Al; 48*h*6: 0.88 Al, 0.12 Ta → 1 Al
$Mg_{82.4}Y_{9.0}Ce_{8.6}$	8, 11, 12	90, 4, 18	4*b*: 0.62 Ce, 0.38 Y → 1 Ce; 4*c*: 0.62 Ce, 0.38 Y → 1 Ce; 16*e*4: 0.62 Ce, 0.38 Y → 1 Ce; 16*e*6: 0.7 → 1 Mg; 24*g*1: 0.86 → 1 Mg; 48*h*2: 0.48 Ce, 0.30 Y, 0.23 Mg → 1 Ce
$Na_{49.2}Ba_{28.8}Li_{22.0}$	7, 10, 3	58, 38, 26	-
Subtype IV (1 structure)			
$Na_{49.1}Sn_{26.3}In_{24.6}$	1, 4, 3	56, 30, 28	48*h*6: 0.83 In, 0.17 Sn → 1 In

Table 28
Details on the performed *ab initio* calculations for structures of space group $Fd\bar{3}m$. The data are given as described for Table 27.

Structure	*e*/atom	atoms/u.c.	Applied idealization steps
$In_{70.7}K_{29.3}$	13, 9	82, 34	-
$Ga_{50.0}Na_{29.3}In_{20.7}$	13, 7, 13	58, 34, 24	-
$Ga_{48.9}Na_{30.4}Cd_{20.7}$	13, 7, 12	48, 36, 32	8*b*: 0.49 → 1 Na; 32*e*1: 0.85 Cd, 0.15 Ga → 1 Cd; 96*g*2: 0.71 Cd, 0.29 Ga → 1 Cd
$Ga_{63.0}Na_{31.0}Ag_{6.0}$	13, 7, 11	48, 36, 32	32*e*1: 0.67 Ga, 0.33 Ag → 1 Ag; 96*g*2: 0.82 Ga, 0.18 Ag → 1 Ag
$Ga_{53.4}Li_{31.0}Cu_{8.6}In_{6.9}$	13, 3, 17, -	72, 36, 8, 0	96*g*4: 0.58 Ga, 0.42 Cu → 1 Ga
$Ga_{47.5}Mg_{31.2}Cu_{21.3}$	13, 8, 17	56, 36, 24	8*a*: 0.56 → 1 Mg; 32*e*1: 0.70 → 1 Ga
$Zn_{61.0}Ca_{35.6}Ni_{3.4}$	12, 8, 16	72, 42, 4	-

8. Electron localization function – (110) layers

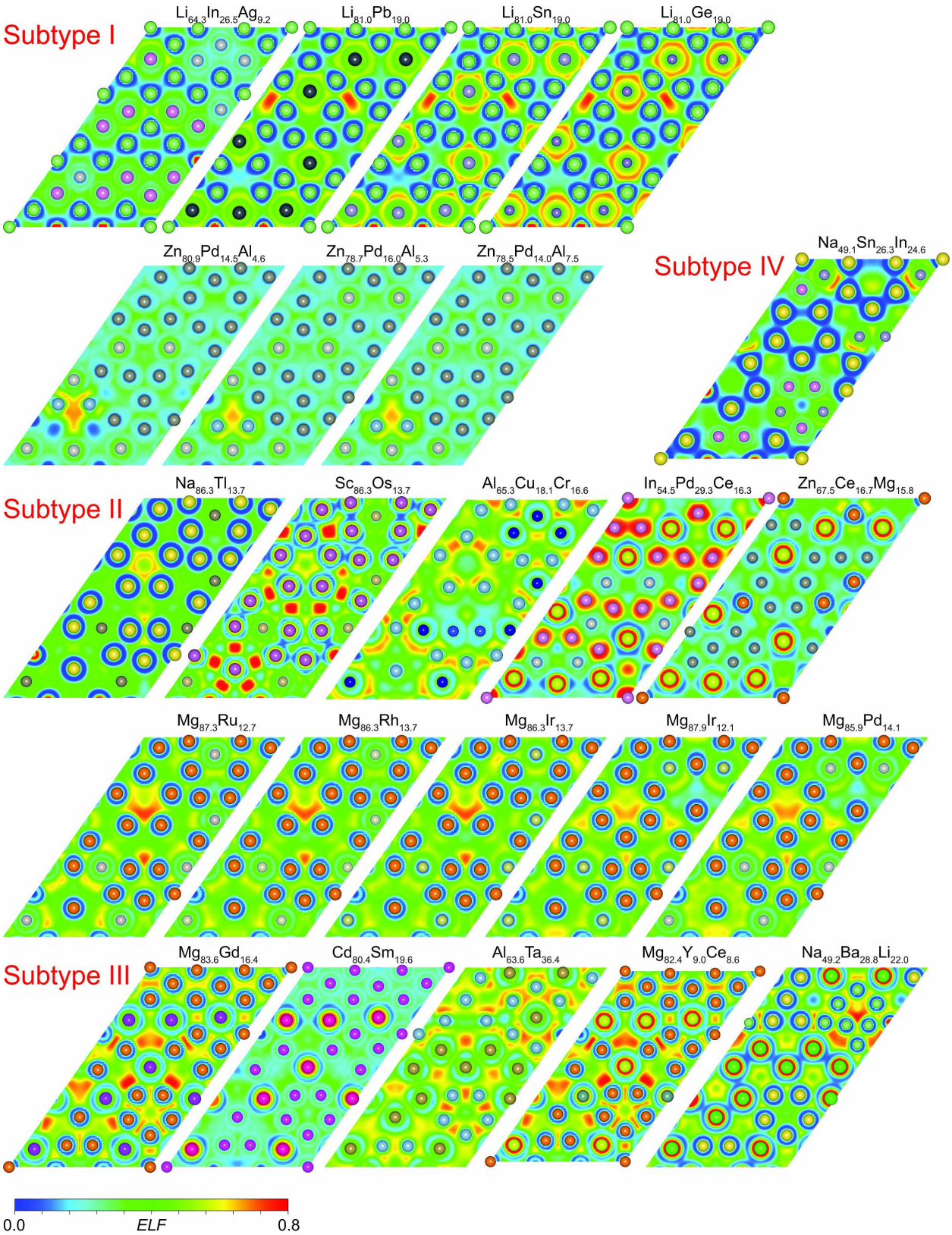

Figure 3
(110) layers of the ELFs of cubic complex intermetallics in the $F\bar{4}3m$ space group – structures with values $ELF > 0.5$.

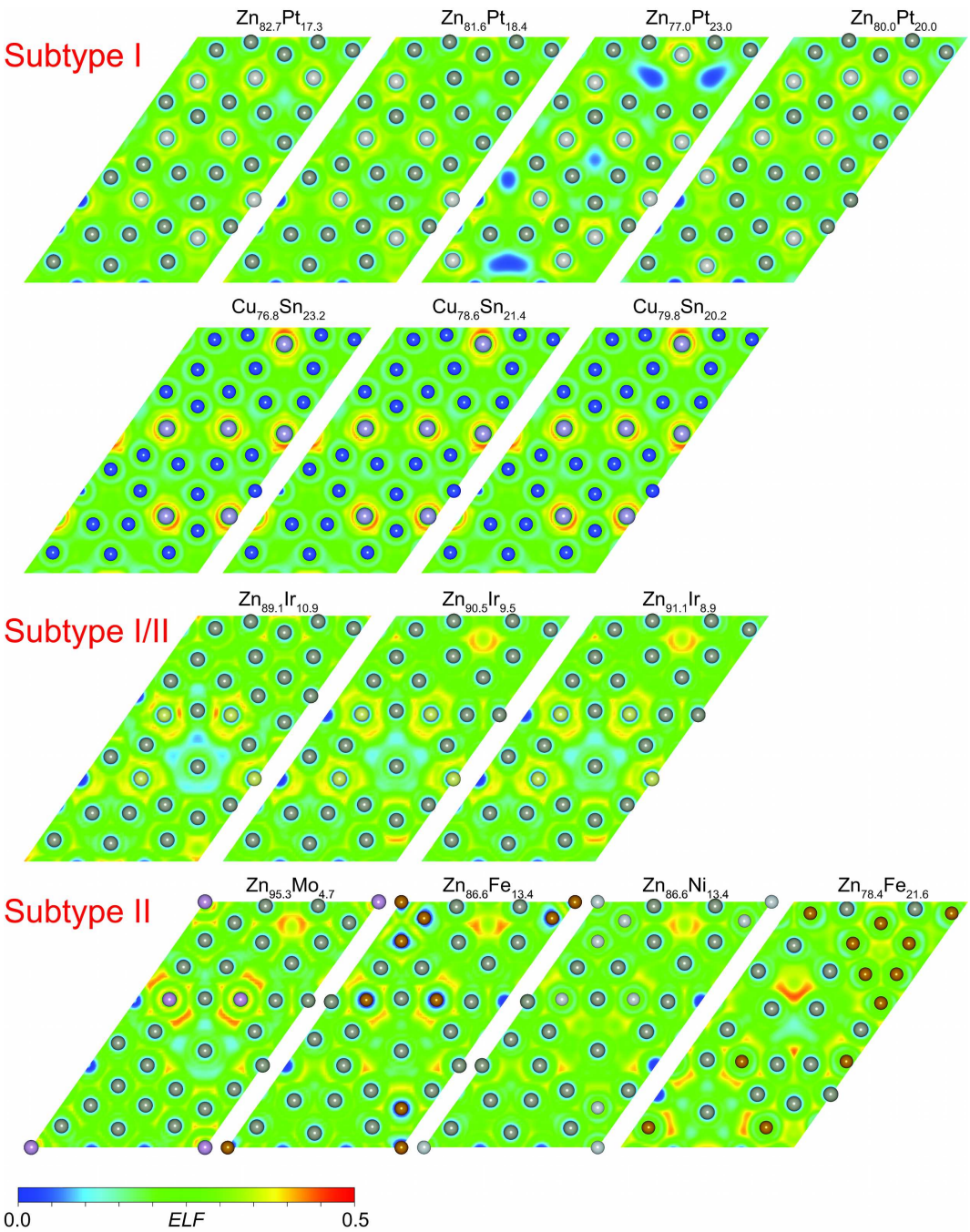

Figure 4
(110) layers of the ELFs of cubic complex intermetallics in the $F\bar{4}3m$ space group – structures only with values $ELF < 0.5$. Due to structural ambiguities as reported, the $Cu_{73.9}Sn_{23.2}Ni_{2.9}$ was simulated as $Cu_{76.8}Sn_{23.2}$ and is also inscribed in this way. Similarly, the structure of $Zn_{86.6}Fe_{6.7}Ni_{6.7}$ was simulated in the variants $Zn_{86.6}Fe_{13.4}$ and $Zn_{86.6}Ni_{13.4}$.

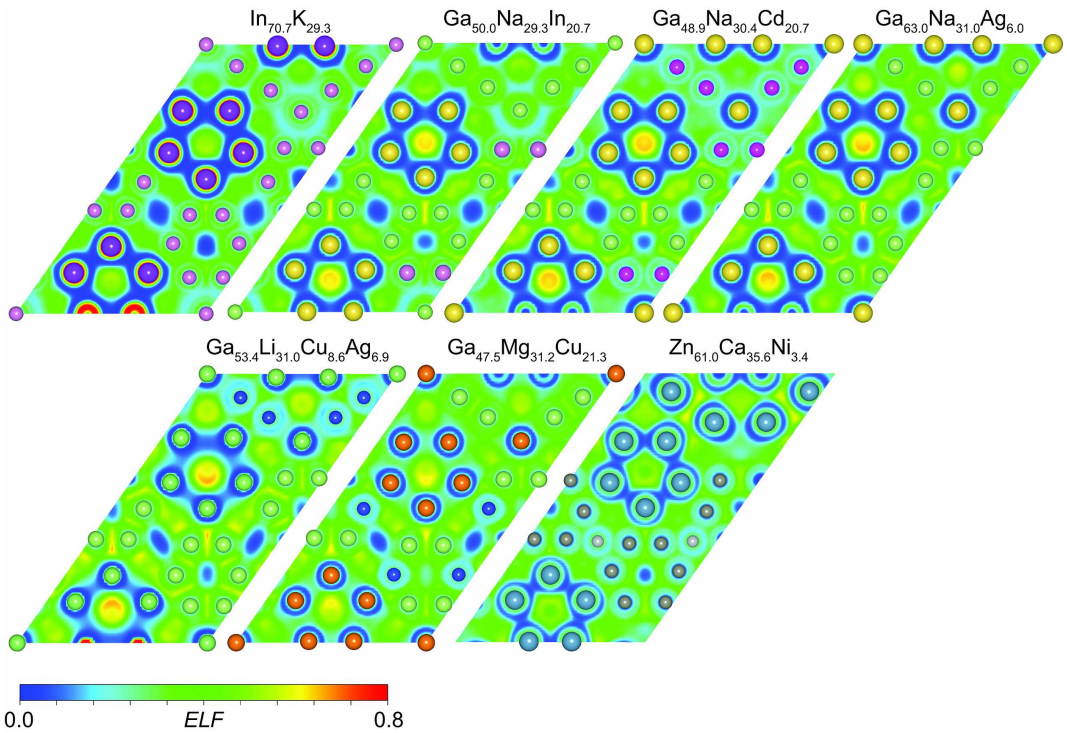

Figure 5
(110) layers of the ELFs of cubic complex intermetallics in the $Fd\bar{3}m$ space group. The structures are labeled with their respective chemical formulas.

9. Bader charge analysis

Table 29
Bader charges of cubic complex intermetallics *cF*464 in space group $F\bar{4}3m$, $(3 \times 3 \times 3)$-fold superstructures of a common basic structure. Given are for all calculated structures the Bader charges, expressed by the electron difference with respect to neutral atoms, for the different atomic sorts. The structures $Cu_{73.9}Sn_{23.2}Ni_{2.9}$ and $Zn_{86.6}Fe_{6.7}Ni_{6.7}$ had to be calculated in the variants $Cu_{76.8}Sn_{23.2}$ and $Zn_{86.6}Fe_{13.4}$, as well as $Zn_{86.6}Ni_{13.4}$, respectively.

	Only atomic basins				With bond basins			
	Majority atoms		Minority atoms		Altered atoms		Bond basins	
Composition	Element	Electrons	Element	Electrons	Element	Electrons	No.×Electrons	Shape
Space group $F\bar{4}3m$ – Subtype I								
$Li_{64.3}In_{26.5}Ag_{9.2}$	Li	−0.9..−0.8	In	+0.8..+1.6	*no bond basins*			
			Ag	+1.0..+1.3				
$Li_{81.0}Pb_{19.0}$	Li	−0.8..−0.7	Pb	+3.1..+3.7	Li	≈ −0.8	4×+0.1	(triangle)
$Li_{81.0}Sn_{19.0}$	Li	−0.8..−0.6	Sn	+3.1..+3.7	Li	≈ −0.8	4×+0.2	(triangle)
$Li_{81.0}Ge_{19.0}$	Li	−0.8..−0.5	Ge	+3.1..+3.6	Li	≈ −0.8	4×+0.3	(triangle)
$Zn_{80.9}Pd_{14.5}Al_{4.6}$	Zn	−0.2..−0.0	Pd	+0.6..+1.1	*no bond basins*			
			Al	≈ −1.2				
$Zn_{82.7}Pt_{17.3}$	Zn	−0.3..−0.1	Pt	+1.0..+1.1	*no bond basins*			
$Zn_{81.6}Pt_{18.4}$	Zn	−0.3..−0.1	Pt	+1.0..+1.1	*no bond basins*			
$Zn_{78.7}Pd_{16.0}Al_{5.3}$	Zn	−0.2..−0.0	Pd	+0.6..+1.1	*no bond basins*			
			Al	≈ −1.2				
$Zn_{77.0}Pt_{23.0}$	Zn	−0.4..−0.3	Pt	+0.9..+1.1	*no bond basins*			
$Zn_{80.0}Pt_{20.0}$	Zn	−0.3..−0.2	Pt	+1.0..+1.1	*no bond basins*			
$Zn_{78.5}Pd_{14.0}Al_{7.5}$	Zn	−0.2..−0.0	Pd	+0.6..+1.2	*no bond basins*			
			Al	≈ −1.3				
$Cu_{76.8}Sn_{23.2}$	Cu	+0.0..+0.1	Sn	−0.3..−0.2	*no bond basins*			
$Cu_{78.6}Sn_{21.4}$	Cu	+0.0..+0.1	Sn	−0.3..−0.2	*no bond basins*			
$Cu_{79.8}Sn_{20.2}$	Cu	+0.0..+0.1	Sn	−0.3..−0.2	*no significant bond basins*			
Space group $F\bar{4}3m$ – Subtype I/II								
$Zn_{89.1}Ir_{10.9}$	Zn	−0.4..+0.1	Ir	≈ +1.2	*no bond basins*			
$Zn_{90.5}Ir_{9.5}$	Zn	−0.3..+0.1	Ir	≈ +1.2	*no bond basins*			
$Zn_{91.1}Ir_{8.9}$	Zn	−0.3..+0.1	Ir	≈ +1.2	*no bond basins*			
Space group $F\bar{4}3m$ – Subtype II								
$Na_{86.3}Tl_{13.7}$	Na	−0.6..−0.0	Tl	+2.4..+2.8	*no bond basins*			
$Sc_{86.3}Os_{13.7}$	Sc	−1.1..+0.4	Os	+3.4..+3.5	Sc	−1.1..−0.5	41×+0.3..+0.4	(covalent bond)
$Mg_{87.3}Ru_{12.7}$	Mg	−1.3..−0.3	Ru	+5.5..+6.7	–	–	6×+0.9	(*p*)
$Mg_{86.3}Rh_{13.7}$	Mg	−1.3..−0.3	Rh	+5.4..+6.5	Rh	−1.3..−0.5	6×+1.1	(*p*)
$Mg_{87.9}Ir_{12.1}$	Mg	−1.4..+0.8	Ir	+5.4..+6.8	–	–	6×+0.4	(*h*)
$Mg_{85.9}Pd_{14.1}$	Mg	−1.3..+0.7	Pd	+4.6..+5.9	–	–	6×+0.5	(*h*)
$Mg_{86.3}Ir_{13.7}$	Mg	−1.4..−0.2	Ir	+5.7..+6.8	Ir	−1.4..−0.5	6×+1.3	(*p*)
$Zn_{95.3}Mo_{4.7}$	Zn	−0.8..+0.2	Mo	−0.1..+0.2	*no bond basins*			
$Al_{65.3}Cu_{18.1}Cr_{16.6}$	Al	−0.7..−0.3	Cr/Cu	+0.6..+2.3	*no bond basins*			
$Zn_{86.6}Fe_{13.4}$	Zn	−0.1..+0.1	Fe	+0.1..+0.3	*no bond basins*			
$Zn_{86.6}Ni_{13.4}$	Zn	−0.2..+0.1	Ni	+0.1..+0.4	*no bond basins*			
$Zn_{78.4}Fe_{21.6}$	Zn	−0.1..+0.0	Fe	+0.1..+0.3	*no bond basins*			
Space group $F\bar{4}3m$ – Subtype II'								
$In_{54.5}Pd_{29.3}Ce_{16.3}$	In	−0.2..+0.3	Pd	+0.8..+1.0	*no bond basins*			
			Ce	−1.4..−1.3				
$Zn_{67.5}Ce_{16.7}Mg_{15.8}$	Zn	+0.2..+0.8	Ce	−1.3..−1.1	*no bond basins*			
			Mg	≈ −1.4				
Space group $F\bar{4}3m$ – Subtype III								
$Mg_{83.6}Gd_{16.4}$	Mg	−0.4..+0.5	Gd	−0.6..−0.3	–	–	17×+0.2..+0.5	(covalent bond)
$Cd_{80.4}Sm_{19.6}$	Cd	+0.1..+0.5	Sm	−1.3..−1.2	*no bond basins*			
$Al_{63.6}Ta_{36.4}$	Al	−0.4..+0.1	Ta	−0.3..+0.6	Al	−0.4..−0.0	15×+0.2	(covalent bond)
$Mg_{82.4}Y_{9.0}Ce_{8.6}$	Mg	−0.6..+0.6	Y	≈ −0.9	–	–	31×+0.1..+0.8	(diverse)
			Ce	−0.4..−0.2				
$Na_{49.2}Ba_{28.8}Li_{22.0}$	Na	−0.1..+0.4	Ba	−0.3..+0.1	Li	≈ −0.8	65×+0.0..+4.0	(diverse)
			Li	−0.8..+3.8				
Space group $F\bar{4}3m$ – Subtype IV								
$Na_{49.1}Sn_{26.3}In_{24.6}$	Na	−0.8..−0.7	In	+0.4..+0.6	*no bond basins*			
			Sn	+0.9..+1.1				

Table 30
Bader charges of cubic complex intermetallics $cF464$ in space group $Fd\bar{3}m$, $(3 \times 3 \times 3)$-fold superstructures of a common basic structure. Given are for all calculated structures the Bader charges, expressed by the electron difference with respect to neutral atoms, for the different atomic sorts.

	Only atomic basins				With bond basins			
	Majority atoms		Minority atoms		Altered atoms		Bond basins	
Composition	Element	Electrons	Element	Electrons	Element	Electrons	No.×Electrons	Shape
Space group $Fd\bar{3}m$								
$In_{70.7}K_{29.3}$	In	$+0.0..+0.3$	K	≈ -0.7	*no bond basins*			
$Ga_{50.0}Na_{29.3}In_{20.7}$	Ga	$+0.0..+0.3$	Na	≈ -0.8	*no bond basins*			
			In	$\approx +0.4$				
$Ga_{48.9}Na_{30.4}Cd_{20.7}$	Ga	$\approx +0.3$	Na	≈ -0.8	*no bond basins*			
			Cd	$\approx +0.4$				
$Ga_{63.0}Na_{31.0}Ag_{6.0}$	Ga	$+0.3..+0.4$	Na	≈ -0.8	*no bond basins*			
			Ag	$+0.4..+0.5$				
$Ga_{53.4}Li_{31.0}Cu_{8.6}In_{6.9}$	Ga	$+0.3..+0.4$	Li	≈ -0.9	*no bond basins*			
			Cu	$\approx +0.6$				
$Ga_{47.5}Mg_{31.2}Cu_{21.3}$	Ga	$+0.5..+0.6$	Mg	≈ -1.5	*no bond basins*			
			Cu	$\approx +0.1$				
$Zn_{61.0}Ca_{35.6}Ni_{3.4}$	Zn	$+0.5..+1.0$	Ca	≈ -1.2	*no bond basins*			
			Ni	$\approx +0.4$				

10. Density of states

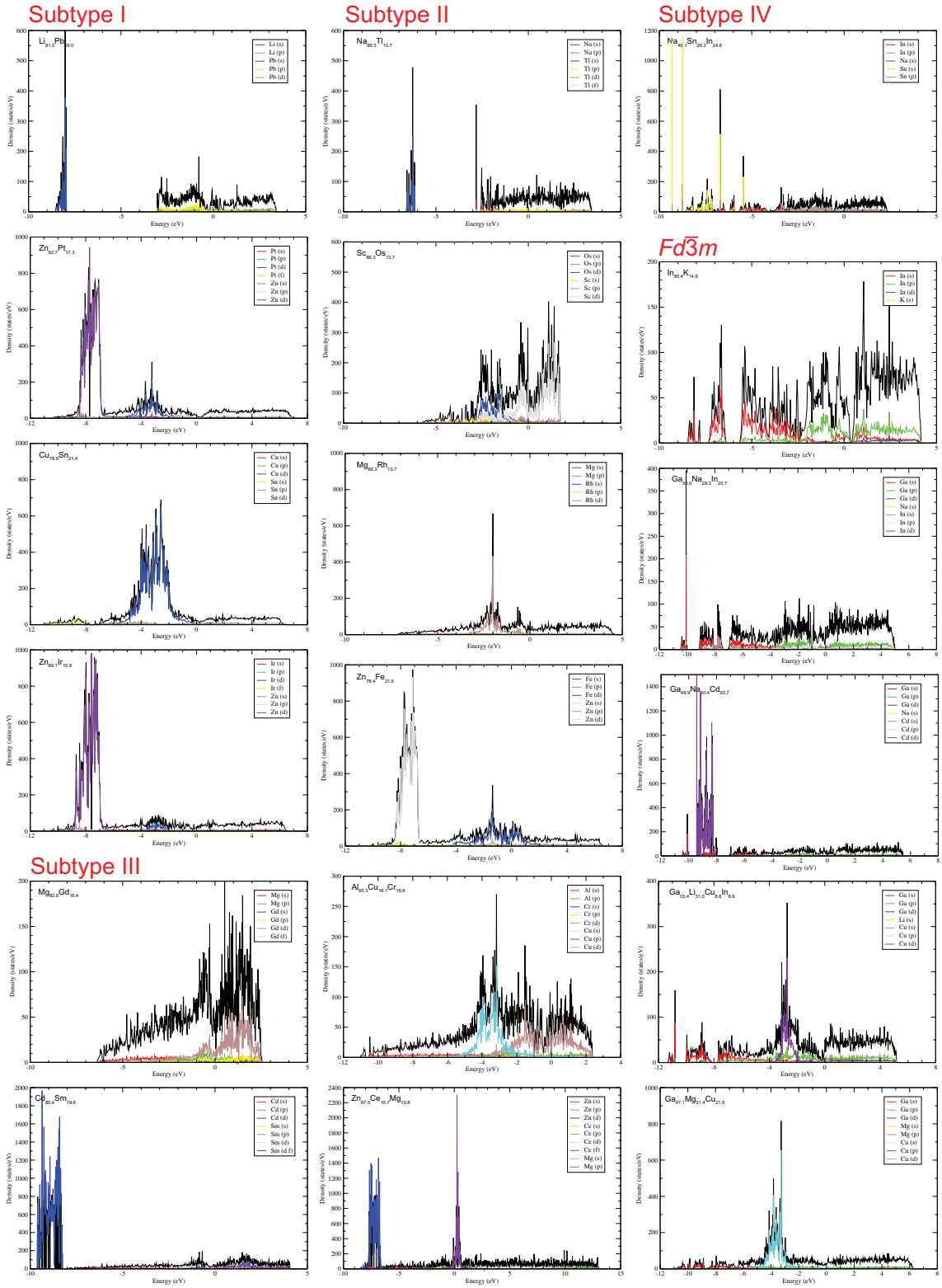

Figure 6
Density of states (DOS) graphs for representatives of the investigated structures ($cF(464-x)$).