Cu	*cF*4	(225) *Fm*-3*m* – a

Cu [1], c.c.p. (cubic close-packed), f.c.c. (face-centered cubic), Strukturbericht notation A1
Structural features: Close-packed layers in c stacking, i.e. consecutive layers are shifted in the same direction. See Fig. I.37.

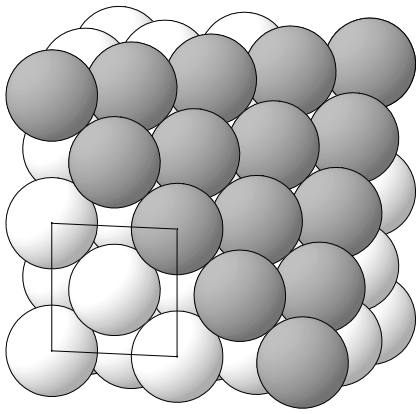

Fig. I.37. **Cu**

Arrangement of Cu atoms emphasizing a close-packed layer perpendicular to [111].

Bragg W.L. (1914) [1]
Cu
$a = 0.36$ nm, $V = 0.0467$ nm^3, $Z = 4$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Cu1	4*a*	*m*-3*m*	0	0	0		cuboctahedron Cu_{12}

Experimental: single crystal, spectrometer, X-rays

References: [1] Bragg W.L. (1914), Philos. Mag. 28, 355-360.

Cu_2MnAl	*cF*16	(225) *Fm*-3*m* – cba

$MnCu_2Al$ [2], Heusler phase, Strukturbericht notation $L2_1$; $NaLi_2Sb$ [3]; $LiRuGa_2$ [5]; $CsLi_2C_{60}$ [4], fulleride-$CsLi_2$

Structural features: $Cu(Mn_4Al_4)$ cubes share all faces to form a 3D-framework. Alternatively: $AlCu_8$ and $MnAl_8$ cubes share all faces to form a 3D-framework. Ordering variant of W (b.c.c.), sequence along <111>: -Cu-Al-Cu-Mn-. $NaLi_2Sb$ contains close-packed Sb layers in c stacking, Na occupies all octahedral and Li all tetrahedral voids. See Fig. I.41.

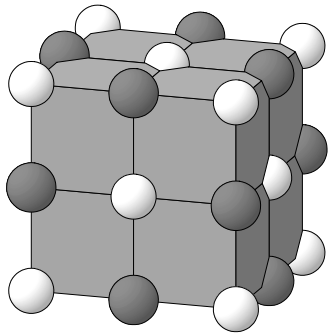

Fig. I.41. **$MnCu_2Al$**

Arrangement of $Cu(Mn_4Al_4)$ cubes (Mn atoms dark, Al atoms light).

Soltys J. (1981) [1]
$AlCu_2Mn$
$a = 0.5958$ nm, $V = 0.2115$ nm^3, $Z = 4$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Cu1	8*c*	-43*m*	$^1/_4$	$^1/_4$	$^1/_4$		rhombic dodecahedron $Al_4Mn_4Cu_6$
Mn2	4*b*	*m*-3*m*	$^1/_2$	$^1/_2$	$^1/_2$		rhombic dodecahedron Cu_8Al_6
Al3	4*a*	*m*-3*m*	0	0	0		rhombic dodecahedron Cu_8Mn_6

Experimental: powder, diffractometer, X-rays

Remarks: The centers of pseudo-spherical C_{60} units are considered for $CsLi_2C_{60}$ (orientational disorder). In the abstract of [3] the Wyckoff positions of the Li and Na sites are misprinted as 8*b* and 4*a* instead of 8*c* and 4*b*, respectively.

References: [1] Soltys J. (1981), Phys. Status Solidi A 66, 485-491. [2] (1931), Strukturberichte 1, 488, 551. [3] Hurng W. (1991), Mater. Res. Bull. 26, 439-442. [4] Hirosawa I., Prassides K., Mizuki J., Tanigaki K., Gevaert M., Lappas A., Cockcroft J.K. (1994), Science (Washington D.C.) 264, 1294-1297. [5] Czybulka A., Petersen A., Schuster H.U. (1990), J. Less-Common Met. 161, 303-312.

Th_6Mn_{23}	*cF*116	(225) *Fm*-3*m* – f^2eda

Th_6Mn_{23} [1], Strukturbericht notation $D8_a$
Structural features: Intergrowth of Ca_3Ag_8- (Th_6 octahedron surrounded by a Mn_8 cube and a Mn_{12} cuboctahedron) and W- (a central Mn atom surrounded by a Mn_8 cube, a Th_6 octahedron and a Mn_{12} cuboctahedron) type nested polyhedra units. See Fig. I.53.

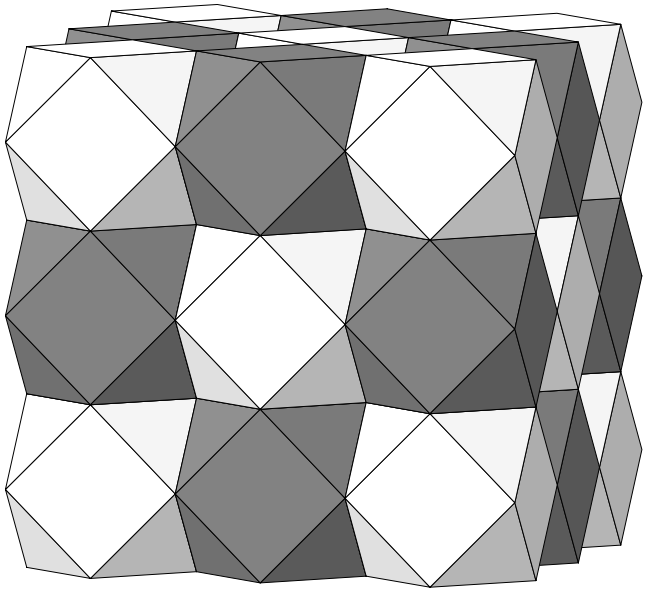

Fig. I.53. **Th_6Mn_{23}**

Arrangement of Mn_{12} cuboctahedra, which represent 27-atom W-type (Mn central atom + Mn_8 cube + Th_6 octahedron + Mn_{12} cuboctahedron; light) and 26-atom Ca_3Ag_8-type (Th_6 octahedron + Mn_8 cube + Mn_{12} cuboctahedron; dark) nested polyhedra units.

Florio J.V. et al. (1952) [1]
$Mn_{23}Th_6$
a = 1.2523 nm, V = 1.9639 nm^3, Z = 4

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Mn1	32*f*	.3*m*	0.122	0.122	0.122		pseudo Frank-Kasper $Mn_{10}Th_3$
Mn2	32*f*	.3*m*	0.322	0.322	0.322		icosahedron Mn_9Th_3
Th3	24*e*	4*m*.*m*	0.297	0	0		7-capped pentagonal prism $Mn_{13}Th_4$
Mn4	24*d*	*m*.*mm*	0	$^1/_4$	$^1/_4$		icosahedron Mn_8Th_4
Mn5	4*a*	*m*-3*m*	0	0	0		square prism (cube) Mn_8

Transformation from published data: origin shift $^1/_2$ $^1/_2$ $^1/_2$
Experimental: single crystal, Weissenberg and rotation photographs, X-rays, R = 0.100

References: [1] Florio J.V., Rundle R.E., Snow A.I. (1952), Acta Crystallogr. 5, 449-457.