

Space group (202) *Fm-3*202
cF48

$\text{Na}_{9.7}[\text{C}_{60}]$	<i>cF48</i>	(202) <i>Fm-3</i> – <i>fcba</i>
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 $\text{Na}_{9.7}\text{C}_{60}$ [1], fulleride- $\text{Na}_{9.7}$

Structural features: Pseudo-spherical C_{60} fullerene units (twelve 5- and twenty 6-membered rings) in a Cu-type (c.c.p.) arrangement; Na in "octahedral" and "tetrahedral" voids (the partly occupied sites forming a centered cube in the former).

Ylldirim T. et al. (1992) [1]

 $\text{CNa}_{9.28}$ $a = 1.459 \text{ nm}$, $V = 3.1057 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Na1	$32f$.3.	0.11	0.11	0.11	0.89	trigonal bipyramid Na_5
Na2	$8c$	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.88	tetrahedron Na_4
$(\text{C}_{60})_3$	$4b$	$m-3.$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		32-vertex polyhedron Na_{32}
Na4	$4a$	$m-3.$	0	0	0	0.4	square prism (cube) Na_8

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: powder, diffractometer, X-rays, $wR_p = 0.099$

Remarks: The atom coordinates correspond to the positions of Na atoms and the centers of C_{60} units. The authors state that the symmetry is lowered due to preferential orientation of the C_{60} units, otherwise the data can be described in space group (225) *Fm-3m*.

References: [1] Ylldirim T., Zhou O., Fischer J.E., Bykovetz N., Strongin R.A., Cichy M.A., Smith A.B. III., Lin C.L., Jelinek R. (1992), *Nature* (London) 360, 568-571.

202
cF56

CuZrF_6	<i>cF56</i>	(202) <i>Fm-3</i> – <i>hba</i>
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 CuZrF_6 **α** [1]

Structural features: Distorted close-packed F layers in c stacking, Cu and Zr in octahedral voids. CuF_6 and ZrF_6 octahedra share vertices to form a 3D-framework; the splitting of the F site is assumed to better accommodate Cu (Jahn-Teller effect).

Propach V., Steffens F. (1978) [1]

 CuF_6Zr $a = 0.7939 \text{ nm}$, $V = 0.5004 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	$48h$	$m..$	0	0.0186	0.2494	0.5	
Zr2	$4b$	$m-3.$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Cu3	$4a$	$m-3.$	0	0	0		

Experimental: powder, diffractometer, neutrons, $R = 0.015$, $T = 393 \text{ K}$

Remarks: Phase stable at $T > 383$ K. Short interatomic distances for partly occupied site(s). Space groups (196) $F23$, (201) $Pn-3$, (216) $F-43m$ and (225) $Fm-3m$ were tested ($R = 0.014, 0.090, 0.013$, and 0.013 , respectively) and rejected considering the smooth transition to the β -phase for which space group (148) $R-3$ was found.

References: [1] Propach V., Steffens F. (1978), Z. Naturforsch. B 33, 268-274.

202
cF88

$K_3Co(NO_2)_6$	cF88	(202) $Fm-3$ – hecba
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$K_3[Co(NO_2)_6]$ [1], Strukturbericht notation J2₄

Structural features: $Co(NO_2)_6$ octahedral units (CoN_6 octahedron, non-linear NO_2 units) and K atoms in a BiF_3 -type arrangement.

Van Driel M., Verweel H.J. (1936) [1]

$CoK_3N_6O_{12}$

$a = 1.046$ nm, $V = 1.1444$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	m..	0	0.1	0.235		single atom N
N2	24e	mm2..	0.195	0	0		non-colinear O ₂
K3	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron O ₁₂
K4	4b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron O ₁₂
Co5	4a	m-3.	0	0	0		octahedron N ₆

Transformation from published data: $y, x, -z$

Experimental: powder, film, X-rays

References: [1] Van Driel M., Verweel H.J. (1936), Z. Kristallogr. 95, 308-314.

202
cF88

$K_2CuPb(NO_2)_6$	cF88	(202) $Fm-3$ – hecba
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$K_2Pb[Cu(NO_2)_6]$ [1]

Structural features: $Cu(NO_2)_6$ octahedral units (CuN_6 octahedron, non-linear NO_2 units) in a Cu-type (c.c.p.) arrangement, Pb in "octahedral", K in "tetrahedral" voids. Ordering variant of $K_3[Co(NO_2)_6]$. See Fig. II.59.

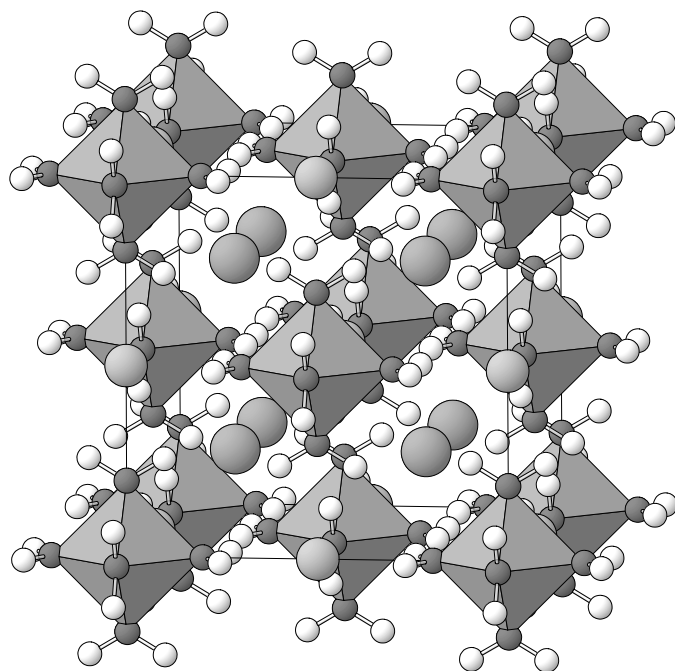
Isaacs N.W., Kennard C.H.L. (1969) [1]

$CuK_2N_6O_{12}Pb$

$a = 1.066$ nm, $V = 1.2114$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	m..	0	0.0986	0.2571		single atom N
N2	24e	mm2..	0.1983	0	0		non-colinear O ₂
K3	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron O ₁₂
Pb4	4b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron O ₁₂
Cu5	4a	m-3.	0	0	0		octahedron N ₆

Experimental: single crystal, diffractometer, neutrons, $R = 0.098$

Fig. II.59. $\text{K}_2\text{Pb}[\text{Cu}(\text{NO}_2)_6]$

Arrangement of $\text{Cu}(\text{NO}_2)_6$ octahedra (N atoms dark, O atoms light), K (large) and Pb (medium) atoms.

References: [1] Isaacs N.W., Kennard C.H.L. (1969), J. Chem. Soc. A 1969, 386-389.

202
 $cF104$

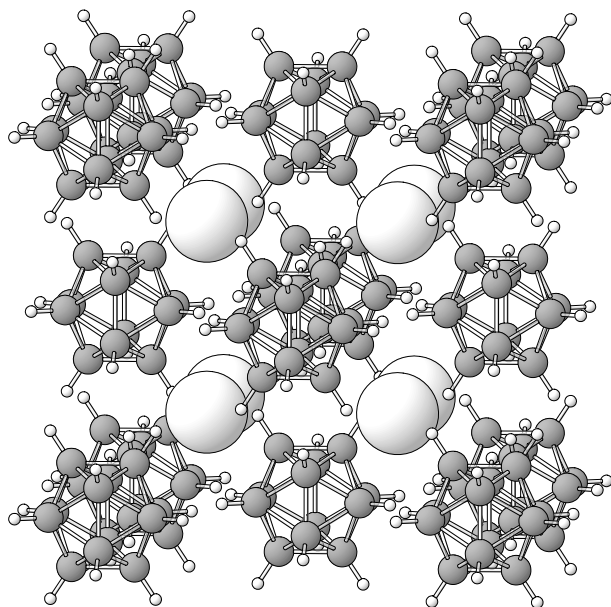
KB_6H_6

$cF104$

(202) $Fm-3 - h^2c$

$\text{K}_2\text{B}_{12}\text{H}_{12}$ [1]

Structural features: $\text{B}_{12}\text{H}_{12}$ icosahedral units (B_{12} icosahedron, one H bonded to each B) and K atoms in a CaF_2 -type arrangement. See Fig. II.60.

Fig. II.60. $\text{K}_2\text{B}_{12}\text{H}_{12}$

Arrangement of $\text{B}_{12}\text{H}_{12}$ units (B atoms dark, H atoms light) and K atoms (large).

Wunderlich J.A., Lipscomb W.N. (1960) [1]
 B_6H_6K

$a = 1.061 \text{ nm}$, $V = 1.1944 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	48h	m..	0	0.0827	0.1359		pentagonal pyramid HB_5
H2	48h	m..	0	0.138	0.22		single atom B
K3	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron H_{12}

Transformation from published data: $y, x, -z$

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.061$

References: [1] Wunderlich J.A., Lipscomb W.N. (1960), J. Am. Chem. Soc. 82, 4427-4428.

202
cF136

$K_2Ba[Ni(NO_2)_6]$	<i>cF136</i>	(202) <i>Fm-3</i> – h^2ecba
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$K_2Ba[Ni(NO_2)_6]$ [1]

Structural features: $Ni(NO_2)_6$ octahedral units (NiN_6 octahedron, non-linear NO_2 units in partial orientational disorder) in a Cu-type (c.c.p.) arrangement, Ba in "octahedral", K in "tetrahedral" voids. Disordered derivative of $K_2Pb[Cu(NO_2)_6]$.

Takagi S. et al. (1975) [1]

$BaK_2N_6NiO_{12}$

$a = 1.078 \text{ nm}$, $V = 1.2527 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	m..	0	0.09848	0.25326	0.733	non-coplanar triangle NO_2
O2	48h	m..	0	0.25309	0.09995	0.267	non-coplanar triangle NO_2
N3	24e	mm2..	0.1929	0	0		square pyramid O_4Ni
K4	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		24-vertex polyhedron O_{24}
Ba5	4b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		24-vertex polyhedron O_{24}
Ni6	4a	m-3.	0	0	0		octahedron N_6

Experimental: single crystal, diffractometer, X-rays, $R = 0.016$

References: [1] Takagi S., Joesten M.D., Lenhert P.G. (1975), Acta Crystallogr. B 31, 1970-1972.

202
cF160

$Cs_3[UO_2]F_5$	<i>cF160</i>	(202) <i>Fm-3</i> – h^2e^2cba
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$Cs_3UO_2F_5$ form I [1]

Structural features: $U(O_2F_5)$ pentagonal bipyramids (orientational disorder, O in axial positions) and Cs atoms in a BiF_3 -type arrangement.

Brusset H., Quy Dao N. (1971) [1]

$Cs_3F_{5.01}O_2U$

$a = 0.9833 \text{ nm}$, $V = 0.9507 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	48h	m..	0	0.069	0.211	0.167	

F2	48h	<i>m.</i>	0	0.18	0.131	0.167	
O3	24e	<i>mm2.</i>	0.183	0	0	0.333	
F4	24e	<i>mm2.</i>	0.222	0	0	0.167	
Cs5	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron F ₁₂
Cs6	4b	<i>m-3.</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron F ₆
U7	4a	<i>m-3.</i>	0	0	0		octahedron O ₆

Transformation from published data: *y,x,-z*

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Brusset H., Quy Dao N. (1971), J. Inorg. Nucl. Chem. 33, 1365-1372.

202
cF240

[C ₆₀]	cF240	(202) <i>Fm-3</i> – i ² h
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C₆₀ rt [1]

Structural features: Pseudo-spherical C₆₀ fullerene units (twelve 5- and twenty 6-membered rings) in a Cu-type (c.c.p.) arrangement.

Dorset D. L., McCourt M.P. (1994) [1]

C₆₀

a = 1.426 nm, *V* = 2.8997 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	96i	1	0.052	0.185	0.165		non-coplanar triangle C ₃
C2	96i	1	0.085	0.105	0.220		non-coplanar triangle C ₃
C3	48h	<i>m.</i>	0	0.052	0.249		non-coplanar triangle C ₃

Transformation from published data: *y,x,-z*

Experimental: single crystal, electron diffraction, R = 0.230

Remarks: Phase stable at T > 249 K. The authors state that the true symmetry is space group (225) *Fm-3m* (orientational disorder).

References: [1] Dorset D. L., McCourt M.P. (1994), Acta Crystallogr. A 50, 344-351.

202
cF264

Mg ₂₆ Ag ₇	cF264	(202) <i>Fm-3</i> – ih ² fecba
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Ag_{7+x}Mg_{26-x} [1]

Structural features: 55-atom Mackay icosahedron units (a central Ag atom surrounded by a (Mg,Ag)₁₂ icosahedron, a (Mg,Ag)₃₀ icosidodecahedron and a large Ag₁₂ icosahedron) in a Cu-type (c.c.p.) arrangement are interconnected via AgMg₁₄ rhombic dodecahedra to form a 3D-framework; additional Mg in voids.

Kreiner G., Spiekermann S. (2001) [1]

Ag_{7.96}Mg_{25.04}

a = 1.7612 nm, *V* = 5.4629 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mg1	96i	1	0.09675	0.25997	0.15471		14-vertex Frank-Kasper Ag ₃ Mg ₁₁
M2	48h	<i>m.</i>	0	0.0884	0.36247		12-vertex polyhedron Ag ₂ Mg ₁₀

Ag3	48h	m..	0	0.15847	0.22495	11-vertex polyhedron Mg ₁₀ Ag
Mg4	32f	.3.	0.09328	0.09328	0.09328	pseudo Frank-Kasper Ag ₄ Mg ₉
Mg5	24e	mm2..	0.21435	0	0	12-vertex polyhedron Ag ₂ Mg ₁₀
M6	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	icosahedron Mg ₁₂
Ag7	4b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	icosahedron Mg ₁₂
Ag8	4a	m-3.	0	0	0	square prism (cube) Mg ₈

M2 = 0.884Mg + 0.116Ag; M6 = 0.737Mg + 0.263Ag

Experimental: single crystal, diffractometer, X-rays, R = 0.023

Remarks: Phase referred to as ε -(AgMg).

References: [1] Kreiner G., Spiekermann S. (2001), Z. Anorg. Allg. Chem. 627, 2460-2468.

202
cF272

[C ₆₀][O ₂]	cF272	(202) <i>Fm-3</i> – i ² hf
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C₆₀O₂ [1], fullerene (O₂)

Structural features: Pseudo-spherical C₆₀ fullerene units (twelve 5- and twenty 6-membered rings) in a Cu-type (c.c.p.) arrangement; one atom of the O₂ molecules is located above a C₆ hexagon, the other one is delocalized.

Bensch W. et al. (1994) [1]

C₆₀O

$a = 1.4152$ nm, $V = 2.8344$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	96i	1	0.0469	0.1722	0.1599		coplanar square C ₃ O
C2	96i	1	0.0845	0.0946	0.2015		coplanar square OC ₃
C3	48h	m..	0	0.0517	0.2349		non-coplanar triangle C ₃
O4	32f	.3.	0.1379	0.1379	0.1379	0.125	coplanar hexagon C ₆

Experimental: single crystal, diffractometer, X-rays, wR = 0.052, T = 300 K

Remarks: Phase stable at T > 256 K. The second O atom of the O₂ molecules was not located. The indication of the occupancy of the O site is ambiguous; we assigned the value corresponding to a maximum O content. Space group (225) *Fm-3m* was tested and rejected.

References: [1] Bensch W., Werner H., Bartl H., Schlögl R. (1994), J. Chem. Soc., Faraday Trans. 90, 2791-2797.

202
cF280

Sr _{2.08} [C ₆₀]	cF280	(202) <i>Fm-3</i> – i ² hfc
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Sr_{2.08}C₆₀ [1], fulleride-Sr_{2.08}

Structural features: Pseudo-spherical C₆₀ fullerene units (twelve 5- and twenty 6-membered rings) in a Cu-type (c.c.p.) arrangement; Sr in "octahedral" and "tetrahedral" voids (the partly occupied positions forming a cube in the former).

Kortan A.R. et al. (1994) [1]

C₆₀Sr_{2.08}

$a = 1.4144$ nm, $V = 2.8296$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	96i	1	0.0502	0.3183	0.1625		non-coplanar triangle C ₃
C2	96i	1	0.0813	0.0997	0.2873		non-coplanar triangle C ₃
C3	48h	m..	0	0.0502	0.2562		non-coplanar triangle C ₃
Sr4	32f	.3.	0.1139	0.1139	0.1139	0.15	trigonal prism C ₆
Sr5	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.44	28-vertex polyhedron C ₂₄ Sr ₄

Transformation from published data: y,x,-z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays

Remarks: On page 502 of [1] the occupancy of former Sr2 is misprinted as 0.88 instead of 0.44 (agreement with the refined composition).

References: [1] Kortan A.R., Kopylov N., Özdas E., Ramirez A.P., Fleming R.M., Haddon R.C. (1994), Chem. Phys. Lett. 223, 501-505.

202
cF296

Li ₃ P ₆ S ₆ N ₇ [H ₂ O] ₁₃	cF296	(202) <i>Fm</i> -3 – h ³ f ⁴ e
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Li₆[P₁₂S₁₂N₁₄]·26H₂O [1]

Structural features: P₁₂S₁₂N₁₄ units formed by twelve P(N₃S) tetrahedra sharing N vertices (a P₁₂N₁₄ cage with one S bonded to each P); Li and H₂O between the cages (partial disorder).

Roth S., Schnick W. (2001) [1]

H₂₆Li₃N₇O₁₃P₆S₆

a = 1.7974 nm, *V* = 5.8068 nm³, *Z* = 8

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	m..	0	0.0809	0.3268		tetrahedron (OH ₂) ₂ ON
P2	48h	m..	0	0.13371	0.07803		tetrahedron N ₃ S
S3	48h	m..	0	0.19715	0.16566		single atom P
N4	32f	.3.	0.07405	0.07405	0.07405		non-coplanar triangle P ₃
O5	32f	.3.	0.1901	0.1901	0.1901		non-coplanar triangle Li ₃
Li6	32f	.3.	0.3011	0.3011	0.3011	0.75	tetrahedron O ₃ (OH ₂)
(OH ₂)7	32f	.3.	0.3689	0.3689	0.3689	0.75	tetrahedron LiO ₃
N8	24e	mm2..	0.176	0	0		non-collinear P ₂
H9	96i	1	0.0215	0.0595	0.3678		
H10	96i	1	0.1623	0.1792	0.2264	0.667	

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, *R* = 0.056, *T* = 293 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. We assume that in the supplementary material deposited for [1] the *x*-coordinate of former H2 is misprinted as 0.485 instead of 0.4785 (four decimals, closer to expected interatomic distances).

References: [1] Roth S., Schnick W. (2001), Z. Anorg. Allg. Chem. 627, 1165-1172.

202
cF296

Fe ₂ Pd ₂₁ Al ₃₉	cF296	(202) <i>Fm</i> -3 – ih ² f ² ecba
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Fe₂Pd₂₁Al₃₉ [1]

Structural features: Commensurate approximant of icosahedral quasicrystals.

Edler F.J. et al. (1998) [1]

$\text{Al}_{38.78}\text{Fe}_{2.15}\text{Pd}_{21.07}$

$a = 1.5515 \text{ nm}$, $V = 3.7347 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	96i	1	0.0995	0.159	0.25		14-vertex Frank-Kasper Pd_5Al_9
Al2	48h	$m..$	0	0.064	0.143	0.4	non-coplanar triangle Al_3
Pd3	48h	$m..$	0	0.241	0.1482		15-vertex polyhedron $\text{Al}_{12}\text{Pd}_3$
Al4	32f	.3.	0.09	0.09	0.09	0.4	non-coplanar triangle Al_3
M5	32f	.3.	0.4028	0.4028	0.4028		pseudo Frank-Kasper Al_7Pd_6
Al6	24e	$mm2..$	0.3095	0	0		pseudo Frank-Kasper Pd_6Al_7
Pd7	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron Al_{12}
M8	4b	$m-3.$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron Pd_8Al_6
M9	4a	$m-3.$	0	0	0		20-vertex polyhedron Al_{20}

$\text{M5} = 0.86\text{Pd} + 0.14\text{Fe}$; $\text{M8} = 0.78\text{Al} + 0.22\text{Fe}$; $\text{M9} = 0.81\text{Fe} + 0.19\text{Pd}$

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.054$, $T = 293 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Edler F.J., Gramlich V., Steurer W. (1998), J. Alloys Compd. 269, 7-12.