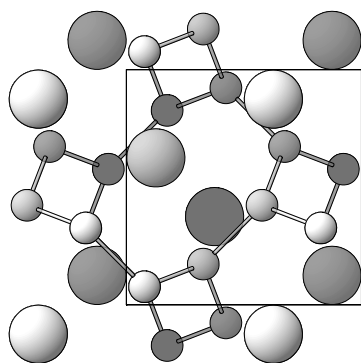


Space group (213) $P4_132$ 213
 $cP12$

SrSi_2	$cP12$	(213) $P4_132 - ca$
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SrSi₂ cubic [2]

Structural features: Si forms a 3D-framework with approximately planar SiSi₃ triangles (helical chains of square cross-section parallel to $\langle 100 \rangle$); Sr in distorted cubes. See Fig. II.28.

Fig. II.28. **SrSi₂ cubic**

Arrangement of Sr (large) and Si (small) atoms.

Pringle G.E. (1972) [1]

 Si_2Sr $a = 0.6515 \text{ nm}$, $V = 0.2765 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	8c	.3.	0.0769	0.0769	0.0769		non-coplanar triangle Si ₃
Sr2	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		pseudo Frank-Kasper Si ₁₄ Sr ₆

Transformation from published data ($P4_332$): new axes -a,-b,-c; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.077$

Remarks: Cell parameter from [3]. The structure was determined independently in [4] (manuscript submitted in 1964, original in Russian published in 1966).

References: [1] Pringle G.E. (1972), Acta Crystallogr. B 28, 2326-2328. [2] Janzon K., Schäfer H., Weiss A. (1965), Angew. Chem. 77, 258-259. [3] Faulring G.M., Malizie E.S. (1966), Adv. X-Ray Anal. 10, 409-421. [4] Kripyakevich P.I., Gladyshevskii E.I. (1967), Sov. Phys. Crystallogr. (Engl. Transl.) 11, 693-696.

213
 $cP20$

Mn	$cP20$	(213) $P4_132 - dc$
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Mn β [2], Strukturbericht notation A13

Structural features: Mn forms a 3D-framework with interpenetrating MnMn₁₂ icosahedra and distorted MnMn₁₄ Frank-Kasper polyhedra (bicapped hexagonal antiprism). See Fig. II.29.

Shoemaker C.B. et al. (1978) [1]

Mn

 $a = 0.6315 \text{ nm}$, $V = 0.2518 \text{ nm}^3$, $Z = 20$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mn1	12 <i>d</i>	..2	$\frac{1}{8}$	0.20224	0.45224		14-vertex Frank-Kasper Mn ₁₄
Mn2	8 <i>c</i>	.3.	0.06361	0.06361	0.06361		icosahedron Mn ₁₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.022

Remarks: Phase stable at 997 < T < 1373 K.

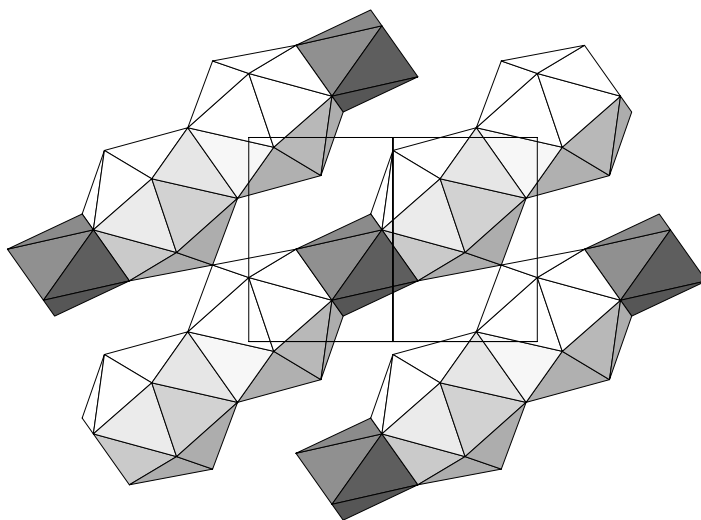


Fig. II.29. **Mn β**

Slab of columns of MnMn₁₂ icosahedra (light) and Mn₆ octahedra (dark) along <111>.

References: [1] Shoemaker C.B., Shoemaker D.P., Hopkins T.E., Yindepit S. (1978), Acta Crystallogr. B 34, 3573-3576. [2] (1937), Strukturberichte 2, 3.

213
cP20

Mg₃Ru₂

cP20

(213) P4₁32 – dc

RuMg_{1.5} [1]

Structural features: Mg and Ru form a dense 3D-framework with interpenetrating Ru(Mg₉Ru₃) icosahedra and distorted Mg(Mg₈Ru₆) Frank-Kasper polyhedra (bicapped hexagonal antiprism). Ordering variant of β-Mn.

Westin L., Edshammar L.E. (1973) [1]

Mg₃Ru₂

a = 0.6929 nm, *V* = 0.3327 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mg1	12 <i>d</i>	..2	$\frac{1}{8}$	0.203	0.453		14-vertex Frank-Kasper Ru ₆ Mg ₈
Ru2	8 <i>c</i>	.3.	0.074	0.074	0.074		icosahedron Ru ₃ Mg ₉

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.170

Remarks: Homogeneity range Mg_{100-x}Ru_x, 23.5 < x < 44.4.

References: [1] Westin L., Edshammar L.E. (1973), Chem. Scr. 3, 15-22.

$\text{Mo}_3\text{Al}_2\text{C}$	$cP24$	(213) $P4_132 - dca$
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$\text{Mo}_3\text{Al}_2\text{C}$ [1]; $\text{W}_2\text{Cr}_9\text{Fe}_{10}\text{C}$ [2]

Structural features: Filled-up derivative of β -Mn with an ordered arrangement of Mo and Al; C in distorted octahedral (Mo_6) voids. See Fig. II.30.

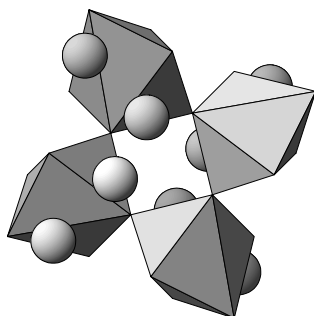


Fig. II.30. **$\text{Mo}_3\text{Al}_2\text{C}$**

Arrangement of CMo_6 octahedra and Al atoms.

Jeitschko W. et al. (1963) [1]

Al_2CMo_3

$a = 0.686 \text{ nm}$, $V = 0.3228 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mo1	12d	..2	$\frac{1}{8}$	0.206	0.456		14-vertex polyhedron $\text{C}_2\text{Al}_6\text{Mo}_6$
Al2	8c	.3.	0.061	0.061	0.061		icosahedron Al_3Mo_9
C3	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron Mo_6

Experimental: powder, film, X-rays

Remarks: Atom coordinates for $\text{W}_2\text{Cr}_9\text{Fe}_{10}\text{C}$ not determined.

References: [1] Jeitschko W., Nowotny H., Benesovsky F. (1963), Monatsh. Chem. 94, 247-251. [2] Goldschmidt H.J. (1957), Acta Crystallogr. 10, 54-54.

$(\text{Mg}_{0.85}\text{Cu}_{0.15})_2\text{Cu}_3(\text{Cu}_{0.2}\text{Si}_{0.8})$	$cP24$	(213) $P4_132 - dca$
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$\text{Mg}_{28.4}\text{Cu}_{57.9}\text{Si}_{13.7}$ [1]

Structural features: Substitution derivative of MgCu_2 (cubic Laves phase). $(\text{Mg,Cu})(\text{Mg,Cu})_4\text{Cu}_9(\text{Cu,Si})_3$ Friauf polyhedra $((\text{Cu,Si})_{12}$ truncated tetrahedron + $(\text{Mg,Cu})_4$ tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework, (Mg,Cu) forming a diamond-type sublattice. Tetrahedrally close-packed structure (Frank-Kasper phase).

Matsunaga T. et al. (1984) [1]

$\text{Cu}_{3.47}\text{Mg}_{1.70}\text{Si}_{0.83}$

$a = 0.69598 \text{ nm}$, $V = 0.3371 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12d	..2	$\frac{1}{8}$	0.13092	0.38092		icosahedron Mg_6
M2	8c	.3.	0.00320	0.00320	0.00320		16-vertex Frank-Kasper Mg_4

M3 4a .32 $\frac{3}{8}$ $\frac{3}{8}$ $\frac{3}{8}$ icosahedron Mg₆

M1 = 0.979Cu + 0.021Si; M2 = 0.85Mg + 0.15Cu; M3 = 0.763Si + 0.237Cu

Experimental: single crystal, diffractometer, X-rays, R = 0.046

References: [1] Matsunaga T., Kodera E., Komura Y. (1984), Acta Crystallogr. C 40, 1668-1670.

213
cP32

CsBe₂F₅ cP32 (213) P4₁32 – dc²a

CsBe₂F₅ β [1]

Structural features: BeF₄ tetrahedra share vertices to form a 3D-framework with 10-rings.

Le Fur Y., Aleonard S. (1972) [1]

Be₂CsF₅

a = 0.7936 nm, *V* = 0.4998 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>d</i>	..2	$\frac{1}{8}$	0.0329	0.2829		non-collinear Be ₂
Be2	8 <i>c</i>	.3.	0.1006	0.1006	0.1006		tetrahedron F ₄
F3	8 <i>c</i>	.3.	0.759	0.759	0.759		single atom Be
Cs4	4 <i>a</i>	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		14-vertex polyhedron F ₁₂ Be ₂

Experimental: powder, diffractometer, neutrons, R = 0.040

Remarks: Phase stable at T < 727 K. Structure analyzed jointly on X-ray and neutron diffraction data. Supersedes a report on β-CsBe₂F₅ with orthorhombic symmetry in [2].

References: [1] Le Fur Y., Aleonard S. (1972), Acta Crystallogr. B 28, 2115-2118. [2] Breusov O.N., Simanov Y.P. (1959), Russ. J. Inorg. Chem. 4, 1190-1194.

213
cP48

Ag₃AuS₂ cP48 (213) P4₁32 – ec³

Ag₃AuS₂ β [1]

Structural features: Single S-Au-S linear units.

Messien P. et al. (1966) [1]

Ag₃AuS₂

a = 0.972 nm, *V* = 0.9183 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	24 <i>e</i>	1	0.042	0.255	0.36		tricapped trigonal prism Ag ₃ S ₄ Au ₂
Au2	8 <i>c</i>	.3.	0.13	0.13	0.13		8-vertex polyhedron Ag ₆ S ₂
S3	8 <i>c</i>	.3.	0.305	0.305	0.305		square prism (cube) SAg ₆ Au
S4	8 <i>c</i>	.3.	0.785	0.785	0.785		square prism (cube) Ag ₆ AuS

Experimental: powder, diffractometer, X-rays, R = 0.220

Remarks: Phase stable at T < 458 K.

References: [1] Messien P., Baiwir M., Tavernier B. (1966), Bull. Soc. R. Sci. Liege 35, 727-733.

213
cP52

$\text{Zn}_2\text{Ge}_3\text{O}_8$	<i>cP52</i>	(213) $P4_132 - \text{edc}^2$
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 $\text{Zn}_2\text{Ge}_3\text{O}_8$ [1], spinel family

Structural features: Close-packed O layers in c stacking; Zn in tetrahedral, Ge in octahedral voids. Edge-linked GeO_6 octahedra share vertices with ZnO_4 tetrahedra to form a defect spinel-type 3D-framework $\text{Zn}_2\text{Ge}_3\text{O}_8$.

Joubert J.C., Durif A. (1963) [1]

 $\text{Ge}_3\text{O}_8\text{Zn}_2$ $a = 0.8213 \text{ nm}$, $V = 0.5540 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>e</i>	1	0.113	0.383	0.363		non-coplanar triangle ZnGe_2
Ge2	12 <i>d</i>	.2	$\frac{1}{8}$	0.137	0.387		octahedron O_6
Zn3	8 <i>c</i>	.3.	0.012	0.012	0.012		tetrahedron O_4
O4	8 <i>c</i>	.3.	0.137	0.137	0.137		tetrahedron ZnGe_3

Transformation from published data ($P4_332$): new axes -a,-b,-cExperimental: powder, film, X-rays, $R = 0.090$

References: [1] Joubert J.C., Durif A. (1963), C. R. Hebd. Seances Acad. Sci. 256, 4403-4405.

213
cP56

$\text{Cu}_3\text{Mn}_3\text{O}_8$	<i>cP56</i>	(213) $P4_132 - \text{edc}^2a$
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 $\text{Cu}_{1.5}\text{Mn}_{1.5}\text{O}_4$ [1], spinel $\text{A}_2[\text{AB}_3]\text{O}_8$

Structural features: Close-packed O layers in c stacking; part of Cu in tetrahedral, Mn and remaining Cu in octahedral voids. Single CuO_4 tetrahedra and edge-linked MnO_6 and CuO_6 octahedra share vertices to form a spinel-type 3D-framework.

Vandenberghe R.E. et al. (1976) [1]

 $\text{Cu}_3\text{Mn}_3\text{O}_8$ $a = 0.828 \text{ nm}$, $V = 0.5677 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>e</i>	1	0.126	0.348	0.358		tetrahedron Mn_2Cu_2
Mn2	12 <i>d</i>	.2	$\frac{1}{8}$	0.129	0.379		octahedron O_6
O3	8 <i>c</i>	.3.	0.133	0.133	0.133		tetrahedron CuMn_3
Cu4	8 <i>c</i>	.3.	0.757	0.757	0.757		tetrahedron O_4
Cu5	4 <i>a</i>	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O_6

Transformation from published data ($P4_332$): new axes -a,-b,-cExperimental: powder, diffractometer, neutrons, $R_B = 0.060$, $T = 293 \text{ K}$ Remarks: Ambiguous data, we interpret the atom coordinates of former B2 as $\frac{3}{8} + \Delta$, $\frac{3}{8}$, $\frac{5}{8} + \Delta$.

References: [1] Vandenberghe R.E., Legrand E., Scheerlinck D., Brabers V.A.M. (1976), Acta Crystallogr. B 32, 2796-2798.

213
cP56

$\text{Li}(\text{Li}_{0.5}\text{Zn}_{0.5})_2\text{Ge}_3\text{O}_8$	<i>cP56</i>	(213) $P4_132 - \text{edc}^2a$
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 $\text{Li}_2\text{ZnGe}_3\text{O}_8$ [2], spinel $\text{A}_2\text{B}_3\text{B}'\text{O}_8$; $\text{CuMg}_{0.5}\text{Mn}_{1.5}\text{O}_4$ [3]

Structural features: Close-packed O layers in c stacking; (Li,Zn) in tetrahedral, Ge and remaining Li in octahedral voids. Single (Li,Zn) O_4 tetrahedra and edge-linked GeO_6 and LiO_6 octahedra share vertices to form a spinel-type 3D-framework. Substitution derivative of MgAl_2O_4 of ideal composition $\text{A}_2\text{B}_3\text{B}'\text{O}_8$.

Kawai H. et al. (1998) [1]

 $\text{Ge}_3\text{Li}_2\text{O}_8\text{Zn}$ $a = 0.81961 \text{ nm}$, $V = 0.5506 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>e</i>	1	0.11896	0.34906	0.3551		tetrahedron Ge_2Li_2
Ge2	12 <i>d</i>	..2	$\frac{1}{8}$	0.12536	0.37536		octahedron O_6
O3	8 <i>c</i>	.3.	0.13653	0.13653	0.13653		tetrahedron Ge_3Li
M4	8 <i>c</i>	.3.	0.75488	0.75488	0.75488		tetrahedron O_4
Li5	4 <i>a</i>	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O_6

 $\text{M4} = 0.5\text{Li} + 0.5\text{Zn}$ Transformation from published data ($P4_332$): new axes -a,-b,-cExperimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.021$ Remarks: A fully ordered structure is reported for $\text{CuMg}_{0.5}\text{Mn}_{1.5}\text{O}_4$ in [3].

References: [1] Kawai H., Tabuchi M., Nagata M., Tukamoto H., West A.R. (1998), J. Mater. Chem. 8, 1273-1280. [2] Durif A., Joubert J.C. (1962), C. R. Hebd. Seances Acad. Sci. 255, 2471-2473. [3] Vandenberghe R.E., Legrand E., Scheerlinck D., Brabers V.A.M. (1976), Acta Crystallogr. B 32, 2796-2798.

213
cP56

$(\text{Li}_{0.1}\text{Fe}_{0.9})(\text{Li}_{0.25}\text{Ti}_{0.1}\text{Fe}_{0.55})_2\text{O}_4$	<i>cP56</i>	(213) $P4_132 - \text{edc}^2a$
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 $\text{Li}_{0.6}\text{Ti}_{0.2}\text{Fe}_{2.2}\text{O}_4$ [1], spinel family

Structural features: Close-packed O layers in c stacking; (Fe,Li) in tetrahedral, (Fe,Li,Ti) in octahedral voids. Single (Fe,Li) O_4 tetrahedra and edge-linked (Fe,Li,Ti) O_6 octahedra share vertices to form a distorted spinel-type 3D-framework. Distorted derivative of MgAl_2O_4 .

Ligenza S. et al. (1988) [1]

 $\text{Fe}_{2.20}\text{Li}_{0.60}\text{O}_4\text{Ti}_{0.20}$ $a = 0.8326 \text{ nm}$, $V = 0.5772 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>e</i>	1	0.124	0.373	0.363		tetrahedron Fe_4
M2	12 <i>d</i>	..2	$\frac{1}{8}$	0.125	0.375		octahedron O_6
M3	8 <i>c</i>	.3.	0.0	0.0	0.0		tetrahedron O_4
O4	8 <i>c</i>	.3.	0.146	0.146	0.146		tetrahedron Fe_4
M5	4 <i>a</i>	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O_6

 $\text{M2} = 0.638\text{Fe} + 0.262\text{Li} + 0.100\text{Ti}$; $\text{M3} = 0.925\text{Fe} + 0.075\text{Li}$; $\text{M5} = 0.638\text{Fe} + 0.262\text{Li} + 0.100\text{Ti}$ Transformation from published data ($P4_332$): new axes -a,-b,-cExperimental: powder, diffractometer, neutrons, $R = 0.064$

References: [1] Ligenza S., Paluchowska B., Konwicky M. (1988), Phys. Status Solidi A 106, K71-K74.

213
cP56

LiFe_5O_8	<i>cP</i> 56	(213) $P4_132 - \text{edc}^2a$
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LiFe_5O_8 [2], spinel $\text{A}_2[\text{A}_3\text{B}]\text{O}_8$; LiGa_5O_8 rt [3]

Structural features: Close-packed O layers in c stacking; part of Fe in tetrahedral, Li and remaining Fe in octahedral voids. Single FeO_4 tetrahedra and edge-linked LiO_6 and FeO_6 octahedra share vertices to form a spinel-type 3D-framework. Substitution derivative of MgAl_2O_4 of ideal composition $\text{A}_2[\text{A}_3\text{B}]\text{O}_8$. See Fig. II.31.

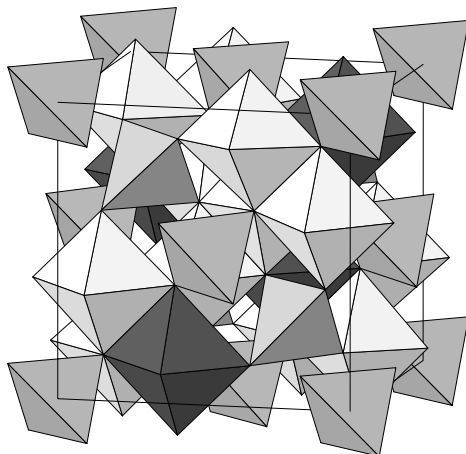


Fig. II.31. **LiFe_5O_8**

Arrangement of LiO_6 (dark) and FeO_6 (light) octahedra and FeO_4 tetrahedra (medium).

Scharner S. et al. (1997) [1]

Fe_5LiO_8

$a = 0.833 \text{ nm}$, $V = 0.5780 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24e	1	0.1232	0.3677	0.3694		tetrahedron Fe_3Li
Fe2	12d	.2	$\frac{1}{8}$	0.1339	0.3839		octahedron O_6
Fe3	8c	.3.	0.0036	0.0036	0.0036		tetrahedron O_4
O4	8c	.3.	0.1368	0.1368	0.1368		tetrahedron Fe_4
Li5	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O_6

Transformation from published data ($P4_332$): new axes -a,-b,-c

Experimental: powder, diffractometer, X-rays, $R_B = 0.047$

References: [1] Scharner S., Weppner W., Schmid Beurmann P. (1997), J. Solid State Chem. 134, 170-181. [2] Braun P.B. (1952), Nature (London) 170, 1123. [3] Joubert J.C., Brunel M., Waintal A., Durif A. (1963), C. R. Hebd. Seances Acad. Sci. 256, 5324-5326.

213
cP60

V_8C_7	<i>cP</i> 60	(213) $P4_132 - \text{ed}^2ca$
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V_8C_7 [2]

Structural features: Close-packed V layers in c stacking, C in octahedral voids. Defect derivative of NaCl with C vacancies arranged in screws. See Fig. II.32.

Rafaja D. et al. (1998) [1]

C_7V_8

$a = 0.83403 \text{ nm}$, $V = 0.5802 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
V1	$24e$	1	0.1189	0.3674	0.3784		square pyramid C_5
C2	$12d$	$\bar{..}2$	$\frac{1}{8}$	0.1296	0.3796		octahedron V_6
C3	$12d$	$\bar{..}2$	$\frac{1}{8}$	0.8254	0.0754		non-collinear V_2
V4	$8c$	$\bar{.}3$	0.1295	0.1295	0.1295		non-coplanar triangle C_3
C5	$4a$	$\bar{.}32$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		tricapped trigonal prism V_6C_3

Transformation from published data ($P4_332$): new axes -a,-b,-c; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.081$

Remarks: Phase stable at $T < 1390 \text{ K}$. In [3] the space group is misprinted as $P4_132$ instead of $P4_332$ (see [4]).

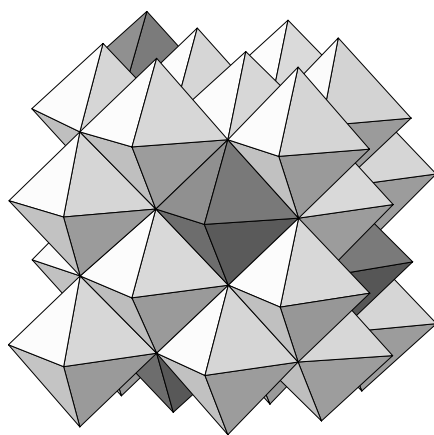


Fig. II.32. V_8C_7

Arrangement of CV_6 (light) and empty V_6 (dark) octahedra.

References: [1] Rafaja D., Lengauer W., Ettmayer P., Lipatnikov V.N. (1998), J. Alloys Compd. 269, 60-62. [2] De Novion C.H., Lorenzelli R., Costa P. (1966), C. R. Seances Acad. Sci., Ser. B 263, 775-778. [3] Henfrey A.W., Fender B.E.F. (1970), Acta Crystallogr. B 26, 1882-1883. [4] (1975), Structure Reports 38A, 68.

213
 $cP60$

$Hg[NH_2][NO_3]$	$cP60$	(213) $P4_132 - ed^3$
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$HgNH_2NO_3$ [1]

Structural features: Planar NO_3 trigonal units.

Randall C.J. et al. (1982) [1]

$HgNO_3$

$a = 1.0254 \text{ nm}$, $V = 1.0782 \text{ nm}^3$, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$24e$	1	0.018	0.127	0.369		single atom N
N2	$12d$	$\bar{..}2$	$\frac{1}{8}$	0.156	0.406		coplanar triangle O_3
O3	$12d$	$\bar{..}2$	$\frac{1}{8}$	0.246	0.496		single atom N

Hg4 12d ..2 $\frac{1}{8}$ 0.9063 0.1563 non-colinear O₂

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

Experimental: single crystal, diffractometer, X-rays, R = 0.090

Remarks: Natural sample from Pitkin County, Colorado. NH₂ not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Randall C.J., Peacor D.R., Rouse R.C., Dunn P.J. (1982), J. Solid State Chem. 42, 221-226.

213
cP64

Li(Li_{0.5}Fe_{0.5})₄Fe₃O₈

cP64

(213) *P*4₁32 – ed²cba

Li₃Fe₅O₈ [1]

Structural features: Close-packed O layers in c stacking, Li and Fe in octahedral voids. Substitution derivative of NaCl of ideal composition A₄A'₃A''B₈.

De Picciotto L.A., Thackeray M.M. (1986) [1]

Fe₅Li₃O₈

a = 0.8389 nm, *V* = 0.5904 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24e	1	0.125	0.375	0.375		octahedron Fe ₅ Li
Fe2	12d	..2	$\frac{1}{8}$	0.125	0.375		octahedron O ₆
M3	12d	..2	$\frac{1}{8}$	0.875	0.125		octahedron O ₆
O4	8c	.3.	0.125	0.125	0.125		octahedron Fe ₆
M5	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		octahedron O ₆
Li6	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O ₆

M3 = 0.50Fe + 0.50Li; M5 = 0.50Fe + 0.50Li

Transformation from published data (*P*4₃32): new axes -a,-b,-c

Experimental: powder, diffractometer, X-rays

Remarks: Space group (227) *Fd*-3*m* was tested and rejected. In table 2a of [1] the space group is misprinted as *P*4₁32 instead of *P*4₃32 (agreement with Wyckoff positions).

References: [1] De Picciotto L.A., Thackeray M.M. (1986), Mater. Res. Bull. 21, 583-592.

213
cP68

LiMg_{0.05}Mn_{1.5}Ni_{0.45}O₄

cP68

(213) *P*4₁32 – ed²c²a

LiMg_{0.05}Ni_{0.45}Mn_{1.5}O₄ [1]

Structural features: Close-packed O layers in c stacking; Li in tetrahedral, (Mn,Ni) in octahedral voids (in part distinct positions for Mn and Ni). Single LiO₄ tetrahedra and edge-linked (Mn,Ni)O₆ octahedra share vertices to form a 3D-framework.

Ooms F.G.B. et al. (2002) [1]

LiMg_{0.04}Mn_{1.54}Ni_{0.40}O₄

a = 0.81703 nm, *V* = 0.5454 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24e	1	0.1226	0.3523	0.3585		
Mn2	12d	..2	$\frac{1}{8}$	0.1216	0.3716	0.975	

Ni3	12d	..2	$\frac{1}{8}$	0.1491	0.3991	0.021	
O4	8c	.3.	0.136	0.136	0.136		
Li5	8c	.3.	0.7584	0.7584	0.7584		tetrahedron O ₄
M6	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	0.971	octahedron O ₆

M6 = 0.749Ni + 0.084Mg + 0.167Mn

Transformation from published data ($P4_332$): new axes -a,-b,-c

Experimental: powder, diffractometer, neutrons, $R_p = 0.059$

Remarks: We changed the z-coordinate of former Mn1 from 0.8718 to 0.8716 to be in agreement with Wyckoff position 12d. Short interatomic distances for partly occupied site(s). Space group (227) $Fd-3m$ was tested and rejected (additional reflections observed by neutron diffraction). We assume that in table 2 of [1] the z-coordinate of former Ni2 is misprinted as 0.0215 instead of 0.8991 (agreement with Wyckoff position 12d).

References: [1] Ooms F.G.B., Wagemaker M., Van Well A.A., Mulder F.M., Kelder E.M., Schoonman J. (2002), Appl. Phys. A: Solids Surf. 74, S1089-S1091.

213
cP72

Ca _{0.5} Al ₃ Te ₅	cP72	(213) $P4_132 - e^2dca$
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CaAl₆Te₁₀ [1]; KAg₄I₅ [2]

Structural features: Te forms a β Mn-type framework; Ca in octahedral, Al in tetrahedral voids (partial disorder).

Klee W., Schäfer H. (1979) [1]

Al₃Ca_{0.50}Te₅

$a = 1.028$ nm, $V = 1.0864$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24e	1	0.0074	0.3055	0.0366	0.25	
Al2	24e	1	0.022	0.3705	0.297	0.25	
Te3	12d	..2	$\frac{1}{8}$	0.1989	0.4489		
Te4	8c	.3.	0.0521	0.0521	0.0521		
Ca5	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	0.5	octahedron Te ₆

Experimental: single crystal, diffractometer, X-rays, $R = 0.026$

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

References: [1] Klee W., Schäfer H. (1979), Z. Naturforsch. B 34, 657-661. [2] Hull S., Keen D.A., Sivia D.S., Berastegui P. (2002), J. Solid State Chem. 165, 363-371.

213
cP72

Ag _{3.8} Sn ₃ S ₈	cP72	(213) $P4_132 - ed^3ca$
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Ag_{3.8}Sn₃S₈ [1]

Structural features: Close-packed S layers in c stacking; Sn and Ag in octahedral voids (splitting of one Ag site). SnS₆ octahedra share edges to form a 3D-framework.

Amiel O. et al. (1995) [1]

Ag_{3.84}S₈Sn₃

$a = 1.08013$ nm, $V = 1.2602$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24e	1	0.1124	0.3488	0.3602		
Sn2	12d	..2	$\frac{1}{8}$	0.1143	0.3643		octahedron S ₆
Ag3	12d	..2	$\frac{1}{8}$	0.8515	0.1015	0.474	
Ag4	12d	..2	$\frac{1}{8}$	0.8551	0.1051	0.474	
S5	8c	.3.	0.1224	0.1224	0.1224		
Ag6	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron S ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 295 K

Remarks: Refinement of the occupancy of site Ag6 showed no significant deviation from unity. Short interatomic distances for partly occupied site(s).

References: [1] Amiel O., Frankel D.C., Wada H. (1995), J. Solid State Chem. 116, 409-421.

213
cP76

Li ₅ Ag _{0.25} Hf ₃ S ₈	cP76	(213) $P4_132 - ed^2c^3a$
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Li₅Ag_{0.25}Hf₃S₈ [1]

Structural features: Close-packed S layers in c stacking; Hf and Ag in octahedral, Li in tetrahedral and distorted octahedral voids (partial disorder). HfS₆ octahedra share edges to form a 3D-framework.

Wada H. et al. (2000) [1]

Ag_{0.25}Hf₃Li_{4.99}S₈

$a = 1.04263$ nm, $V = 1.1334$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24e	1	0.127	0.375	0.372		7-vertex polyhedron Li ₄ Hf ₂ Ag
Hf2	12d	..2	$\frac{1}{8}$	0.131	0.381		8-vertex polyhedron Li ₂ S ₆
Li3	12d	..2	$\frac{1}{8}$	0.91	0.16	0.33	tetrahedron S ₂ Li ₂
Li4	8c	.3.	0.0	0.0	0.0		monocapped trigonal prism S ₄ Li ₃
S5	8c	.3.	0.127	0.127	0.127		8-vertex polyhedron Li ₅ Hf ₃
Li6	8c	.3.	0.25	0.25	0.25		square prism (cube) S ₄ AgHf ₃
Ag7	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	0.25	8-vertex polyhedron Li ₂ S ₆

Transformation from published data ($P4_132$): new axes -a,-b,-c

Experimental: powder, diffractometer, X-rays, R_B = 0.080

Remarks: In part the same authors refined also the structure Li₅Ag_{0.094}Hf₃S₈ the same year [2].

References: [1] Wada H., Sakamaki K., Ishii M. (2000), Solid State Ionics 136/137, 469-472. [2] Wada H., Sakamaki K. (2000), J. Alloys Compd. 302, 101-111.

213
cP80

RbAg ₄ I ₅	cP80	(213) $P4_132 - e^2dc^2a$
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RbAg₄I₅ (see remark)

Structural features: I forms a β Mn-type framework; Rb in octahedral, Ag in tetrahedral voids (disorder). See Fig. II.33.

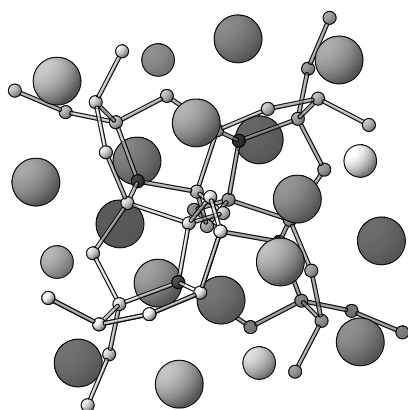
Hull S. et al. (2002) [1]

 $\text{Ag}_4\text{I}_5\text{Rb}$ $a = 1.12393 \text{ nm}$, $V = 1.4198 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	24e	1	0.004	0.3535	0.286	0.254	
Ag2	24e	1	0.0293	0.2293	0.2008	0.396	tetrahedron Ag_4
I3	12d	..2	$\frac{1}{8}$	0.1773	0.4273		
I4	8c	.3.	0.0307	0.0307	0.0307		
Ag5	8c	.3.	0.175	0.175	0.175	0.05	non-coplanar triangle Ag_3
Rb6	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		8-vertex polyhedron I_6Ag_2

Experimental: powder, diffractometer, neutrons, $R_B = 0.003$, $T = 298 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). Refinement of the occupancies of the additional Ag sites reported in [2] and [3] showed no significant deviation from zero.

Fig. II.33. RbAg_4I_5

Arrangement of partly occupied Ag sites (24-fold sites small light, 8-fold site small dark), Rb (medium) and I (large) atoms.

References: [1] Hull S., Keen D.A., Sivia D.S., Berastegui P. (2002), J. Solid State Chem. 165, 363-371.
 [2] Geller S. (1967), Science (Washington D.C.) 157, 310-312. [3] Bradley J.N., Greene P.D. (1967), Trans. Faraday Soc. 63, 2516-2521.

213
cP80

$\text{RbCu}_4\text{I}_2\text{Cl}_3$	$cP80$	$(213) P4_132 - e^2dc^2a$
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 $\text{RbCu}_4\text{Cl}_3\text{I}_2$ [1]Structural features: I and Cl form a β Mn-type framework; Rb in octahedral, Cu in tetrahedral voids (disorder).

Geller S. et al. (1979) [1]

 $\text{Cl}_3\text{Cu}_{3.89}\text{I}_2\text{Rb}$ $a = 1.0032 \text{ nm}$, $V = 1.0096 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	24e	1	0.0214	0.2081	0.2023	0.339	tetrahedron Cu_4
Cu2	24e	1	0.0368	0.5841	0.2526	0.294	
Cl3	12d	..2	$\frac{1}{8}$	0.1504	0.4004		
I4	8c	.3.	0.0103	0.0103	0.0103		
Cu5	8c	.3.	0.161	0.161	0.161	0.044	non-coplanar triangle Cu_3

Rb6 4a .32 $\frac{3}{8}$ $\frac{3}{8}$ $\frac{3}{8}$ octahedron Cl₆

Experimental: single crystal, diffractometer, X-rays, R = 0.072

Remarks: Short interatomic distances for partly occupied site(s). The structure of partly disordered RbCu₄I_{1.8}Cl_{3.2} in the temperature range 50-300 K is studied in [2].

References: [1] Geller S., Akridge J.R., Wilber S.A. (1979), Phys. Rev. B: Condens. Matter 19, 5396-5402. [2] Kanno R., Ohno K., Kawamoto Y., Takeda Y., Yamamoto O., Kamiyama T., Asano H., Izumi F., Kondo S. (1993), J. Solid State Chem. 102, 79-92.

213
cP80

K₃Si₆N₅[NH]₆

cP80

(213) P4₁32 – e²dc²a

K₃Si₆N₅(NH)₆ [1]; K₃P₆N₁₁ [2]

Structural features: Si(N,NH)₄ tetrahedra share vertices to form a 3D-framework; K in voids.

Peters D. et al. (1990) [1]

H₆K₃N₁₁Si₆

a = 1.0789 nm, *V* = 1.2559 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	24 <i>e</i>	1	0.0253	0.3792	0.2785		non-colinear Si ₂
Si2	24 <i>e</i>	1	0.08827	0.23531	0.31417		tetrahedron N ₄
N3	12 <i>d</i>	..2	$\frac{1}{8}$	0.2147	0.4647		non-colinear Si ₂
N4	8 <i>c</i>	.3.	0.217	0.217	0.217		non-coplanar triangle Si ₃
K5	8 <i>c</i>	.3.	0.79146	0.79146	0.79146		6-vertex polyhedron N ₆
K6	4 <i>a</i>	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		colinear N ₂
H7	24 <i>e</i>	1	0.0438	0.6398	0.3062		

Transformation from published data (P4₃32): new axes -a,-b,-c; origin shift $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.017, T = 293 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the *y*-coordinate of former N(2) is misprinted as 0.2853 instead of -0.2853 (checked on interatomic distances).

References: [1] Peters D., Paulus E.F., Jacobs H. (1990), Z. Anorg. Allg. Chem. 584, 129-137. [2] Jacobs H., Nymwegen R. (1997), Z. Anorg. Allg. Chem. 623, 429-433.

213
cP84

RbAg₄I₅

cP84

(213) P4₁32 – e²dc²ba

RbAg₄I₅ [1]

Structural features: I forms a β Mn-type framework; Rb in octahedral, Ag in tetrahedral and trigonal bipyramidal voids (disorder).

Geller S. (1967) [1]

Ag_{4.03}I₅Rb

a = 1.124 nm, *V* = 1.4200 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	24 <i>e</i>	1	0.0036	0.3506	0.2846	0.229	non-colinear Ag ₂
Ag2	24 <i>e</i>	1	0.0299	0.2287	0.202	0.391	tetrahedron Ag ₄

I3	12d	..2	$\frac{1}{8}$	0.178	0.428		13-vertex polyhedron Ag ₁₁ Rb ₂
I4	8c	.3.	0.0306	0.0306	0.0306		14-vertex polyhedron Ag ₁₄
Ag5	8c	.3.	0.1739	0.1739	0.1739	0.111	non-coplanar triangle Ag ₃
Ag6	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$	0.084	trigonal bipyramid I ₅
Rb7	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron I ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.083

Remarks: Short interatomic distances for partly occupied site(s). An additional partly occupied Ag site is reported in [2]. Refinement of the occupancies of this additional site and the site in Wyckoff position 4b showed not significant deviation from zero in [3].

References: [1] Geller S. (1967), Science (Washington D.C.) 157, 310-312. [2] Bradley J.N., Greene P.D. (1967), Trans. Faraday Soc. 63, 2516-2521. [3] Hull S., Keen D.A., Sivia D.S., Berastegui P. (2002), J. Solid State Chem. 165, 363-371.

213
cP96

RbAg ₄ I ₅	cP96	(213) $P4_132 - e^2d^2c^2ba$
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RbAg₄I₅ (see remark)

Structural features: I forms a β Mn-type framework; Rb in octahedral, Ag in tetrahedral and trigonal bipyramidal voids (disorder).

Bradley J.N., Greene P.D. (1967) [1]

Ag₄I₅Rb

$a = 1.122$ nm, $V = 1.4125$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	24e	1	0.011	0.357	0.297	0.222	non-collinear Ag ₂
Ag2	24e	1	0.033	0.232	0.197	0.222	tetrahedron Ag ₄
I3	12d	..2	$\frac{1}{8}$	0.177	0.427		15-vertex polyhedron Ag ₁₃ Rb ₂
Ag4	12d	..2	$\frac{1}{8}$	0.8	0.05	0.222	non-collinear Ag ₂
I5	8c	.3.	0.036	0.036	0.036		17-vertex polyhedron Ag ₁₇
Ag6	8c	.3.	0.18	0.18	0.18	0.222	non-coplanar triangle Ag ₃
Ag7	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$	0.222	pseudo Frank-Kasper I ₅ Ag ₁₂ Rb ₃
Rb8	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		coplanar triangle Ag ₃

Transformation from published data ($P4_332$): new axes -a,-b,-c; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, film, X-rays

Remarks: Short interatomic distances: d(Rb8-Ag4) = 0.278 nm. Short interatomic distances for partly occupied site(s). Supersedes a similar structure proposal where site Ag4 was not detected [2]. Refinement of the occupancy of sites Ag4 and Ag7 showed not significant deviation from zero in [3].

References: [1] Bradley J.N., Greene P.D. (1967), Trans. Faraday Soc. 63, 2516-2521. [2] Geller S. (1967), Science (Washington D.C.) 157, 310-312. [3] Hull S., Keen D.A., Sivia D.S., Berastegui P. (2002), J. Solid State Chem. 165, 363-371.

213
cP100

Ag ₄ Hf ₃ S ₈	cP100	(213) $P4_132 - e^3dc^2$
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Ag₄Hf₃S₈ [1]; Ag₄Zr₃S₈ [2]

Structural features: Close-packed S layers in c stacking; Hf in octahedral, Ag in tetrahedral and trigonal voids (disorder). HfS₆ octahedra share edges to form a 3D-framework.

Amiel O., Wada H. (1995) [1]

 $\text{Ag}_4\text{Hf}_3\text{S}_8$ $a = 1.09051 \text{ nm}$, $V = 1.2968 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	24e	1	0.063	0.282	0.571	0.167	
Ag2	24e	1	0.08	0.2695	0.5357	0.167	
S3	24e	1	0.1076	0.4073	0.3558		
Hf4	12d	.2	$\frac{1}{8}$	0.8851	0.1352		octahedron S_6
S5	8c	.3.	0.1211	0.1211	0.1211		tetrahedron AgHf_3
Ag6	8c	.3.	0.2573	0.2573	0.2573		tetrahedron S_4

Transformation from published data ($P4_332$): new axes -a,-b,-c; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.042$, $T = 296 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). The same data are also reported in [3].

References: [1] Amiel O., Wada H. (1995), J. Solid State Chem. 115, 112-119. [2] Amiel O., Frankel D.C., Wada H. (1995), J. Solid State Chem. 116, 409-421. [3] Wada H., Sakamaki K. (2000), J. Alloys Compd. 302, 101-111.

213
 $cP120$

$\text{SrCuTe}_2\text{O}_6$	$cP120$	(213) $P4_132 - e^4dca$
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 $\text{SrCuTe}_2\text{O}_6$ [1]Structural features: TeO_3 ψ -tetrahedra share vertices with CuO_4 squares to form a 3D-framework.

Wulff L., Müller Buschbaum H. (1997) [1]

 $\text{CuO}_6\text{SrTe}_2$ $a = 1.2473 \text{ nm}$, $V = 1.9405 \text{ nm}^3$, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24e	1	0.0283	0.1195	0.2745		single atom Te
Te2	24e	1	0.0812	0.4405	0.3383		non-coplanar triangle O_3
O3	24e	1	0.1797	0.3287	0.3727		non-colinear TeCu
O4	24e	1	0.1882	0.5218	0.2666		non-colinear TeCu
Cu5	12d	.2	$\frac{1}{8}$	0.2259	0.4759		coplanar square O_4
Sr6	8c	.3.	0.1954	0.1954	0.1954		tricapped trigonal prism O_9
Sr7	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O_6

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.024$

References: [1] Wulff L., Müller Buschbaum H. (1997), Z. Naturforsch. B 52, 1341-1344.

213
 $cP124$

K_6Sn_{25}	$cP124$	(213) $P4_132 - e^3d^2c^3b$
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 K_6Sn_{25} [1], clathrate chiral; $\text{Ba}_6\text{Ge}_{25}$ [2]Structural features: Sn forms a 3D-framework (SnSn_4 tetrahedra and SnSn_3 ψ -tetrahedra) with helical chains of condensed 20-vertex polyhedra (pentagonal dodecahedra) centered by K; additional K in smaller voids.

Fässler T.F., Kronseder C. (1998) [1]

K_6Sn_{25}

$a = 1.6202 \text{ nm}$, $V = 4.2531 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	24e	1	0.0019	0.2039	0.0438		tetrahedron Sn_4
Sn2	24e	1	0.067	0.3742	0.2604		tetrahedron Sn_4
Sn3	24e	1	0.1667	0.3391	0.4016		non-coplanar triangle Sn_3
Sn4	12d	..2	$\frac{1}{8}$	0.17	0.42		tetrahedron Sn_4
K5	12d	..2	$\frac{1}{8}$	0.81	0.06		22-vertex polyhedron $Sn_{20}K_2$
Sn6	8c	.3.	0.0315	0.0315	0.0315		non-coplanar triangle Sn_3
K7	8c	.3.	0.19	0.19	0.19		20-vertex polyhedron Sn_{20}
Sn8	8c	.3.	0.3252	0.3252	0.3252		tetrahedron Sn_4
K9	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		octahedron Sn_6

Transformation from published data ($P4_332$): new axes -a,-b,-c; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.084$, $T = 293 \text{ K}$

Remarks: The structure of Ba_6Ge_{25} was determined independently in [3].

References: [1] Fässler T.F., Kronseder C. (1998), Z. Anorg. Allg. Chem. 624, 561-568. [2] Fukuoka H., Iwai K., Yamanaka S., Abe H., Yoza K., Häming L. (2000), J. Solid State Chem. 151, 117-121. [3] Carrillo Cabrera W., Curda J., Von Schnering H.G., Paschen S., Grin Y. (2000), Z. Kristallogr., New Cryst. Struct. 215, 207-208.

213
cP124

$Ba_6(In_{0.36}Ge_{0.64})_{11}Ge_{14}$

cP124

(213) $P4_132 - e^3d^2c^3b$

$Ba_6In_4Ge_{21}$ [1]

Structural features: Ge and In form a 3D-framework ((Ge,In)(Ge,In)₄ tetrahedra and :Ge(Ge,In)₃ ψ -tetrahedra) with helical chains of condensed 20-vertex polyhedra (pentagonal dodecahedra) centered by Ba; additional Ba in other voids. Ordering variant of K_6Sn_{25} .

Von Schnering H.G. et al. (1998) [1]

$Ba_6Ge_{20.94}In_{4.06}$

$a = 1.4739 \text{ nm}$, $V = 3.2019 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24e	1	0.00291	0.20412	0.04185		tetrahedron Ge_4
Ge2	24e	1	0.06842	0.3763	0.26009		tetrahedron Ge_4
Ge3	24e	1	0.16528	0.33782	0.39597		non-coplanar triangle Ge_3
M4	12d	..2	$\frac{1}{8}$	0.17357	0.42357		tetrahedron Ge_4
Ba5	12d	..2	$\frac{1}{8}$	0.81392	0.06392		22-vertex polyhedron $Ge_{20}Ba_2$
Ge6	8c	.3.	0.03218	0.03218	0.03218		non-coplanar triangle Ge_3
Ba7	8c	.3.	0.19206	0.19206	0.19206		20-vertex polyhedron Ge_{20}
M8	8c	.3.	0.32535	0.32535	0.32535		tetrahedron Ge_4
Ba9	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		7-capped pentagonal prism $Ge_{11}Ba_6$

$M1 = 0.58Ge + 0.42In$; $M4 = 0.68Ge + 0.32In$; $M8 = 0.71Ge + 0.29In$

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.032$, $T = 293 \text{ K}$

Remarks: Composition $Ba_{6.2}In_{4.3}Ge_{20.7}$ from chemical analysis. A similar model with site Ba5 split into Wyckoff position 24e is also proposed.

References: [1] Von Schnering H.G., Kröner R., Carrillo Cabrera W., Peters K., Nesper R. (1998), Z. Kristallogr., New Cryst. Struct. 213, 665-666.

213
cP124

$(\text{Ca}_{0.1}\text{Pb}_{0.9})_3(\text{Cu}_{0.93}\text{Sb}_{0.07})_3\text{Te}_6\text{Cl}_{0.92}\text{O}_{18}$	cP124	(213) $P4_132 - e^4dcba$
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(Cu,Sb)₃(Pb,Ca)₃Te₆O₁₈Cl_{0.92} [1], choloalite

Structural features: TeO_3 ψ -tetrahedra and (Cu,Sb)(O₄Cl) square pyramids (Cl in apical position) share vertices to form a 3D-framework; (Pb,Ca) in voids.

Lam A.E. et al. (1999) [1]

$\text{Ca}_{0.30}\text{Cl}_{0.92}\text{Cu}_{2.79}\text{O}_{18}\text{Pb}_{2.70}\text{Sb}_{0.21}\text{Te}_6$

$a = 1.252 \text{ nm}$, $V = 1.9625 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24e	1	0.0261	0.1205	0.2682		single atom Te
Te2	24e	1	0.0812	0.4406	0.3401		non-coplanar triangle O ₃
O3	24e	1	0.1759	0.3274	0.3738		non-colinear TeCu
O4	24e	1	0.1857	0.52	0.2613		non-colinear CuTe
M5	12d	..2	$\frac{1}{8}$	0.2321	0.4821		coplanar square O ₄
Pb6	8c	.3.	0.1927	0.1927	0.1927		tricapped trigonal prism O ₉
Cl7	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$	0.92	coplanar triangle Cu ₃
M8	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O ₆

M5 = 0.93Cu + 0.07Sb; M8 = 0.70Pb + 0.30Ca

Experimental: single crystal, diffractometer, X-rays, R = 0.053

Remarks: Natural specimen from Mina La Oriental, Moctezuma, Mexico. Composition $\text{Cu}_{2.81}\text{Sb}_{0.26}\text{Pb}_{2.65}\text{Ca}_{0.17}\text{Zn}_{0.09}\text{Te}_{6.15}\text{O}_{18.41}\text{Cl}_{0.64}$ from electron microprobe analysis.

References: [1] Lam A.E., Groat L.A., Grice J.D., Ercit T.S. (1999), Can. Mineral. 37, 721-729.

213
cP136

K_8Sn_{25}	cP136	(213) $P4_132 - e^4dc^3b$
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K₈Sn₂₅ [1], clathrate chiral

Structural features: Sn forms a 3D-framework (SnSn₄ tetrahedra and SnSn_3 ψ -tetrahedra) with helical chains of condensed 20-vertex polyhedra (pentagonal dodecahedra) centered by K; additional K in octahedral voids and in channels (partial disorder). See Fig. II.34.

Zhao J.T., Corbett J.D. (1994) [1]

$\text{K}_{7.38}\text{Sn}_{25}$

$a = 1.6294 \text{ nm}$, $V = 4.3260 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	24e	1	0.0007	0.2037	0.0442		tetrahedron Sn ₄
Sn2	24e	1	0.0658	0.3723	0.2603		tetrahedron Sn ₄
Sn3	24e	1	0.1673	0.3364	0.3988		non-coplanar triangle Sn ₃
K4	24e	1	0.209	0.5615	0.287	0.73	single atom K
Sn5	12d	..2	$\frac{1}{8}$	0.1669	0.4169		tetrahedron Sn ₄
Sn6	8c	.3.	0.0324	0.0324	0.0324		octahedron Sn ₃ K ₃
K7	8c	.3.	0.1903	0.1903	0.1903		20-vertex polyhedron Sn ₂₀
Sn8	8c	.3.	0.3246	0.3246	0.3246		tetrahedron Sn ₄

K9 4b .32 $\frac{7}{8}$ $\frac{7}{8}$ $\frac{7}{8}$ 7-capped pentagonal prism Sn_{11}K_6

Experimental: single crystal, diffractometer, X-rays, $wR = 0.036$

Remarks: Homogeneity range $\text{K}_{100-x}\text{Sn}_x$, $74.6 < x < 76.2$ at 633 K.

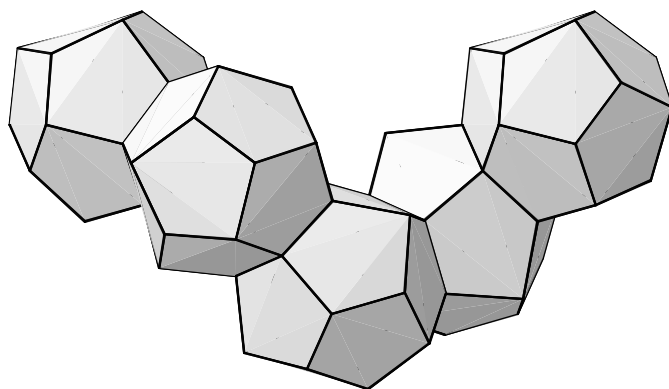


Fig. II.34. K_8Sn_{25}

Arrangement of KSn_{20} pentagonal dodecahedra.

References: [1] Zhao J.T., Corbett J.D. (1994), Inorg. Chem. 33, 5721-5726.

213
cP136

$\text{Ba}_6(\text{In}_{0.36}\text{Ge}_{0.64})_{11}\text{Ge}_{14}$

cP136

(213) $P4_132 - e^4dc^3b$

Ba₆In₄Ge₂₁ [2], clathrate chiral

Structural features: Ge and In form a 3D-framework ((Ge,In)(Ge,In)₄ tetrahedra and :Ge(Ge,In)₃ ψ-tetrahedra) with helical chains of condensed 20-vertex polyhedra (pentagonal dodecahedra) centered by Ba; additional Ba in other voids. Ordering variant of K_8Sn_{25} .

Kim S.J. et al. (2000) [1]

$\text{Ba}_6\text{Ge}_{21.94}\text{In}_{3.06}$

$a = 1.47409 \text{ nm}$, $V = 3.2031 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24e	1	0.0027	0.2041	0.0417		tetrahedron Ge ₃
M2	24e	1	0.0683	0.3759	0.2602		tetrahedron Ge ₄
Ge3	24e	1	0.1651	0.3374	0.3959		non-coplanar triangle Ge ₃
Ba4	24e	1	0.1863	0.5628	0.3589	0.5	
M5	12d	..2	$\frac{1}{8}$	0.1732	0.4232		tetrahedron Ge ₄
M6	8c	.3.	0.032	0.032	0.032		non-coplanar triangle Ge ₃
Ba7	8c	.3.	0.192	0.192	0.192		20-vertex polyhedron Ge ₁₉
M8	8c	.3.	0.3254	0.3254	0.3254		tetrahedron Ge ₄
Ba9	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		octahedron Ge ₆

M1 = 0.723Ge + 0.277In; M2 = 0.984Ge + 0.016In; M5 = 0.736Ge + 0.264In; M6 = 0.937Ge + 0.063In; M8 = 0.809Ge + 0.191In

Transformation from published data ($P4_132$): new axes -a,-b,-c

Experimental: single crystal, diffractometer, X-rays, $R = 0.021$, $T = 293 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). A similar model with site Ba4 in Wyckoff position 12d is also proposed in [2].

References: [1] Kim S.J., Hu S., Uher C., Hogan T., Huang B., Corbett J.D., Kanatzidis M.G. (2000), J. Solid State Chem. 153, 321-329. [2] Von Schnering H.G., Kröner R., Carrillo Cabrera W., Peters K., Nesper R. (1998), Z. Kristallogr., New Cryst. Struct. 213, 665-666.

213
cP140

$\text{Na}_3\text{FeP}_8\text{O}_{23}$	<i>cP140</i>	(213) $P4_132 - e^4d^2c^2a$
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Na₃FeP₈O₂₃ [1]

Structural features: P₈O₂₃ units consisting of eight vertex-linked PO₄ tetrahedra (cage with three 6-membered rings) share vertices with FeO₆ octahedra to form a 3D-framework.

Chudinova N.N. et al. (1989) [1]

FeNa₃O₂₃P₈

$a = 1.1915 \text{ nm}$, $V = 1.6915 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24 <i>e</i>	1	0.0069	0.4046	0.424		non-collinear P ₂
O2	24 <i>e</i>	1	0.0681	0.2367	0.3128		single atom P
P3	24 <i>e</i>	1	0.1083	0.3187	0.3954		tetrahedron O ₄
O4	24 <i>e</i>	1	0.2092	0.3872	0.3699		single atom P
Na5	12 <i>d</i>	..2	$\frac{1}{8}$	0.043	0.293		octahedron O ₆
O6	12 <i>d</i>	..2	$\frac{1}{8}$	0.2669	0.5169		non-collinear P ₂
P7	8 <i>c</i>	..3.	0.019	0.019	0.019		tetrahedron O ₄
O8	8 <i>c</i>	..3.	0.0899	0.0899	0.0899		single atom P
Fe9	4 <i>a</i>	..32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, $R = 0.027$

References: [1] Chudinova N.N., Palkina K.K., Karmanovskaya N.B., Maximova S.I., Chibiskova N.T. (1989), Dokl. Akad. Nauk SSSR 306, 635-638.

213
cP148

$\text{Na}_2\text{Ba}_4\text{Ge}_{25}$	<i>cP148</i>	(213) $P4_132 - e^4d^2c^3b$
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Na₂Ba₄Ge₂₅ [1], clathrate chiral

Structural features: Ge forms a 3D-framework (GeGe₄ tetrahedra and :GeGe₃ ψ -tetrahedra) with helical chains of condensed 20-vertex polyhedra (pentagonal dodecahedra) centered by Ba; Na and additional Ba in other voids (partial disorder).

Carrillo Cabrera W. et al. (2001) [1]

Ba₄Ge₂₅Na₂

$a = 1.44703 \text{ nm}$, $V = 3.0299 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	24 <i>e</i>	1	0.0017	0.2038	0.0433		tetrahedron Ge ₄
Ge2	24 <i>e</i>	1	0.0664	0.3768	0.2591		tetrahedron Ge ₄
Ge3	24 <i>e</i>	1	0.1662	0.3389	0.3964		non-coplanar triangle Ge ₃
M4	24 <i>e</i>	1	0.189	0.562	0.347	0.237	
Ge5	12 <i>d</i>	..2	$\frac{1}{8}$	0.1725	0.4225		tetrahedron Ge ₄
M6	12 <i>d</i>	..2	$\frac{1}{8}$	0.8134	0.0634	0.525	
Ge7	8 <i>c</i>	..3.	0.0318	0.0318	0.0318		non-coplanar triangle Ge ₃
Ba8	8 <i>c</i>	..3.	0.1913	0.1913	0.1913		20-vertex polyhedron Ge ₂₀

Ge9	8c	.3.	0.3256	0.3256	0.3256	tetrahedron Ge ₄
Ba10	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$	octahedron Ge ₆

M4 = 0.667Na + 0.333Ba; M6 = 0.667Na + 0.333Ba

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

Experimental: single crystal, diffractometer, X-rays, R = 0.052, T = 293 K

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

References: [1] Carrillo Cabrera W., Curda J., Peters K., Paschen S., Grin Y., von Schnering H.G. (2001), Z. Kristallogr., New Cryst. Struct. 216, 183-184.

213
cP156

Rb ₅ Na ₃ Sn ₂₅	cP156	(213) $P4_132 - e^5dc^3$
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Rb₅Na₃Sn₂₅ [1], clathrate chiral

Structural features: Sn forms a 3D-framework (SnSn₄ tetrahedra and :SnSn₃ ψ-tetrahedra) with helical chains of condensed 20-vertex polyhedra (pentagonal dodecahedra) centered by Rb; Na and additional Rb in other voids (partial disorder).

Bobev S., Sevov S.C. (2000) [1]

Na₃Rb₅Sn₂₅

$a = 1.64127 \text{ nm}$, $V = 4.4212 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	24e	1	0.00134	0.20503	0.04408		tetrahedron Sn ₄
Na2	24e	1	0.024	0.3385	0.524	0.5	
Sn3	24e	1	0.06632	0.3737	0.26037		tetrahedron Sn ₄
Sn4	24e	1	0.16655	0.33694	0.39925		trigonal bipyramid Sn ₃ Na ₂
Rb5	24e	1	0.1938	0.5607	0.3234	0.5	
Sn6	12d	..2	$\frac{1}{8}$	0.16808	0.41808		tetrahedron Sn ₄
Sn7	8c	.3.	0.03431	0.03431	0.03431		non-coplanar triangle Sn ₃
Rb8	8c	.3.	0.18962	0.18962	0.18962		20-vertex polyhedron Sn ₂₀
Sn9	8c	.3.	0.32489	0.32489	0.32489		tetrahedron Sn ₄

Experimental: single crystal, diffractometer, X-rays, R = 0.027, T = 294 K

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

References: [1] Bobev S., Sevov S.C. (2000), Inorg. Chem. 39, 5930-5937.

213
cP164

K ₃ Pr ₂ [NO ₃] ₉	cP164	(213) $P4_132 - e^5d^3c$
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K₃Pr₂(NO₃)₉ [1]

Structural features: Pr(NO₃)₆ icosahedral units (a central PrO₁₂ icosahedron sharing edges with six NO₃ trigonal units) are interconnected to form a 3D-framework.

Carnall W.T. et al. (1973) [1]

K₃N₉O₂₇Pr₂

$a = 1.352 \text{ nm}$, $V = 2.4713 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24e	1	0.0541	0.39	0.4392		single atom N
O2	24e	1	0.0836	0.4966	0.3245		single atom N
O3	24e	1	0.092	0.0961	0.2426		single atom N
N4	24e	1	0.1022	0.4145	0.3624		non-coplanar triangle O ₃
O5	24e	1	0.16	0.3571	0.3228		single atom N
N6	12d	..2	$\frac{1}{8}$	0.0148	0.2648		coplanar triangle O ₃
K7	12d	..2	$\frac{1}{8}$	0.1884	0.4384		8-vertex polyhedron O ₈
O8	12d	..2	$\frac{1}{8}$	0.9471	0.1971		single atom N
Pr9	8c	.3.	0.04952	0.04952	0.04952		icosahedron O ₁₂

Transformation from published data (*P*₄32): new axes -a,-b,-c

Experimental: single crystal, diffractometer, X-rays, R = 0.058

References: [1] Carnall W.T., Siegel S., Ferraro J.R., Tani B., Gebert E. (1973), Inorg. Chem. 12, 560-564.

213
cP176

K ₅ NaFe ₂ [C ₂ O ₄] ₆	cP176	(213) <i>P</i> ₄ 32 – e ⁶ dc ² a
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K_{2.5}Na_{0.5}Fe(C₂O₄)₃ [2]

Structural features: Single Fe(C₂O₄)₃ units consisting of a FeO₆ octahedron sharing vertices with three planar O₂C-CO₂ units (FeC₂O₂ rings).

Wartchow R. (1997) [1]

C₁₂Fe₂K₅NaO₂₄

a = 1.3536 nm, *V* = 2.4801 nm³, *Z* = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24e	1	0.004	0.1576	0.0257		single atom C
O2	24e	1	0.0456	0.2357	0.3112		single atom C
C3	24e	1	0.0507	0.48	0.2936		coplanar triangle O ₂ C
O4	24e	1	0.1224	0.4541	0.4524		single atom C
C5	24e	1	0.1376	0.4421	0.3588		coplanar triangle O ₂ C
O6	24e	1	0.2093	0.4045	0.3206		single atom C
K7	12d	..2	$\frac{1}{8}$	0.24307	0.49307		square antiprism O ₈
Fe8	8c	.3.	0.01093	0.01093	0.01093		octahedron O ₆
K9	8c	.3.	0.17085	0.17085	0.17085		octahedron O ₆
Na10	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		trigonal prism O ₆

Transformation from published data (*P*₄32): new axes -a,-b,-c

Experimental: single crystal, diffractometer, X-rays, R = 0.028, T = 293 K

Remarks: An error in [2] is corrected in [3].

References: [1] Wartchow R. (1997), Z. Kristallogr. 212, 57. [2] Henneicke S., Wartchow R. (1994), Z. Kristallogr. Suppl. 8, 365. [3] Henneicke S., Wartchow R. (1997), Z. Kristallogr. 212, 56.

213
cP252

Zn ₆ Ru	cP252	(213) <i>P</i> ₄ 32 – e ⁸ d ⁴ ca
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RuZn₆ [1]

Structural features: RuZn_{12} icosahedra are interconnected to form a 3D-framework.

Edström V.A., Westman S. (1971) [1]

RuZn_6

$a = 1.55575 \text{ nm}$, $V = 3.7655 \text{ nm}^3$, $Z = 36$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	24e	1	0.0099	0.6018	0.2870		12-vertex polyhedron $\text{Ru}_2\text{Zn}_{10}$
Zn2	24e	1	0.0245	0.6147	0.4607		12-vertex polyhedron $\text{Zn}_{10}\text{Ru}_2$
Ru3	24e	1	0.0406	0.3258	0.3994		icosahedron Zn_{12}
Zn4	24e	1	0.1014	0.4359	0.2874		12-vertex polyhedron $\text{Zn}_{10}\text{Ru}_2$
Zn5	24e	1	0.1130	0.4521	0.4750		12-vertex polyhedron $\text{Zn}_{10}\text{Ru}_2$
Zn6	24e	1	0.1157	0.2251	0.2636		icosahedron $\text{Zn}_{10}\text{Ru}_2$
Zn7	24e	1	0.2102	0.3315	0.3506		icosahedron $\text{Zn}_{10}\text{Ru}_2$
Zn8	24e	1	0.2717	0.4767	0.2881		icosahedron $\text{Zn}_{10}\text{Ru}_2$
Zn9	12d	..2	$\frac{1}{8}$	0.0259	0.2759		12-vertex polyhedron $\text{Zn}_{10}\text{Ru}_2$
Zn10	12d	..2	$\frac{1}{8}$	0.1810	0.4310		icosahedron $\text{Zn}_{10}\text{Ru}_2$
Zn11	12d	..2	$\frac{1}{8}$	0.2985	0.5485		pseudo Frank-Kasper Zn_9Ru_2
Zn12	12d	..2	$\frac{1}{8}$	0.8325	0.0825		12-vertex polyhedron $\text{Ru}_2\text{Zn}_{10}$
Ru13	8c	.3.	0.1225	0.1225	0.1225		icosahedron Zn_{12}
Ru14	4a	.32	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{3}{8}$		icosahedron Zn_{12}

Experimental: single crystal, diffractometer, X-rays, $R = 0.074$

References: [1] Edström V.A., Westman S. (1971), Chem. Scr. 1, 137-143.

213
cP260

$[\text{CN}_3\text{H}_6]_2[\text{SO}_4]$	cP260	(213) $P4_32 - e^8 d^4 c^2 b$
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$[\text{C}(\text{NH}_2)_3]_2\text{SO}_4$ [1]

Structural features: Planar $\text{C}(\text{NH}_2)_3$ (guanidinium) trigonal units and SO_4 tetrahedra.

Dera P. et al. (2000) [1]

$\text{C}_2\text{H}_{12}\text{N}_6\text{O}_4\text{S}$

$a = 1.7764 \text{ nm}$, $V = 5.6056 \text{ nm}^3$, $Z = 20$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24e	1	0.0154	0.0724	0.1251		single atom S
O2	24e	1	0.0634	0.254	0.4693		single atom S
N3	24e	1	0.0693	0.4008	0.3982		single atom C
N4	24e	1	0.099	0.1009	0.2674		single atom C
N5	24e	1	0.111	0.4856	0.3115		single atom C
C6	24e	1	0.1133	0.4161	0.3426		non-coplanar triangle N_3
O7	24e	1	0.1512	0.2133	0.3749		single atom S
N8	24e	1	0.1533	0.3637	0.3075		single atom C
C9	12d	..2	$\frac{1}{8}$	0.0303	0.2803		coplanar triangle N_3
S10	12d	..2	$\frac{1}{8}$	0.2036	0.4536		tetrahedron O_4
N11	12d	..2	$\frac{1}{8}$	0.4263	0.6763		single atom C
N12	12d	..2	$\frac{1}{8}$	0.9812	0.2312		single atom C
O13	8c	.3.	0.0066	0.0066	0.0066		single atom S
S14	8c	.3.	0.0555	0.0555	0.0555		tetrahedron O_4
C15	4b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		coplanar triangle N_3
H16	24e	1	0.0088	0.687	0.3919		

H17	24e	1	0.0442	0.4362	0.4196
H18	24e	1	0.065	0.3552	0.4138
H19	24e	1	0.0737	0.2895	0.5908
H20	24e	1	0.0804	0.5189	0.3288
H21	24e	1	0.0817	0.1127	0.2237
H22	24e	1	0.0997	0.1339	0.3028
H23	24e	1	0.1401	0.4965	0.2744
H24	24e	1	0.1504	0.3175	0.3217
H25	24e	1	0.1822	0.3759	0.2706

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

Experimental: single crystal, diffractometer, X-rays, R = 0.103, T = 293 K

Remarks: Diguanidinium sulfate. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Dera P., Katrusiak A., Szafranski M. (2000), Pol. J. Chem. 74, 1637-1644.