

Space group (214) $I4_132$ 214
 $cI48$ Ag_3AuTe_2 $cI48$ (214) $I4_132$ – fea**AuAg₃Te₂** rt [2], petzite

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

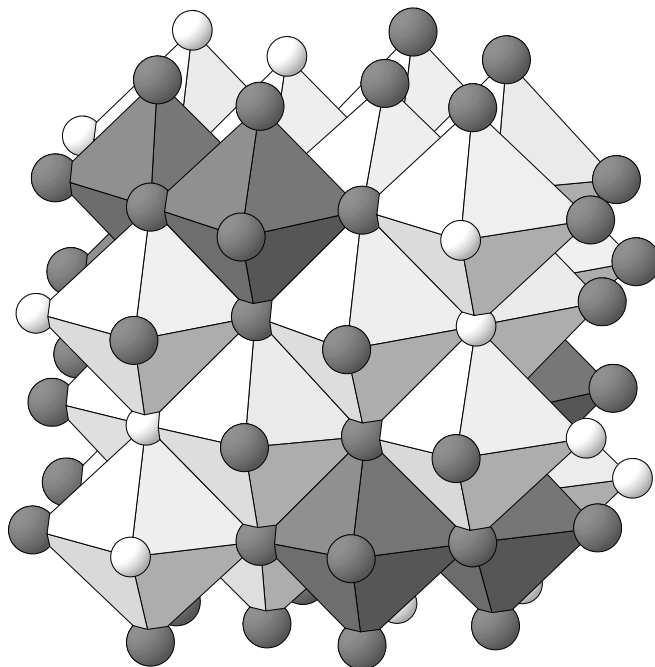
Shapur Chamid et al. (1978) [1]

 Ag_3AuTe_2 $a = 1.0385 \text{ nm}$, $V = 1.1200 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	$24f$	2..	0.361	0	$\frac{1}{4}$		bicapped square prism $\text{Te}_4\text{Au}_2\text{Ag}_4$
Te2	$16e$.3.	0.27	0.27	0.27		7-vertex polyhedron AuAg_6
Au3	$8a$.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		8-vertex polyhedron Te_2Ag_6

Experimental: single crystal, diffractometer, X-rays, $R = 0.089$ Remarks: Natural specimen from the Zhana-Tyube deposit, northern Kazakhstan. Composition $\text{Au}_{0.96}\text{Ag}_{2.92}\text{Cu}_{0.08}\text{Fe}_{0.03}\text{Te}_{2.01}$ from chemical analysis. Phase stable at $T < 423\text{-}523 \text{ K}$.

References: [1] Shapur Chamid, Pobedinskaya E.A., Spiridonov E.M., Belov N.V. (1978), Sov. Phys. Crystallogr. (Engl. Transl.) 23, 267-269. [2] Frueh A.J. Jr. (1959), Am. Mineral. 44, 693-701.

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 $cI56$ Ca_3PI_3 $cI56$ (214) $I4_132$ – hga**Ca₃PI₃** [1]; Gd_3CCl_3 [2]Fig. II.27. **Ca₃PI₃**Arrangement of $\text{Ca}(\text{P}_2\text{I}_4)$ (P atoms light, I atoms dark) and empty I_6 (dark) octahedra.

Structural features: Close-packed PI_3 layers in c stacking; Ca in octahedral voids. Alternatively: PCa_6 octahedra share edges to form a 3D-framework. See Fig. II.27.

Hamon C. et al. (1974) [1]

$\text{Ca}_3\text{I}_3\text{P}$

$a = 1.2315 \text{ nm}$, $V = 1.8677 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	24h	..2	$\frac{1}{8}$	0.616	0.634		4-vertex polyhedron Ca_4
Ca2	24g	..2	$\frac{1}{8}$	0.108	0.358		octahedron P_2I_4
P3	8a	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		octahedron Ca_6

Experimental: powder, X-rays, $R = 0.092$

References: [1] Hamon C., Marchand R., Laurent Y., Lang J. (1974), Bull. Soc. Fr. Mineral. Cristallogr. 97, 6-12. [2] Warkentin E., Simon A. (1983), Rev. Chim. Miner. 20, 488-495.

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cI184

$\text{Na}_{6.5}\text{Al}_{12}(\text{Si}_{0.54}\text{P}_{0.46})_{12}\text{O}_{48}[\text{H}_2\text{O}]_8$	cI184	(214) $I4_132 - i^2\text{hgdcba}$
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$\text{Na}_{13}\text{Al}_{24}\text{Si}_{13}\text{P}_{11}\text{O}_{96}\cdot 16\text{H}_2\text{O}$ [1], zeolite ANA

Structural features: AlO_4 and $(\text{Si,P})\text{O}_4$ tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; Na and H_2O in non-intersecting channels along $\langle 111 \rangle$.

Artioli G. et al. (1984) [1]

$\text{Al}_{12}\text{H}_{16}\text{Na}_{6.30}\text{O}_{56}\text{P}_{5.40}\text{Si}_{6.60}$

$a = 1.3729 \text{ nm}$, $V = 2.5877 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48i	1	0.0256	0.1079	0.3533		non-collinear SiAl
O2	48i	1	0.1247	0.2853	0.3959		non-collinear SiAl
M3	24h	..2	$\frac{1}{8}$	0.6635	0.5865		tetrahedron O_4
Al4	24g	..2	$\frac{1}{8}$	0.1612	0.4112		tetrahedron O_4
Na5	12d	2.22	$\frac{5}{8}$	0	$\frac{1}{4}$	0.475	octahedron $(\text{OH}_2)_2\text{O}_4$
Na6	12c	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$	0.575	octahedron $(\text{OH}_2)_2\text{O}_4$
$(\text{OH}_2)7$	8b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		coplanar triangle Na_3
$(\text{OH}_2)8$	8a	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		coplanar triangle Na_3

$\text{M3} = 0.55\text{Si} + 0.45\text{P}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.042$, $T = 295 \text{ K}$

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

References: [1] Artioli G., Pluth J.J., Smith J.V. (1984), Acta Crystallogr. C 40, 214-217.

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cI320

$\text{La}_3\text{Rh}_4\text{Sn}_{13}$	cI320	(214) $I4_132 - i^4h^2g^2\text{eba}$
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$\text{La}_3\text{Rh}_4\text{Sn}_{13}$ [1]; $\text{Pr}_3\text{Rh}_4\text{Sn}_{13}$ (see remark)

Structural features: RhSn_6 trigonal prisms share vertices to form a 3D-framework; La in cuboctahedral and additional Sn in icosahedral voids.

Bordet P. et al. (1991) [1]

 $\text{La}_3\text{Rh}_4\text{Sn}_{13}$ $a = 1.94918 \text{ nm}$, $V = 7.4055 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	48i	1	0.0003	0.1432	0.4257		pseudo Frank-Kasper $\text{Rh}_2\text{Sn}_8\text{La}_3$
Sn2	48i	1	0.001	0.1532	0.0773		14-vertex Frank-Kasper $\text{Rh}_2\text{Sn}_9\text{La}_3$
Sn3	48i	1	0.0924	0.2497	0.329		14-vertex Frank-Kasper $\text{Rh}_2\text{Sn}_9\text{La}_3$
Sn4	48i	1	0.251	0.3281	0.4039		14-vertex Frank-Kasper $\text{Rh}_2\text{Sn}_9\text{La}_3$
La5	24h	..2	$\frac{1}{8}$	0.2495	0.0005		16-vertex polyhedron $\text{Sn}_{12}\text{Rh}_4$
Rh6	24h	..2	$\frac{1}{8}$	0.625	0.625		tricapped trigonal prism Sn_6La_3
Rh7	24g	..2	$\frac{1}{8}$	0.125	0.375		tricapped trigonal prism Sn_6La_3
La8	24g	..2	$\frac{1}{8}$	0.2495	0.4995		16-vertex polyhedron $\text{Sn}_{12}\text{Rh}_4$
Sn9	16e	.3.	0.0011	0.0011	0.0011		icosahedron Sn_{12}
Rh10	8b	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		tricapped trigonal prism Sn_6La_3
Rh11	8a	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		tricapped trigonal prism Sn_6La_3

Experimental: powder, diffractometer, X-rays, $wR_p = 0.085$

Remarks: Referred to as phase I' in the literature. Supersedes structure proposals in space groups (199) $I2_13$ and (93) $P4_222$ [3]. A report on $\text{Pr}_3\text{Rh}_4\text{Sn}_{13}$ with phase I ($\text{Yb}_3\text{Rh}_4\text{Sn}_{13}$) type structure [2] is superseded in [3]. The description of the superseded structure proposal in space group (93) $P4_222$ in [3] does not take into consideration all symmetry elements of the proposed model; the correct space group is (131) $P4_2/mmc$ with half cell volume.

References: [1] Bordet P., Cox D.E., Espinosa G.P., Hodeau J.L., Marezio M. (1991), Solid State Commun. 78, 359-366. [2] Vandenberg J.M. (1980), Mater. Res. Bull. 15, 835-847. [3] Hodeau J.L., Marezio M., Remeika J.P., Chen C.H. (1982), Solid State Commun. 42, 97-102.

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cI448

$\text{Na}_{27}\text{Yb}_{6.75}[\text{OH}]_{47.25}[\text{H}_2\text{O}]_{16.75}$	cI448	(214) $I4_132 - i^5h^2g^2f^3edc$
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 $\text{Na}_4\text{Yb}(\text{OH})_7 \cdot 2.5\text{H}_2\text{O}$ [1]Structural features: Close-packed (OH,OH₂) layers in c stacking; Na and Yb in octahedral voids.

Nevskii N.N. et al. (1982) [1]

 $\text{H}_{80.77}\text{Na}_{27}\text{O}_{64}\text{Yb}_{6.74}$ $a = 1.9418 \text{ nm}$, $V = 7.3217 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48i	1	0.121	0.251	0.123		square pyramid Na_3Yb_2
Yb2	48i	1	0.125	0.243	0.258	0.208	octahedron (OH) ₆
M3	48i	1	0.126	0.245	0.372		square pyramid Yb_2Na_3
M4	48i	1	0.127	0.376	0.255		square pyramid Na_3Yb_2
M5	48i	1	0.243	0.373	0.383		non-coplanar triangle YbNa_2
Na6	24h	..2	$\frac{1}{8}$	0.249	0.001		octahedron (OH) ₆
Na7	24h	..2	$\frac{1}{8}$	0.626	0.624		octahedron (OH) ₆
Na8	24g	..2	$\frac{1}{8}$	0.121	0.371		octahedron (OH) ₆
Na9	24g	..2	$\frac{1}{8}$	0.253	0.503		octahedron (OH) ₆
M10	24f	2..	0.004	0	$\frac{1}{4}$		octahedron Na_3Yb_3
Yb11	24f	2..	0.384	0	$\frac{1}{4}$	0.208	octahedron (OH) ₆
M12	24f	2..	0.512	0	$\frac{1}{4}$		coplanar square Yb_2Na_2
M13	16e	.3.	0.001	0.001	0.001		non-coplanar triangle Yb_3

Yb14	12 <i>d</i>	2.22	$\frac{5}{8}$	0	$\frac{1}{4}$	octahedron (OH) ₆
Na15	12 <i>c</i>	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$	octahedron (OH) ₆

M1 = 0.738OH + 0.262OH₂; M3 = 0.738OH + 0.262OH₂; M4 = 0.738OH + 0.262OH₂; M5 = 0.738OH + 0.262OH₂; M10 = 0.738OH + 0.262OH₂; M12 = 0.738OH + 0.262OH₂; M13 = 0.738OH + 0.262OH₂

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

Experimental: single crystal, diffractometer, X-rays, R = 0.063

Remarks: Space group (230) *Ia*-3*d* was tested and rejected (R = 0.10). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Nevskii N.N., Ivanov Emin B.N., Nevskiaia N.A., Belov N.V. (1982), Dokl. Akad. Nauk SSSR 262, 880-883.

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cI832

U ₄ O ₉	cI832	(214) <i>I</i> 4 ₁ 32 – i ¹⁴ g ² e ³ dcba
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U₄O₉ [1]

Structural features: Filled-up derivative of CaF₂ (fluorite) with additional O in octahedral voids (in part displaced from the octahedron center along <110>); part of U displaced along <111>.

Masaki N., Doi K. (1972) [1]

O₉U₄

a = 2.1764 nm, *V* = 10.3090 nm³, *Z* = 64

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
U1	48 <i>i</i>	1	0.0	0.125	0.125		11-vertex polyhedron O ₁₁
U2	48 <i>i</i>	1	0.0	0.125	0.375		monocapped square prism O ₉
O3	48 <i>i</i>	1	0.0625	0.0625	0.1875		anticuboctahedron U ₄ O ₈
O4	48 <i>i</i>	1	0.0625	0.0625	0.3125		anticuboctahedron O ₈ U ₄
O5	48 <i>i</i>	1	0.0625	0.1875	0.3125		pentacapped trigonal prism U ₄ O ₇
O6	48 <i>i</i>	1	0.0625	0.1875	0.4375		pentacapped trigonal prism U ₄ O ₇
O7	48 <i>i</i>	1	0.0625	0.3125	0.3125		fourcapped trigonal prism U ₄ O ₆
O8	48 <i>i</i>	1	0.0625	0.3125	0.4375		fourcapped trigonal prism U ₄ O ₆
U9	48 <i>i</i>	1	0.125	0.25	0.375		square prism (cube) O ₈
O10	48 <i>i</i>	1	0.1875	0.1875	0.3125		pentacapped trigonal prism U ₄ O ₇
O11	48 <i>i</i>	1	0.1875	0.3125	0.3125		fourcapped trigonal prism U ₄ O ₆
O12	48 <i>i</i>	1	0.1875	0.3125	0.4375		pentacapped trigonal prism O ₇ U ₄
U13	48 <i>i</i>	1	0.25	0.375	0.375		10-vertex polyhedron O ₁₀
O14	48 <i>i</i>	1	0.3125	0.3125	0.4375		anticuboctahedron U ₄ O ₈
O15	24 <i>g</i>	.2	$\frac{1}{8}$	0.108	0.358		anticuboctahedron O ₈ U ₄
U16	24 <i>f</i>	2..	0.0	0	$\frac{1}{4}$		monocapped square prism O ₉
U17	24 <i>f</i>	2..	0.5	0	$\frac{1}{4}$		monocapped square prism O ₉
O18	16 <i>e</i>	.3.	0.0625	0.0625	0.0625		pentacapped trigonal prism U ₄ O ₇
U19	16 <i>e</i>	.3.	0.262	0.262	0.262		square prism (cube) O ₈
O20	16 <i>e</i>	.3.	0.3125	0.3125	0.3125		pentacapped trigonal prism U ₄ O ₇
O21	12 <i>d</i>	2.22	$\frac{5}{8}$	0	$\frac{1}{4}$		rhombic dodecahedron O ₈ U ₆
O22	12 <i>c</i>	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$		rhombic dodecahedron O ₈ U ₆
O23	8 <i>b</i>	.32	$\frac{7}{8}$	$\frac{7}{8}$	$\frac{7}{8}$		rhombic dodecahedron O ₈ U ₆
O24	8 <i>a</i>	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		rhombic dodecahedron O ₈ U ₆

Transformation from published data (*I*4₁32 *): origin shift $\frac{1}{2} \frac{3}{4} 0$

Experimental: single crystal, diffractometer, neutrons, R = 0.200

Remarks: Atom coordinates are published for 64 atoms in the unit cell; we derived the coordinates of the remaining sites considering an idealized CaF_2 -type atom arrangement. The published data refer to a non-conventional space group setting with the origin of the cell shifted by $\frac{1}{2} \frac{1}{4} 0$ from the description in the International Tables for Crystallography. In [1] the y -coordinate of the published U site is misprinted as 0.262 instead of -0.262 (agreement with Wyckoff position 16e).

References: [1] Masaki N., Doi K. (1972), Acta Crystallogr. B 28, 785-791.