

Space group (197) *I*23197
*cI*38(Li_{0.5}Cu_{0.5})_{2.67}Nb₄O₁₂*cI*38(197) *I*23 – fcb**LiCuNb₃O₉** [1], perovskite familyStructural features: NbO₆ octahedra share vertices to form a distorted perovskite-type framework; (Li,Cu) in approximately square planar coordination.

Sato M., Hama Y. (1993) [1]

Cu_{0.67}Li_{0.67}Nb₂O₆ $a = 0.75286 \text{ nm}$, $V = 0.4267 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>f</i>	1	0.0018	0.1858	0.3067		non-coplanar triangle Nb ₂ Cu
Nb2	8 <i>c</i>	.3.	0.2621	0.2621	0.2621		octahedron O ₆
M3	6 <i>b</i>	222..	0	1/2	1/2	0.889	coplanar square O ₄

M3 = 0.5Cu + 0.5Li

Transformation from published data: -*y*, -*x*, *z*Experimental: powder, diffractometer, X-rays, $R = 0.027$ Remarks: Space groups (204) *Im*-3, (211) *I*432, (217) *I*-43*m*, and (229) *Im*-3*m* were tested and rejected ($R = 0.1291, 0.1379, 0.1107$, and 0.1378 , respectively).

References: [1] Sato M., Hama Y. (1993), J. Mater. Chem. 3, 233-236.

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*cI*40Ni_{0.97}Ga_{3.62}*cI*40(197) *I*23 – edc²**NiGa₄** [1], γ -brassStructural features: 14-atom γ brass-type nested polyhedra units (a Ni₄ inner tetrahedron surrounded by a Ga₄ outer tetrahedron and a Ga₆ octahedron) in a matrix of additional Ga atoms.

Liang J., Xie S. (1983) [1]

Ga_{3.62}Ni_{0.97} $a = 0.84295 \text{ nm}$, $V = 0.5990 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	12 <i>e</i>	2..	0.2482	1/2	0	0.905	16-vertex Frank-Kasper Ga ₁₂ Ni ₄
Ga2	12 <i>d</i>	2..	0.3524	0	0	0.905	tricapped trigonal prism Ga ₇ Ni ₂
Ni3	8 <i>c</i>	.3.	0.1655	0.1655	0.1655	0.973	pseudo Frank-Kasper Ga ₁₃
Ga4	8 <i>c</i>	.3.	0.3332	0.3332	0.3332	0.905	pseudo Frank-Kasper Ni ₄ Ga ₉

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

Experimental: powder, Debye-Scherrer film, X-rays

Remarks: Symmetry doubtful, we recommend space group (217) *I*-43*m* be tested.

References: [1] Liang J., Xie S. (1983), Sci. Sin., Ser. A (Engl. Ed.) 26, 1305-1313.

Ag₅Hg_{7.55}*cI52*(197) *I23* – *fd*c²**Ag₅Hg_{7.55}** [2], moschellandsbergite, γ -brass

Structural features: 26-atom γ brass-type nested polyhedra units (a Hg₄ inner tetrahedron surrounded by an Ag₄ outer tetrahedron, an Ag₆ octahedron and a distorted Hg₁₂ cuboctahedron with disordered vacancies) in a W-type (b.c.c.) arrangement.

Fairhurst C.W., Cohen J.B. (1972) [1]

Ag₅Hg_{7.55} $a = 1.00506 \text{ nm}$, $V = 1.0153 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Hg1	24 <i>f</i>	1	0.0291	0.2957	0.3359	0.925	icosahedron Ag ₆ Hg ₆
Ag2	12 <i>d</i>	2..	0.355	0	0		pseudo Frank-Kasper Hg ₁₀ Ag ₃
Hg3	8 <i>c</i>	.3.	0.1151	0.1151	0.1151		pseudo Frank-Kasper Ag ₇ Hg ₆
Ag4	8 <i>c</i>	.3.	0.3285	0.3285	0.3285		pseudo Frank-Kasper Hg ₁₀ Ag ₃

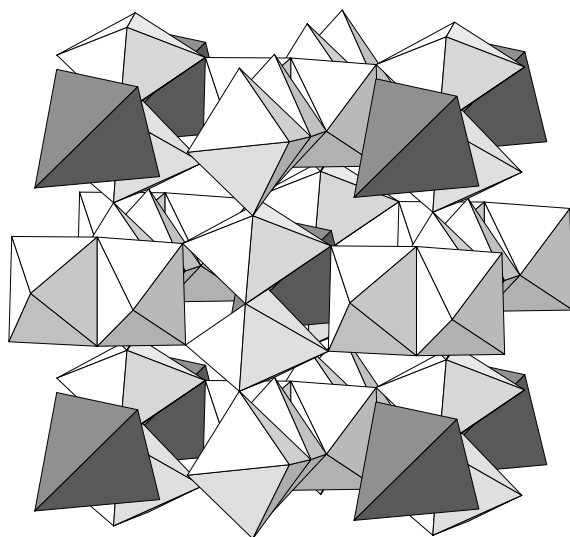
Experimental: single crystal, diffractometer, X-rays, $R = 0.143$

Remarks: Cell parameter from [3]. Orthorhombic symmetry was tested and rejected in [2].

References: [1] Fairhurst C.W., Cohen J.B. (1972), *Acta Crystallogr. B* 28, 371-378. [2] Baird H.W., Muller F.A. (1969), *J. Biomed. Mater. Res.* 3, 375-382. [3] Dreiner R. (1958), thesis, Aachen (Germany).

La₄Re₆O₁₉*cI58*(197) *I23* – *fed*ca**La₄Re₆O₁₉** [2]

Structural features: Pairs of edge-linked ReO₆ octahedra ($d(\text{Re-Re}) = 0.242 \text{ nm}$) share vertices to form a 3D-framework; OLa₄ tetrahedra in voids. See Fig. II.83.

Fig. II.83. **La₄Re₆O₁₉**

Arrangement of OLa₄ tetrahedra (dark) and ReO₆ octahedra (light).

Longo J.M., Sleight A.W. (1968) [1]

$\text{La}_4\text{O}_{19}\text{Re}_6$

$a = 0.90308 \text{ nm}$, $V = 0.7365 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24f	1	0.16	0.479	0.228		non-colinear Re_2
Re2	12e	2..	0.1341	$\frac{1}{2}$	0		7-vertex polyhedron O_6Re
O3	12d	2..	0.331	0	0		non-colinear Re_2
La4	8c	.3.	0.1613	0.1613	0.1613		10-vertex polyhedron O_{10}
O5	2a	23.	0	0	0		tetrahedron La_4

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

Experimental: powder, diffractometer, X-rays, $R = 0.027$

References: [1] Longo J.M., Sleight A.W. (1968), Inorg. Chem. 7, 108-111. [2] Morrow N.L., Katz L. (1968), Acta Crystallogr. B 24, 1466-1471.

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cI58

$\text{Ba}_4\text{Os}_6\text{ClO}_{18}$ cI58 (197) I23 – fedca

$\text{Ba}_4\text{Os}_6\text{O}_{18}\text{Cl}$ [1]

Structural features: Pairs of edge-linked OsO_6 octahedra ($d(\text{Os}-\text{Os}) = 0.256 \text{ nm}$) share vertices to form a 3D-framework; ClBa_4 tetrahedra in voids. Ordering variant of $\text{La}_4\text{Re}_6\text{O}_{19}$.

Plaisier J.R. et al. (1996) [1]

$\text{Ba}_4\text{ClO}_{18}\text{Os}_6$

$a = 0.938 \text{ nm}$, $V = 0.8253 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24f	1	0.1426	0.489	0.2093		non-colinear Os_2
Os2	12e	2..	0.13642	$\frac{1}{2}$	0		octahedron O_6
O3	12d	2..	0.34	0	0		non-colinear Os_2
Ba4	8c	.3.	0.18382	0.18382	0.18382		10-vertex polyhedron O_9Cl
Cl5	2a	23.	0	0	0		fourcapped trigonal prism Ba_4O_6

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.019$

References: [1] Plaisier J.R., De Graaff R.A.G., Ijdo D.J.W. (1996), Mater. Res. Bull. 31, 279-282.

197
cI60

Bi_2O_3 cI60 (197) I23 – f²d

$\text{Bi}_2\text{O}_3 \gamma$ [1], sillénite

Structural features: BiO_4 tetrahedra share vertices to form a 3D-framework.

Sillén L.G. (1937) [1]

Bi_2O_3

$a = 1.008 \text{ nm}$, $V = 1.0242 \text{ nm}^3$, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Bi1	24f	1	0.02	0.32	0.18		tetrahedron O_4

O2	24 <i>f</i>	1	0.08	0.21	0.36	non-coplanar triangle Bi ₃
O3	12 <i>d</i>	2..	0.19	0	0	non-colinear Bi ₂

Experimental: powder, film, X-rays

Remarks: Phase stable at ht, stabilized by small amounts of Al, Si or Fe (?). A second model proposed in the same paper but assumed to be stabilized by metal atoms, Bi₁₂MO₂₀ (Pearson symbol cI66), was later accepted also for pure Bi₂O₃ (see [2], [3]).

References: [1] Sillén L.G. (1937), Ark. Kemi Mineral. Geol. 12A(18), 1-15. [2] Harwig H.A. (1978), Z. Anorg. Allg. Chem. 444, 151-166. [3] Radaev S.F., Simonov V.I., Kargin Y.F. (1992), Acta Crystallogr. B 48, 604-609.

197
cI64

Li ₃ NbO ₄	cI64	(197) I23 – f ² c ²
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Li₃NbO₄ [1]

Structural features: Close-packed O layers in c stacking, Nb and Li occupy all octahedral voids. Units of four edge-linked NbO₆ octahedra (central Nb₄O₄ cube). Substitution derivative of NaCl.

Grenier J.C., Bassi G. (1965) [1]

Li₃NbO₄

a = 0.8429 nm, *V* = 0.5989 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	24 <i>f</i>	1	0.113	0.13	0.379		octahedron O ₆
O2	24 <i>f</i>	1	0.133	0.368	0.377		octahedron NbLi ₅
O3	8 <i>c</i>	.3.	0.111	0.111	0.111		octahedron Nb ₃ Li ₃
Nb4	8 <i>c</i>	.3.	0.357	0.357	0.357		octahedron O ₆

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

Experimental: powder, diffractometer, neutrons, *R* = 0.060

References: [1] Grenier J.C., Bassi G. (1965), Bull. Soc. Fr. Mineral. Cristallogr. 88, 345-346.

197
cI64

Hf ₁₀ Ta ₃ S ₃	cI64	(197) I23 – fedc ²
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Hf₁₀Ta₃S₃ [1]

Structural features: γ brass-type metal clusters (a Ta₄ inner tetrahedron surrounded by a (Hf,Ta)₄ outer tetrahedron, a Hf₆ octahedron and a Hf₁₂ cuboctahedron); S in distorted octahedral voids.

Marking G.A., Franzen H.F. (1993) [1]

Hf_{10.10}S₃Ta_{2.90}

a = 1.0832 nm, *V* = 1.2709 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Hf1	24 <i>f</i>	1	0.0671	0.2816	0.2964		non-colinear S ₂
S2	12 <i>e</i>	2..	0.173	1/2	0		octahedron Hf ₆
Hf3	12 <i>d</i>	2..	0.3368	0	0		pseudo Frank-Kasper S ₂ Ta ₂ Hf ₉
Ta4	8 <i>c</i>	.3.	0.0971	0.0971	0.0971		icosahedron Hf ₉ Ta ₃

M5 8c .3. 0.3399 0.3399 0.3399 icosahedron Ta₃Hf₉

M5 = 0.55Hf + 0.45Ta

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

Experimental: twinned crystal, diffractometer, X-rays, R = 0.034, T = 296 K

Remarks: Occupation of the metal atom sites from bond order calculations.

References: [1] Marking G.A., Franzen H.F. (1993), J. Am. Chem. Soc. 115, 6126-6130.

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cI66

Bi_{12.8}O_{19.2}

cI66

(197) I23 – f²c²a

Bi₂O₃ γ (see remark), sillénite

Structural features: :BiO₅ ψ-octahedra share atoms to form a 3D-framework, additional Bi in tetrahedral voids (O vacancies reduce the coordination to a ψ-tetrahedron).

Radaev S.F. et al. (1992) [1]

Bi_{12.83}O_{19.04}

$a = 1.02501$ nm, $V = 1.0769$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24f	1	0.0038	0.3635	0.2524		single atom Bi
Bi2	24f	1	0.0096	0.176	0.3203		5-vertex polyhedron O ₅
O3	8c	.3.	0.1874	0.1874	0.1874		non-coplanar triangle Bi ₃
O4	8c	.3.	0.3885	0.3885	0.3885	0.76	tetrahedron Bi ₄
Bi5	2a	23.	0	0	0	0.83	tetrahedron O ₄

Experimental: powder, diffractometer, neutrons, R = 0.034, T = 293 K

Remarks: Metastable phase observed at ht, may be stabilized by impurities. The authors state that, contrary to other reports, sillénite does not contain Bi⁵⁺ but electroneutrality is realized thanks to O vacancies. Supersedes a structure proposal in the same space group with 4-coordinated Bi in [3]; the present model was proposed in the same paper but assumed to be stabilized by impurities (Bi₁₂MO₂₀). A refinement on M-free γ-Bi₂O₃ is reported in [2].

References: [1] Radaev S.F., Simonov V.I., Kargin Y.F. (1992), Acta Crystallogr. B 48, 604-609. [2] Harwig H.A. (1978), Z. Anorg. Allg. Chem. 444, 151-166. [3] Sillén L.G. (1937), Ark. Kemi Mineral. Geol. 12A(18), 1-15.

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cI66

Bi₁₂SiO₂₀

cI66

(197) I23 – f²c²a

Bi₁₂SiO₂₀ [2], sillénite; Bi₁₂AlO₂₀ [2]; Bi₁₂FeO₂₀ [2]

Structural features: :BiO₃ ψ-tetrahedra share atoms to form a 3D-framework, single SiO₄ tetrahedra in large voids. Distorted ordering variant of γ-Bi₂O₃. See Fig. II.84.

Horowitz H.S. et al. (1989) [1]

Bi₁₂O₂₀Si

$a = 1.01132$ nm, $V = 1.0343$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24f	1	0.0157	0.2484	0.3643		non-collinear Bi ₂
Bi2	24f	1	0.1824	0.3241	0.4832		non-coplanar triangle O ₃

O3	8c	.3.	0.0939	0.0939	0.0939	single atom Si
O4	8c	.3.	0.3031	0.3031	0.3031	non-coplanar triangle Bi ₃
Si5	2a	23.	0	0	0	tetrahedron O ₄

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

Experimental: powder, diffractometer, neutrons, $R_B = 0.012$

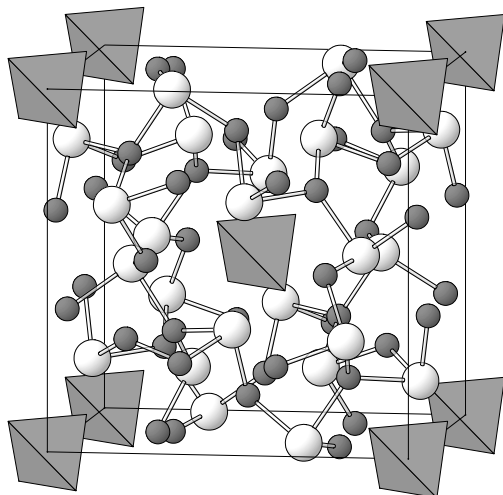


Fig. II.84. **Bi₁₂SiO₂₀**

Arrangement of SiO₄ tetrahedra and :BiO₃ ψ -tetrahedra (Bi atoms large, O atoms small).

References: [1] Horowitz H.S., Jacobson A.J., Newsam J.M., Lewandowski J.T., Leonowicz M.E. (1989), Solid State Ionics 32/33, 678-690. [2] Sillén L.G. (1937), Ark. Kemi Mineral. Geol. 12A(18), 1-15.

197
cI72

$V_{0.89}Bi_{12.03}O_{20.27}$

$cI72$

(197) $I23 - f^2c^2ba$

Bi₁₂(V_{0.89}Bi_{0.03}□_{0.08})O_{20.27} [2], sillénite family

Structural features: :BiO₃ ψ -tetrahedra share atoms to form a 3D-framework; single VO₄ tetrahedra in large voids, additional O in smaller voids.

Radaev S.F., Simonov V.I. (1992) [1]

Bi_{12.03}O_{20.27}V_{0.89}

$a = 1.0247$ nm, $V = 1.0759$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24f	1	0.00943	0.25252	0.36617		non-colinear Bi ₂
Bi2	24f	1	0.17765	0.3226	0.47707		octahedron O ₆
O3	8c	.3.	0.09718	0.09718	0.09718		single atom V
O4	8c	.3.	0.29993	0.29993	0.29993		non-coplanar triangle Bi ₃
O5	6b	222..	0	1/2	1/2	0.09	icosahedron Bi ₄ O ₈
M6	2a	23.	0	0	0	0.92	tetrahedron O ₄

$M6 = 0.97V + 0.03Bi$

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

Experimental: single crystal, diffractometer, neutrons, $R = 0.015$

Remarks: The same data are reported in [2].

References: [1] Radaev S.F., Simonov V.I. (1992), Sov. Phys. Crystallogr. (Engl. Transl.) 37, 484-499.
 [2] Radaev S.F., Muradyan L.A., Sarin V.A., Kanepit V.N., Yudin A.N., Mar'in A.A., Simonov V.I. (1989), Dokl. Akad. Nauk SSSR 307, 606-610.

197
cI74

$V_{0.5}Bi_{12.5}O_{20}$	<i>cI74</i>	(197) <i>I23</i> – f^2c^3a
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$Bi_{12}(V_{0.5}Bi_{0.5})O_{20}$ [1], sillénite family

Structural features: $:BiO_3$ ψ -tetrahedra share atoms to form a 3D-framework; single smaller $V^{5+}O_4$ and larger $Bi^{3+}O_4$ tetrahedra in voids (disorder, split site).

Yudin A.N. et al. (1989) [1]

$Bi_{12.50}O_{20}V_{0.50}$

$a = 1.0222$ nm, $V = 1.0681$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>f</i>	1	0.006	0.257	0.37		non-collinear Bi_2
Bi2	24 <i>f</i>	1	0.1774	0.3225	0.4764		non-coplanar triangle O_3
O3	8 <i>c</i>	.3.	0.098	0.098	0.098	0.5	
O4	8 <i>c</i>	.3.	0.121	0.121	0.121	0.5	
O5	8 <i>c</i>	.3.	0.299	0.299	0.299		non-coplanar triangle Bi_3
M6	2 <i>a</i>	23.	0	0	0		tetrahedron O_4

$M6 = 0.5Bi + 0.5V$

Experimental: powder, diffractometer, X-rays, $R = 0.059$

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

References: [1] Yudin A.N., Pobedinskaya E.A., Terent'eva L.E., Petrova I.V., Kaplunnik L.N., Malakhova G.V. (1989), Inorg. Mater. 25, 1451-1454.

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cI74

$Ga_{0.5}Bi_{12.5}O_{19.5}$	<i>cI74</i>	(197) <i>I23</i> – f^2c^3a
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$Bi_{12}(Ga_{0.5}Bi_{0.5})O_{19.50}$ [2], sillénite family

Structural features: $:BiO_3$ ψ -tetrahedra share atoms to form a 3D-framework; single GaO_4 tetrahedra and additional $:BiO_3$ ψ -tetrahedra in large voids (disorder, Bi displaced from the center of the void).

Radaev S.F., Simonov V.I. (1992) [1]

$Bi_{12.50}Ga_{0.50}O_{19.52}$

$a = 1.0183$ nm, $V = 1.0559$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>f</i>	1	0.01448	0.24808	0.36474		non-collinear Bi_2
Bi2	24 <i>f</i>	1	0.18228	0.32387	0.48614		non-coplanar triangle O_3
Bi3	8 <i>c</i>	.3.	0.018	0.018	0.018	0.125	
O4	8 <i>c</i>	.3.	0.10656	0.10656	0.10656	0.88	
O5	8 <i>c</i>	.3.	0.31036	0.31036	0.31036		non-coplanar triangle Bi_3
Ga6	2 <i>a</i>	23.	0	0	0	0.5	

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

Experimental: single crystal, diffractometer, neutrons, $R = 0.013$

Remarks: The same data are reported in [2]. Short interatomic distances for partly occupied site(s).

References: [1] Radaev S.F., Simonov V.I. (1992), Sov. Phys. Crystallogr. (Engl. Transl.) 37, 484-499.
[2] Radaev S.F., Muradian L.A., Kargin I.F., Sarin V.A., Rider E.E., Simonov V.I. (1989), Dokl. Akad. Nauk SSSR 306, 624-627.

197
c/82

$\text{Tl}_{0.5}\text{Bi}_{12.5}\text{O}_{19.5}$	<i>c</i> /82	(197) <i>I</i> 23 – $\text{f}^2\text{c}^4\text{a}$
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Bi₁₂(Tl_{0.5}Bi_{0.5})O_{19.50} [1], sillénite family

Structural features: :BiO₃ ψ -tetrahedra share atoms to form a 3D-framework; single TlO₄ tetrahedra and additional :BiO₃ ψ -tetrahedra in large voids (disorder, Bi displaced from the center of the void).

Radaev S.F. et al. (1994) [1]

$\text{Bi}_{12.50}\text{O}_{19.52}\text{Tl}_{0.50}$

$a = 1.0221 \text{ nm}$, $V = 1.0678 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>f</i>	1	0.01179	0.25181	0.3651		non-collinear Bi ₂
Bi2	24 <i>f</i>	1	0.18079	0.32348	0.48546		non-coplanar triangle O ₃
Bi3	8 <i>c</i>	.3.	0.0175	0.0175	0.0175	0.125	
O4	8 <i>c</i>	.3.	0.107	0.107	0.107	0.38	
O5	8 <i>c</i>	.3.	0.1195	0.1195	0.1195	0.5	
O6	8 <i>c</i>	.3.	0.3123	0.3123	0.3123		non-coplanar triangle Bi ₃
Tl7	2 <i>a</i>	23.	0	0	0	0.5	

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

Experimental: single crystal, diffractometer, neutrons, *w*R = 0.015, *T* = 293 K

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

References: [1] Radaev S.F., Trömel M., Kargin Y.F., Marin A.A., Rider E.E., Sarin V.A. (1994), Acta Crystallogr. C 50, 656-659.

197
c/166

$(\text{Rb}_{0.125}\text{Tl}_{0.875})_{12}\text{Be}_{12}[\text{AsO}_4]_{12}$	<i>c</i> /166	(197) <i>I</i> 23 – $\text{f}^6\text{c}^2\text{b}$
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Rb₃Tl₂₁Be₂₄As₂₄O₉₆ [1], zeolite RHO(BeAs)-Tl,Rb

Structural features: BeO₄ and AsO₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; (Tl,Rb) between 8-rings and near the centers of 6-rings. See Fig. II.85.

Parise J.B. et al. (1994) [1]

$\text{As}_{12}\text{Be}_{12}\text{O}_{48}\text{Rb}_{1.06}\text{Tl}_{7.80}$

$a = 1.3998 \text{ nm}$, $V = 2.7428 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Be1	24 <i>f</i>	1	0.0679	0.2148	0.3661		tetrahedron O ₄
As2	24 <i>f</i>	1	0.0699	0.3688	0.2203		tetrahedron O ₄
O3	24 <i>f</i>	1	0.0967	0.2593	0.2635		non-collinear BeAs
O4	24 <i>f</i>	1	0.1055	0.106	0.3741		non-collinear BeAs
O5	24 <i>f</i>	1	0.116	0.2776	0.4502		non-collinear BeAs
O6	24 <i>f</i>	1	0.1233	0.4528	0.285		non-collinear BeAs

M7	8c	.3.	0.1395	0.1395	0.1395	0.84	non-coplanar triangle O ₃
M8	8c	.3.	0.3101	0.3101	0.3101	0.79	non-coplanar triangle O ₃
M9	6b	222..	0	1/2	1/2	0.78	tetrahedron O ₄

M7 = 0.88Tl + 0.12Rb; M8 = 0.88Tl + 0.12Rb; M9 = 0.88Tl + 0.12Rb

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

Experimental: powder, diffractometer, neutrons, $R_B = 0.074$, $T = 300$ K

Remarks: Composition $\text{Tl}_{19.0}\text{Na}_{0.90}\text{Rb}_{2.50}\text{Be}_{25.2}\text{As}_{22.8}\text{O}_{96}$ from chemical analysis. Part of non framework cations not located.

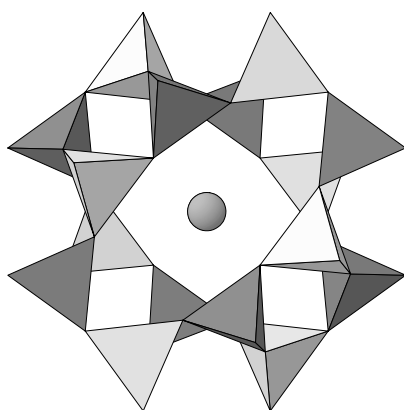


Fig. II.85. **Rb₃Tl₂₁Be₂₄As₂₄O₉₆**

Detail of a RHO-type zeolite: double 8-ring of AsO₄ (light) and BeO₄ (dark) tetrahedra around a (Tl,Rb) atom.

References: [1] Parise J.B., Corbin D.R., Abrams L., Northrup P., Rakovan J., Nenoff T.M., Stucky G.D. (1994), Zeolites 14, 25-34.

197
cI168

Cd₆Yb

cI168

(197) $I23 - f^6edc^3$

YbCd₆ [1]; **HfNi_{2.15}Ga_{3.85}** [2]

Structural features: YbCd₁₇ polyhedra (bicapped double pentagonal antiprism) are interconnected to form a 3D-framework; the centering atoms form large Yb₁₂ icosahedra. See Fig. II.86.

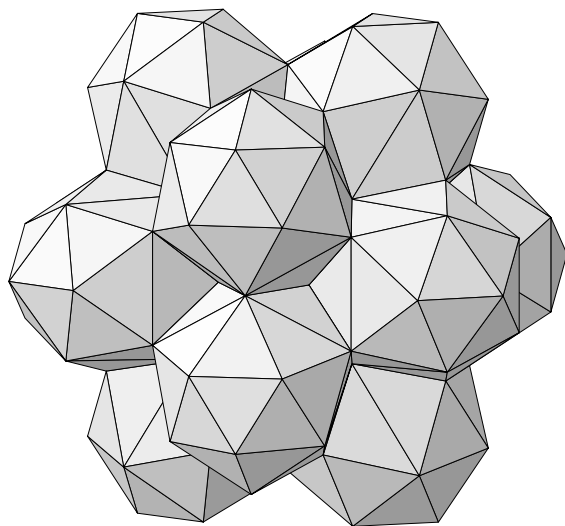


Fig. II.86. **Cd₆Yb**

Arrangement of YbCd₁₇ polyhedra.

Palenzona A. (1971) [1]

Cd_6Yb

$a = 1.5638 \text{ nm}$, $V = 3.8242 \text{ nm}^3$, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	24 <i>f</i>	1	0.0	0.0914	0.2305		pseudo Frank-Kasper Cd_8Yb_3
Yb2	24 <i>f</i>	1	0.0	0.3014	0.1879		7-capped pentagonal prism Cd_{17}
Cd3	24 <i>f</i>	1	0.0945	0.5000	0.1512		icosahedron Cd_9Yb_3
Cd4	24 <i>f</i>	1	0.1140	0.2010	0.3434		pseudo Frank-Kasper $\text{Cd}_{10}\text{Yb}_3$
Cd5	24 <i>f</i>	1	0.1566	0.3860	0.2990		15-vertex Frank-Kasper $\text{Cd}_{12}\text{Yb}_3$
Cd6	12 <i>e</i>	2..	0.1956	$\frac{1}{2}$	0		icosahedron $\text{Cd}_{10}\text{Yb}_2$
Cd7	12 <i>d</i>	2..	0.4065	0	0		15-vertex Frank-Kasper $\text{Cd}_{13}\text{Yb}_2$
Cd8	8 <i>c</i>	.3.	0.0700	0.0700	0.0700		7-vertex polyhedron Cd_7
Cd9	8 <i>c</i>	.3.	0.1645	0.1645	0.1645		bicapped square prism Cd_7Yb_3
Cd10	8 <i>c</i>	.3.	0.3355	0.3355	0.3355		tricapped trigonal prism Cd_6Yb_3

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

Experimental: single crystal, photographs, X-rays

Remarks: The atom coordinates, except for Cd8, were taken from [2] ($\text{Ru}_2\text{Be}_{17}$). In [1] the z -coordinate of former Cd(5) is misprinted as 0.5 instead of 0 (private communication from the author). In [2] the space group is misprinted as 123 instead of $I23$; impossibly short interatomic distances indicate probable additional misprint.

References: [1] Palenzona A. (1971), J. Less-Common Met. 25, 367-372. [2] Markiv V.Y., Belyavina N.N. (1983), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1983(12), 30-33.

197
cI168

$\text{Au}_{28.4}\text{Ce}_6\text{Sn}_{5.4}$	<i>cI168</i>	(197) $I23 - f^5\text{edc}^3$
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$\text{Ce}_3\text{Au}_{14.2}\text{Sn}_{2.7}$ [1]

Structural features: $\text{Ce}(\text{Au}_{14}\text{Sn}_2)$ polyhedra (monocapped double pentagonal antiprism) share atoms to form a 3D-framework where the centering atoms form large Ce_{12} icosahedra; additional Sn in cubic voids (partial disorder).

Boulet P. et al. (2001) [1]

$\text{Au}_{28.28}\text{Ce}_6\text{Sn}_{5.44}$

$a = 1.5118 \text{ nm}$, $V = 3.4553 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Au1	24 <i>f</i>	1	0.0	0.0901	0.2433	0.88	tricapped trigonal prism Au_5SnCe_3
Ce2	24 <i>f</i>	1	0.0	0.303	0.1878		18-vertex polyhedron $\text{Au}_{14}\text{Sn}_4$
Au3	24 <i>f</i>	1	0.0943	0.5	0.1526		icosahedron $\text{Sn}_2\text{Au}_7\text{Ce}_3$
Au4	24 <i>f</i>	1	0.1069	0.1981	0.3477		pseudo Frank-Kasper $\text{Sn}_3\text{Au}_7\text{Ce}_3$
Au5	24 <i>f</i>	1	0.1596	0.389	0.2983		pseudo Frank-Kasper $\text{Sn}_2\text{Au}_8\text{Ce}_3$
Sn6	12 <i>e</i>	2..	0.1878	$\frac{1}{2}$	0		icosahedron $\text{Au}_{10}\text{Ce}_2$
Au7	12 <i>d</i>	2..	0.4085	0	0		15-vertex Frank-Kasper $\text{Au}_{11}\text{Sn}_2\text{Ce}_2$
Sn8	8 <i>c</i>	.3.	0.1486	0.1486	0.1486		bicapped square prism SnAu_6Ce_3
Sn9	8 <i>c</i>	.3.	0.243	0.243	0.243	0.22	square prism (cube) SnAu_7
Au10	8 <i>c</i>	.3.	0.3466	0.3466	0.3466		bicapped square prism SnAu_6Ce_3

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

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

Remarks: $\text{Ce}_6\text{Au}_{29-x}\text{Sn}_{5+y}$. Space group (204) $Im\bar{3}$ was tested and rejected.

References: [1] Boulet P., Mazzone D., Noel H., Rogl P., Ferro R. (2001), J. Alloys Compd. 317/318, 350-356.

197
cI174

$\text{K}_{0.6}\text{Na}_{0.1}\text{Li}_{5.8}\text{Ca}_{2.75}\text{Be}_{12}[\text{PO}_4]_{12}$	<i>cI174</i>	(197) <i>I</i> 23 – f^6c^3b
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$\text{Li}_8(\text{Ca}_{5.5}\text{Li}_{3.6}\text{K}_{1.2}\text{Na}_{0.2}\square_{13.5})\text{Be}_{24}\text{P}_{24}\text{O}_{96}$ [1], pahasapaite dehydrated, zeolite RHO(BeP)-Li,Ca
Structural features: BeO_4 and PO_4 tetrahedra share vertices to form a distorted RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Ca between 8-rings, Li and (Li,K,Na) near the centers of 6-rings.

Corbin D.R. et al. (1991) [1]

$\text{Be}_{12}\text{Ca}_{2.59}\text{K}_{0.60}\text{Li}_{7.50}\text{Na}_{0.10}\text{O}_{48}\text{P}_{12}$

$a = 1.31 \text{ nm}$, $V = 2.2481 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	24 <i>f</i>	1	0.06093	0.36774	0.21202		tetrahedron O ₄
Be2	24 <i>f</i>	1	0.0622	0.2201	0.3684		tetrahedron O ₄
O3	24 <i>f</i>	1	0.0864	0.2595	0.2509		non-coplanar triangle PBeLi
O4	24 <i>f</i>	1	0.1028	0.103	0.3797		non-coplanar PBe
O5	24 <i>f</i>	1	0.1094	0.4436	0.2859		non-coplanar PBe
O6	24 <i>f</i>	1	0.1168	0.2973	0.4468		non-coplanar PBe
Li7	8 <i>c</i>	.3.	0.1393	0.1393	0.1393	0.3	
Li8	8 <i>c</i>	.3.	0.1796	0.1796	0.1796	0.75	
M9	8 <i>c</i>	.3.	0.3092	0.3092	0.3092		
Ca10	6 <i>b</i>	222..	0	1/2	1/2	0.864	tetrahedron O ₄

$\text{M9} = 0.825\text{Li} + 0.15\text{K} + 0.025\text{Na}$

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.037$, $T = 296 \text{ K}$

Remarks: Natural specimen from the Tip Top mine, Cluster, South Dakota, dehydrated. Short interatomic distances for partly occupied site(s).

References: [1] Corbin D.R., Abrams L., Jones G.A., Harlow R.L., Dunn P.J. (1991), Zeolites 11, 364-367.

197
cI178

$\text{Be}_{12}\text{Tl}_{12}[\text{PO}_4]_{12}$	<i>cI178</i>	(197) <i>I</i> 23 – f^6dc^2b
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$\text{Be}_{24}\text{Tl}_{24}\text{P}_{24}\text{O}_{96}$ [1], zeolite RHO(BeP)-Tl

Structural features: BeO_4 and PO_4 tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Tl between 8-rings and near the centers of 8- and 6-rings (disorder).

Parise J.B. et al. (1994) [1]

$\text{Be}_{12}\text{O}_{48}\text{P}_{12}\text{Tl}_{10.59}$

$a = 1.36469 \text{ nm}$, $V = 2.5416 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Be1	24 <i>f</i>	1	0.07	0.371	0.222		tetrahedron O ₄

P2	24f	1	0.0768	0.226	0.3771		tetrahedron O ₄
O3	24f	1	0.099	0.27	0.276		non-colinear PBe
O4	24f	1	0.105	0.467	0.282		non-colinear PBe
O5	24f	1	0.116	0.122	0.379		non-colinear PBe
O6	24f	1	0.128	0.29	0.452		non-colinear PBe
Tl7	12d	2..	0.203	0	0	0.083	non-colinear Tl ₂
Tl8	8c	.3.	0.1399	0.1399	0.1399		octahedron O ₃ Tl ₃
Tl9	8c	.3.	0.3111	0.3111	0.3111	0.773	6-vertex polyhedron O ₆
Tl10	6b	222..	0	1/2	1/2		tetrahedron O ₄

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

Experimental: powder, diffractometer, neutrons, $R_p = 0.076$, $T = 300$ K

Remarks: Composition $\text{Ti}_{21.0}\text{Na}_{0.81}\text{Li}_{1.06}\text{Be}_{24.5}\text{P}_{23.5}\text{O}_{96}$ from chemical analysis.

References: [1] Parise J.B., Corbin D.R., Abrams L., Northrup P., Rakovan J., Nenoff T.M., Stucky G.D. (1994), Zeolites 14, 25-34.

197
cI190

$\text{Cs}_4\text{Na}_8\text{Al}_{12}[\text{GeO}_4]_{12}$

$cI190$

(197) $I23 - f^7c^2b$

Cs₈Na₁₆Al₂₄Ge₂₄O₉₆ [1], zeolite RHO(Ge)-Na,Cs

Structural features: AlO_4 and GeO_4 tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs between 8-rings and near the centers of 6-rings, Na near the centers of 8- and 6-rings (disorder).

Johnson G.M. et al. (1999) [1]

$\text{Al}_{12}\text{Cs}_{3.97}\text{Ge}_{12}\text{Na}_{7.43}\text{O}_{48}$

$a = 1.46737$ nm, $V = 3.1595$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Na1	24f	1	0.0493	0.0515	0.6078	0.286	
Al2	24f	1	0.0653	0.2192	0.3687		tetrahedron O ₄
Ge3	24f	1	0.0657	0.3689	0.218		tetrahedron O ₄
O4	24f	1	0.088	0.263	0.261		non-colinear GeAl
O5	24f	1	0.1038	0.1117	0.3719		non-colinear AlGe
O6	24f	1	0.114	0.4496	0.2858		non-colinear GeAl
O7	24f	1	0.1176	0.2918	0.4468		non-colinear AlGe
Na8	8c	.3.	0.1708	0.1708	0.1708		non-coplanar triangle O ₃
Cs9	8c	.3.	0.3102	0.3102	0.3102	0.673	
Cs10	6b	222..	0	1/2	1/2	0.427	

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

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.056$, $T = 298$ K

Remarks: The structure was refined on a combined set of neutron and synchrotron X-ray diffraction data. Short interatomic distances for partly occupied site(s). In table 3 of [1] the Wyckoff position of the 24-fold sites is misprinted as 24g instead of 24f.

References: [1] Johnson G.M., Tripathi A., Parise J.B. (1999), Microporous Mesoporous Mater. 28, 139-154.

197
cI192

$\text{Li}_2\text{CaBe}_4[\text{PO}_4]_4$	<i>cI192</i>	(197) <i>I23</i> – f^7c^3
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Li₂CaBe₄(PO₄)₄ [1], pahasapaite dehydrated, zeolite RHO(BeP)-Li,CaStructural features: BeO₄ and PO₄ tetrahedra share vertices to form a distorted RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Ca between 8-rings (split site), Li near and above the centers of 6-rings (disorder).

Parise J.B. et al. (1994) [1]

 $\text{Be}_4\text{CaLi}_2\text{O}_{16}\text{P}_4$ $a = 1.309 \text{ nm}$, $V = 2.2429 \text{ nm}^3$, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ca1	24 <i>f</i>	1	0.0109	0.0208	0.5131	0.25	
P2	24 <i>f</i>	1	0.0605	0.3678	0.2129		tetrahedron O ₄
Be3	24 <i>f</i>	1	0.062	0.2205	0.3678		tetrahedron O ₄
O4	24 <i>f</i>	1	0.0848	0.2585	0.2497		
O5	24 <i>f</i>	1	0.1021	0.38	0.1038		non-colinear PBe
O6	24 <i>f</i>	1	0.1079	0.4427	0.2858		non-colinear PBe
O7	24 <i>f</i>	1	0.1148	0.2975	0.4469		non-colinear PBe
Li8	8 <i>c</i>	.3.	0.158	0.158	0.158	0.5	
Li9	8 <i>c</i>	.3.	0.182	0.182	0.182	0.5	
Li10	8 <i>c</i>	.3.	0.316	0.316	0.316	0.5	

Transformation from published data: $y, x, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.052$, $T = 298 \text{ K}$ Remarks: Natural specimen from the Tip Top Mine, Custer, South Dakota. Composition $\text{Ca}_{5.5}\text{Li}_{11.6}\text{K}_{1.2}\text{Na}_{0.2}\text{Be}_{24}\text{P}_{24}\text{O}_{96}$ from chemical analysis. Short interatomic distances for partly occupied site(s).

References: [1] Parise J.B., Corbin D.R., Abrams L., Northrup P., Rakovan J., Nenoff T.M., Stucky G.D. (1994), Zeolites 14, 25-34.

197
cI202

$\text{Rb}_{12}\text{Be}_{12}\text{As}_{12}\text{O}_{48}[\text{H}_2\text{O}]_{1.6}$	<i>cI202</i>	(197) <i>I23</i> – f^6dc^5b
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Rb₂₄Be₂₄As₂₄O₉₆·3.2H₂O [1], zeolite RHO(BeAs)-RbStructural features: BeO₄ and AsO₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Rb between 8-rings, additional Rb and H₂O in the cages (disorder).

Parise J.B. et al. (1992) [1]

 $\text{As}_{12}\text{Be}_{12}\text{D}_{3.20}\text{O}_{49.60}\text{Rb}_{11.98}$ $a = 1.4001 \text{ nm}$, $V = 2.7446 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Be1	24 <i>f</i>	1	0.0689	0.3717	0.2173		tetrahedron O ₄
As2	24 <i>f</i>	1	0.07263	0.22554	0.37251		tetrahedron O ₄
O3	24 <i>f</i>	1	0.1012	0.2704	0.2651		non-colinear BeAs
O4	24 <i>f</i>	1	0.1055	0.4571	0.2852		non-colinear BeAs
O5	24 <i>f</i>	1	0.1101	0.1118	0.3735		non-colinear BeAs
O6	24 <i>f</i>	1	0.1321	0.2906	0.4533		non-colinear BeAs

Rb7	12d	2..	0.244	0	0	0.25	8-vertex polyhedron (OD ₂) ₄ O ₂ Rb ₂
(OD ₂)8	8c	.3.	0.059	0.059	0.059	0.07	tetrahedron Rb(OD ₂) ₃
Rb9	8c	.3.	0.1284	0.1284	0.1284	0.87	
(OD ₂)10	8c	.3.	0.256	0.256	0.256	0.1	
Rb11	8c	.3.	0.3097	0.3097	0.3097		
(OD ₂)12	8c	.3.	0.434	0.434	0.434	0.23	non-coplanar triangle (OD ₂) ₃
Rb13	6b	222..	0	1/2	1/2		tetrahedron O ₄

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

Experimental: powder, diffractometer, neutrons, $R_p = 0.034$

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the y- and z-coordinates of former D₂O(1) and the z-coordinate of former D₂O(3) are misprinted as 0, 0 and 0.411 instead of 0.244, 0.244 and 0.441, respectively (agreement with Wyckoff position 8c).

References: [1] Parise J.B., Corbin D.R., Gier T.E., Harlow R.L., Abrams L., Dreele R.B.V. (1992), Zeolites 12, 360-368.

197
cI234

HK ₃ Ge ₇ O ₁₆ [H ₂ O] ₄	cI234	(197) I23 – f ⁸ edc ² a
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K₃HGe₇O₁₆·4H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked GeO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; K and H₂O in a system of interconnected channels (partial disorder). Superstructure caused by small distortions of the framework.

Bialek R., Gramlich V. (1992) [1]

Ge₇H_{6.50}K_{2.24}O_{19.25}

$a = 1.5418$ nm, $V = 3.6651$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	24f	1	0.0001	0.2412	0.2576		tetrahedron O ₄
O2	24f	1	0.0568	0.3038	0.1893		non-colinear Ge ₂
O3	24f	1	0.066	0.1777	0.3245		non-colinear Ge ₂
(OH ₂)4	24f	1	0.0876	0.3951	0.4386		non-colinear O ₂
O5	24f	1	0.1674	0.4374	0.1969		non-colinear Ge ₂
Ge6	24f	1	0.1768	0.3191	0.1848		octahedron O ₆
O7	24f	1	0.1885	0.3004	0.3152		non-coplanar triangle Ge ₃
O8	24f	1	0.3159	0.435	0.3226		non-colinear Ge ₂
K9	12e	2..	0.1998	1/2	0	0.57	8-vertex polyhedron O ₆ (OH ₂) ₂
K10	12d	2..	0.2409	0	0	0.92	bicapped square prism O ₈ (OH ₂) ₂
O11	8c	.3.	0.1933	0.1933	0.1933		non-coplanar triangle Ge ₃
Ge12	8c	.3.	0.3201	0.3201	0.3201		octahedron O ₆
(OH ₂)13	2a	23.	0	0	0		octahedron K ₆

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

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

Remarks: H not belonging to H₂O was not located. The average structure was refined in space group (215) $P-43m$ with $1/8$ cell volume. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bialek R., Gramlich V. (1992), Z. Kristallogr. 198, 67-77.

197
cI244

$\text{K}_{0.6}\text{Na}_{0.1}\text{Li}_{5.8}\text{Ca}_{2.75}\text{Be}_{12}[\text{PO}_4]_{12}[\text{H}_2\text{O}]_{19}$	<i>cI244</i>	(197) <i>I23</i> – f^9dc^2
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Li₈(Ca,Li,K,N)_{18.5}Be₂₄P₂₄O₉₆·38H₂O [1], pahasapaite, zeolite RHO(BeP)-Li,Ca

Structural features: BeO₄ and PO₄ tetrahedra share vertices to form a distorted RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; (Ca,etc.) near the centers of 8-rings, Li above the centers of 6-rings, H₂O between 8-rings and in the cages (disorder).

Rouse R.C. et al. (1989) [1]

 $\text{Be}_{12}\text{Ca}_{2.75}\text{H}_{38}\text{K}_{0.60}\text{Li}_{5.80}\text{Na}_{0.10}\text{O}_{67}\text{P}_{12}$ $a = 1.3781 \text{ nm}$, $V = 2.6172 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24 <i>f</i>	1	0.0301	0.0357	0.3615	0.438	
O2	24 <i>f</i>	1	0.0329	0.3791	0.2041		non-colinear PBe
O3	24 <i>f</i>	1	0.0383	0.216	0.3889		non-colinear PBe
(OH ₂)4	24 <i>f</i>	1	0.0504	0.0765	0.2459	0.5	
(OH ₂)5	24 <i>f</i>	1	0.0714	0.1095	0.2171	0.5	
Be6	24 <i>f</i>	1	0.121	0.4207	0.2675		tetrahedron O ₄
P7	24 <i>f</i>	1	0.124	0.2771	0.4224		tetrahedron O ₄
O8	24 <i>f</i>	1	0.1245	0.3781	0.3766		non-colinear PBe
O9	24 <i>f</i>	1	0.2178	0.2246	0.3914		non-coplanar triangle PBeLi
(OH ₂)10	12 <i>d</i>	2..	0.4768	0	0	0.5	
Li11	8 <i>c</i>	.3.	0.3013	0.3013	0.3013		tetrahedron O ₃ (OH ₂)
(OH ₂)12	8 <i>c</i>	.3.	0.3851	0.3851	0.3851		single atom Li

M1 = 0.524Ca + 0.343Li + 0.114K + 0.019Na

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.035

Remarks: Natural specimen from the Tip Top mine, Custer, South Dakota. Composition (Ca_{5.5}Li_{3.6}K_{1.2}Na_{0.2}□_{13.5})Li₈Be₂₄P₂₄O₉₆·38H₂O from chemical analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Rouse R.C., Peacor D.R., Merlino S. (1989), Am. Mineral. 74, 1195-1202.

197
cI258

$\text{HCs}_3\text{Ti}_4[\text{GeO}_4]_3\text{O}_4[\text{H}_2\text{O}]_4$	<i>cI258</i>	(197) <i>I23</i> – $f^8e^2d^2c^2a$
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Cs₃H(TiO)₄(GeO₄)₃·4H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked TiO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; Cs and H₂O in a system of interconnected channels.

Behrens E.A. et al. (1998) [1]

 $\text{Cs}_3\text{Ge}_3\text{H}_{6.50}\text{O}_{19.25}\text{Ti}_4$ $a = 1.59606 \text{ nm}$, $V = 4.0658 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	24 <i>f</i>	1	0.0023	0.2469	0.2562		tetrahedron O ₄
O2	24 <i>f</i>	1	0.0613	0.1885	0.1858		non-colinear GeTi
(OH ₂)3	24 <i>f</i>	1	0.0632	0.4155	0.098		square pyramid Cs ₃ O ₂

O4	24f	1	0.0686	0.3107	0.3182	non-collinear GeTi
Ti5	24f	1	0.1821	0.3193	0.3219	octahedron O ₆
O6	24f	1	0.1822	0.3037	0.4403	non-collinear GeTi
O7	24f	1	0.1836	0.438	0.3138	non-collinear GeTi
O8	24f	1	0.1878	0.1986	0.3103	non-coplanar triangle Ti ₃
Cs9	12e	2..	0.1925	1/2	0	0.5
Cs10	12e	2..	0.2421	1/2	0	0.5
Cs11	12d	2..	0.2239	0	0	0.5
Cs12	12d	2..	0.2839	0	0	0.5
Ti13	8c	.3.	0.1844	0.1844	0.1844	octahedron O ₆
O14	8c	.3.	0.314	0.314	0.314	non-coplanar triangle Ti ₃
(OH ₂)15	2a	23.	0	0	0	octahedron Cs ₆

Experimental: powder, diffractometer, X-rays, $R_B = 0.060$

Remarks: Part of H₂O and H not belonging to H₂O was not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Behrens E.A., Poojary D.M., Clearfield A. (1998), Chem. Mater. 10, 959-967.

197
cI264

HK ₃ Ge ₇ O ₁₆ [H ₂ O] _{3.14}	cI264	(197) I23 – f ⁸ e ² d ² c ³
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K₃HGe₇O₁₆·3.14H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked GeO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; K and H₂O in a system of interconnected channels.

Roberts M.A., Fitch A.N. (1996) [1]

Ge₇H_{6.28}K₃O_{19.14}

$a = 1.53496$ nm, $V = 3.6165$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	24f	1	0.0003	0.2401	0.2567		tetrahedron O ₄
O2	24f	1	0.0622	0.3172	0.2001		non-collinear Ge ₂
O3	24f	1	0.0698	0.173	0.3157		non-collinear Ge ₂
(OH ₂)4	24f	1	0.0935	0.3877	0.4309	0.713	single atom K
Ge5	24f	1	0.1767	0.3195	0.1849		octahedron O ₆
O6	24f	1	0.178	0.439	0.187		non-collinear Ge ₂
O7	24f	1	0.195	0.3013	0.3131		non-coplanar triangle Ge ₃
O8	24f	1	0.305	0.435	0.329		non-collinear Ge ₂
K9	12e	2..	0.201	1/2	0	0.617	
K10	12e	2..	0.266	1/2	0	0.383	
K11	12d	2..	0.237	0	0	0.712	
K12	12d	2..	0.348	0	0	0.288	
(OH ₂)13	8c	.3.	0.0766	0.0766	0.0766		bicapped square prism K ₃ O ₄ (OH ₂) ₃
O14	8c	.3.	0.193	0.193	0.193		non-coplanar triangle Ge ₃
Ge15	8c	.3.	0.3189	0.3189	0.3189		octahedron O ₆

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

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

Remarks: H not belonging to H₂O was not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Roberts M.A., Fitch A.N. (1996), Z. Kristallogr. 211, 378-387.