

Space group (199) $I2_13$ 199
 $cI16$

UCo	$cI16$	(199) $I2_13 - a^2$
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UCo [1], Strukturbericht notation B_a

Structural features: U and Co atoms in a distorted CsCl-type arrangement.

Baenziger N.C. et al. (1950) [1]

CoU

 $a = 0.63557 \text{ nm}$, $V = 0.2567 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
U1	$8a$.3.	0.0347	0.0347	0.0347		pentacapped trigonal prism Co ₈ U ₃
Co2	$8a$.3.	0.294	0.294	0.294		pentacapped trigonal prism U ₈ Co ₃

Experimental: powder, film, X-rays

Remarks: In [2] the cell parameter is misprinted as 0.63577 nm instead of 0.63557 nm.

References: [1] Baenziger N.C., Rundle R.E., Snow A.I., Wilson A.S. (1950), Acta Crystallogr. 3, 34-40.
[2] (1954), Structure Reports 13, 94.199
 $cI28$

K ₂ Pb ₂ O ₃	$cI28$	(199) $I2_13 - ba^2$
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K₂Pb₂O₃ [1]Structural features: :PbO₃ ψ -tetrahedra share vertices to form a 3D-framework.

Martens K.P., Hoppe R. (1977) [1]

K₂O₃Pb₂ $a = 0.8419 \text{ nm}$, $V = 0.5967 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$12b$	2..	0.2887	0	$\frac{1}{4}$		non-colinear Pb ₂
K2	$8a$.3.	0.0232	0.0232	0.0232		octahedron O ₆
Pb3	$8a$.3.	0.2562	0.2562	0.2562		non-coplanar triangle O ₃

Experimental: single crystal, diffractometer, X-rays, $R = 0.060$

References: [1] Martens K.P., Hoppe R. (1977), Z. Anorg. Allg. Chem. 437, 116-122.

199
 $cI28$

Hg ₃ S ₂ Cl ₂	$cI28$	(199) $I2_13 - ba^2$
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Hg₃S₂Cl₂ **a** [2], corderoite

Structural features: Approximately linear S-Hg-S units share atoms to form a 3D-framework; four Cl atoms complete the octahedral coordination around Hg. See Fig. II.67.

Frueh A.J., Gray N. (1968) [1]

Cl₂Hg₃S₂ $a = 0.8949 \text{ nm}$, $V = 0.7167 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	12b	2..	0.3029	0	$\frac{1}{4}$		10-vertex polyhedron $S_2Cl_4Hg_4$
Cl2	8a	.3.	0.0107	0.0107	0.0107		non-coplanar triangle Hg_3
S3	8a	.3.	0.2709	0.2709	0.2709		non-coplanar triangle Hg_3

Experimental: single crystal, diffractometer, X-rays, $wR = 0.077$

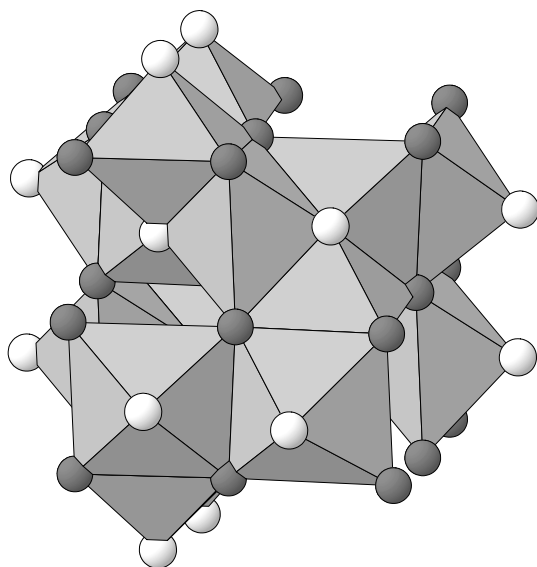


Fig. II.67. $Hg_3S_2Cl_2 \alpha$

Arrangement of $Hg(S_2Cl_4)$ (S atoms light, Cl atoms dark) octahedra.

References: [1] Frueh A.J., Gray N. (1968), Acta Crystallogr. B 24, 156-157. [2] Puff H., Küster J. (1962), Naturwissenschaften 49, 299b.

199
c/36

NO_2	$c/36$	(199) $I2_13 - cb$
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N_2O_4 [2], Strukturbericht notation C26a

Structural features: Mutually perpendicular O-N-O linear molecules.

Vegard L. (1931) [1]

NO_2

$a = 0.777 \text{ nm}$, $V = 0.4691 \text{ nm}^3$, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.000	0.072	0.347		single atom N
N2	12b	2..	0.347	0	$\frac{1}{4}$		colinear O_2

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: powder, film, X-rays, $T = 77 \text{ K}$

Remarks: The structure was determined independently in space group (204) $Im-3$ and found to contain N_2O_4 molecules [3] (confirmed in [4]).

References: [1] Vegard L. (1931), Z. Phys. 68, 184-203. [2] Vegard L. (1930), Nature (London) 126, 916. [3] Hendricks S.B. (1931), Z. Phys. 70, 699-700. [4] Broadley J.S., Monteath Robertson J. (1949), Nature (London) 164, 915.

199
cI48

$\text{Ba}_3\text{Fe}_2\text{Cl}_2\text{O}_5$	<i>cI48</i>	(199) $I2_13 - b^2a^3$
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Ba₃Fe₂O₅Cl₂ [1]

Structural features: FeO₄ tetrahedra share vertices to form an open 3D-framework embedded in a 3D-framework of interconnected ClBa₆ octahedra.

Leib W., Müller Buschbaum H. (1985) [1]

$\text{Ba}_3\text{Cl}_2\text{Fe}_2\text{O}_5$

$a = 0.99705 \text{ nm}$, $V = 0.9912 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	12b	2..	0.3445	0	$\frac{1}{4}$		coplanar triangle O ₃
O2	12b	2..	0.609	0	$\frac{1}{4}$		non-colinear Fe ₂
Cl3	8a	.3.	0.0573	0.0573	0.0573		tetrahedron OBa ₃
O4	8a	.3.	0.2377	0.2377	0.2377		single atom Fe
Fe5	8a	.3.	0.3448	0.3448	0.3448		tetrahedron O ₄

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

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

References: [1] Leib W., Müller Buschbaum H. (1985), Z. Anorg. Allg. Chem. 521, 51-56.

199
cI64

$[\text{H}_3\text{O}]\text{SbF}_6$	<i>cI64</i>	(199) $I2_13 - c^2a^2$
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(H₃O)SbF₆ [1]

Structural features: SbF₆ octahedra and :OH₃ ψ-tetrahedra in a CsCl-type arrangement.

Larson E.M. et al. (1991) [1]

$\text{F}_6\text{H}_3\text{OSb}$

$a = 1.012 \text{ nm}$, $V = 1.0364 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	24c	1	0.1038	0.1443	0.298		single atom Sb
F2	24c	1	0.1779	0.3822	0.3547		single atom Sb
O3	8a	.3.	0.0015	0.0015	0.0015		octahedron F ₆
Sb4	8a	.3.	0.25016	0.25016	0.25016		octahedron F ₆
H5	24c	1	0.059	0.072	0.548		

Experimental: single crystal, diffractometer, X-rays, wR = 0.046, T = 238 K

Remarks: An alternative model in space group (206) *Ia-3* could not be excluded. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Larson E.M., Abney K.D., Larson A.C., Eller P.G. (1991), Acta Crystallogr. B 47, 206-209.

199
cI64

$\text{Cs}_2\text{Ba}_2[\text{CO}_3]_3$	<i>cI64</i>	(199) $I2_13 - cb^2a^2$
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Cs₂Ba₂(CO₃)₃ [1]

Structural features: Single mutually perpendicular planar CO₃ units.

Hagen S., Jansen M. (1993) [1]

Ba₂C₃Cs₂O₉

$a = 1.0349$ nm, $V = 1.1084$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.1069	0.2344	0.4711		single atom C
O2	12b	2..	0.2852	0	$\frac{1}{4}$		single atom C
C3	12b	2..	0.4095	0	$\frac{1}{4}$		coplanar triangle O ₃
Cs4	8a	.3.	0.06002	0.06002	0.06002		trigonal prism O ₆
Ba5	8a	.3.	0.29177	0.29177	0.29177		octahedron O ₆

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

Experimental: single crystal, diffractometer, X-rays, wR = 0.026

References: [1] Hagen S., Jansen M. (1993), Z. Anorg. Allg. Chem. 619, 461-465.

199
c/80

Sm ₂ O ₃	c/80	(199) $I2_13 - c^2b^2a$
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Sm₂O₃ form C [2]; (Li_{1-x}Mg_x)₃N_{2-x} [5]

Structural features: Distorted SmO₆ octahedra share six edges with neighboring octahedra to form a 3D-framework. Distorted derivative of bixbyite.

Zav'yalova A.A. et al. (1976) [1]

O₃Sm₂

$a = 1.093$ nm, $V = 1.3058$ nm³, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.105	0.350	0.150		non-collinear Sm ₂
O2	24c	1	0.141	0.405	0.409		non-collinear Sm ₂
Sm3	12b	2..	0.275	0	$\frac{1}{4}$		octahedron O ₆
Sm4	12b	2..	0.803	0	$\frac{1}{4}$		octahedron O ₆
Sm5	8a	.3.	0.002	0.002	0.002		octahedron O ₆

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: thin film, electron diffraction, R = 0.180

Remarks: Phase stable at $T < 1253$ K. We took the non-refinable atom coordinates from [4]. Space group (206) $Ia-3$ was tested and rejected (weak additional reflections). The structure was, however, later successfully refined in this space group [3] (bixbyite type).

References: [1] Zav'yalova A.A., Imamov R.M., Ragimli N.A., Semiletov S.A. (1976), Sov. Phys. Crystallogr. (Engl. Transl.) 21, 411-413. [2] Zachariasen W.H. (1927), Nor. Geol. Tidsskr. 9, 310-316. [3] Bartos A., Lieb K.P., Uhrmacher M., Wiarda D. (1993), Acta Crystallogr. B 49, 165-169. [4] (1978), Structure Reports 42A, 443. [5] Yamane H., Okabe T.H., Ishiyama O., Maseda Y., Shimada M. (2001), J. Alloys Compd. 319, 124-130.

199
c/80

Gd(Gd _{0.17} Bi _{0.83}) ₃ O ₆	c/80	(199) $I2_13 - c^2b^2a$
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Bi_{0.65}Gd_{0.35}O_{1.5} [1]

Structural features: GdO_6 and $(\text{Bi,Gd})\text{O}_6$ octahedra share edges to form a 3D-framework. Ordering variant of Sm_2O_3 of ideal composition $\text{AA}'_3\text{O}_6$.

Watanabe A. (1995) [1]

$\text{Bi}_{2.61}\text{Gd}_{1.39}\text{O}_6$

$a = 1.1051 \text{ nm}$, $V = 1.3496 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.1	0.163	0.38		single atom Bi
O2	24c	1	0.13	0.35	0.412		non-colinear BiO
M3	12b	2..	0.271	0	$\frac{1}{4}$		octahedron O_6
M4	12b	2..	0.771	0	$\frac{1}{4}$		6-vertex polyhedron O_6
Gd5	8a	.3.	0.02	0.02	0.02		6-vertex polyhedron O_6

$\text{M3} = 0.87\text{Bi} + 0.13\text{Gd}$; $\text{M4} = 0.87\text{Bi} + 0.13\text{Gd}$

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: powder, diffractometer, X-rays, $R_B = 0.155$

References: [1] Watanabe A. (1995), J. Solid State Chem. 120, 32-37.

199
cI84

$\text{Na}_2\text{Ca}_3\text{Al}_2\text{F}_{14}$	<i>cI84</i>	(199) $I2_13 - c^2ba^3$
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$\text{Na}_2\text{Ca}_3\text{Al}_2\text{F}_{14}$ [1]

Structural features: Single AlF_6 octahedra; additional F in Ca_3Na tetrahedra, which share vertices (Ca) to form a 3D-framework.

Courbion G., Ferey G. (1988) [1]

$\text{Al}_2\text{Ca}_3\text{F}_{14}\text{Na}_2$

$a = 1.0257 \text{ nm}$, $V = 1.0791 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	24c	1	0.0562	0.3887	0.1294		single atom Al
F2	24c	1	0.1127	0.386	0.4373		single atom Al
Ca3	12b	2..	0.7833	0	$\frac{1}{4}$		8-vertex polyhedron F_8
Al4	8a	.3.	0.0018	0.0018	0.0018		octahedron F_6
Na5	8a	.3.	0.1653	0.1653	0.1653		8-vertex polyhedron F_7Al
F6	8a	.3.	0.2886	0.2886	0.2886		7-vertex polyhedron NaCa_3F_3

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

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

References: [1] Courbion G., Ferey G. (1988), J. Solid State Chem. 76, 426-431.

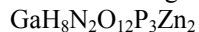
199
cI160

$[\text{NH}_4]_2(\text{Zn}_{0.67}\text{Ga}_{0.33})_3[\text{PO}_4]_3$	<i>cI160</i>	(199) $I2_13 - c^6a^2$
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$(\text{NH}_4)_{0.67}\text{Zn}_{0.67}\text{Ga}_{0.33}\text{PO}_4$ [1], zeolite ANA(Zn,Ga,P)- NH_4

Structural features: $(\text{Zn,Ga})\text{O}_4$ and PO_4 tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; NH_4 in non-intersecting channels along $\langle 111 \rangle$.

Zabukovec Logar N. et al. (2001) [1]



$a = 1.3456 \text{ nm}$, $V = 2.4364 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.0575	0.1475	0.3215		non-colinear PZn
M2	24c	1	0.07851	0.37803	0.34935		tetrahedron O ₄
O3	24c	1	0.0974	0.4895	0.1095		non-colinear PZn
O4	24c	1	0.1208	0.2777	0.4419		non-colinear PZn
P5	24c	1	0.132	0.1699	0.4055		tetrahedron O ₄
O6	24c	1	0.1583	0.3628	0.2359		non-colinear PZn
N7	8a	.3.	0.1234	0.1234	0.1234		non-coplanar triangle O ₃
N8	8a	.3.	0.3576	0.3576	0.3576		trigonal prism O ₆
H9	24c	1	0.0886	0.142	0.2008		
H10	24c	1	0.1293	0.341	0.5595		
H11	8a	.3.	0.0779	0.0779	0.0779		
H12	8a	.3.	0.3167	0.3167	0.3167		

$\text{M2} = 0.667\text{Zn} + 0.333\text{Ga}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.025$, $T = 293 \text{ K}$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 3 of [1] the z -coordinate of former O(3) and the y -coordinate of former O(1) are misprinted as 0.8215 and 0.7332 instead of 0.7359 and 0.7223, respectively (checked on interatomic distances).

References: [1] Zabukovec Logar N., Mrak M., Kaucic V., Golobic A. (2001), J. Solid State Chem. 156, 480-486.

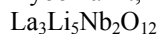
199
cI184

$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$	$cI184$	$(199) I2_13 - c^6b^2a^2$
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$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$ [1]

Structural features: Single NbO₆ octahedra and distorted LaO₈ cubes share atoms to form a 3D-framework. See Fig. II.68.

Hyooma H., Hayashi K. (1988) [1]



$a = 1.2797 \text{ nm}$, $V = 2.0957 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.033	0.4451	0.1426		non-coplanar triangle NbLi ₂
O2	24c	1	0.0489	0.3524	0.4707		non-colinear NbLi
Li3	24c	1	0.0574	0.3536	0.2831	0.667	6-vertex polyhedron O ₅ La
O4	24c	1	0.1076	0.194	0.2784		4-vertex polyhedron NbLi ₃
Li5	24c	1	0.1325	0.2039	0.4467		octahedron O ₆
O6	24c	1	0.2183	0.3957	0.3008		tetrahedron NbLi ₃
La7	12b	2..	0.1265	0	$\frac{1}{4}$		cuboctahedron O ₈ Li ₄
La8	12b	2..	0.6236	0	$\frac{1}{4}$		icosahedron O ₈ Li ₄
Nb9	8a	.3.	0.0	0.0	0.0		octahedron O ₆
Nb10	8a	.3.	0.25	0.25	0.25		octahedron O ₆

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: single crystal, diffractometer, X-rays, wR = 0.051, T = 298 K

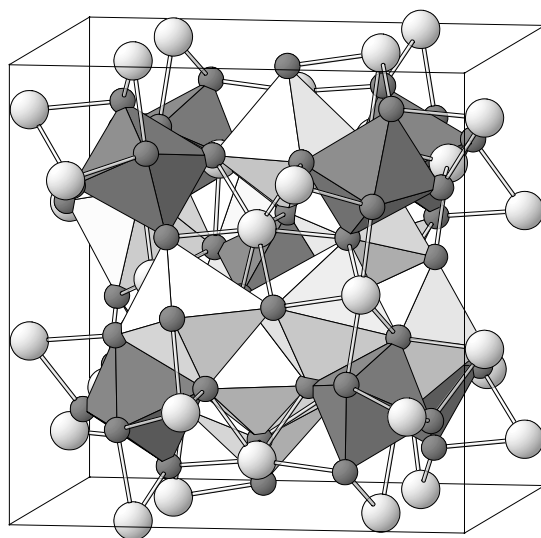


Fig. II.68. **Li₅La₃Nb₂O₁₂**

Arrangement of NbO₆ (dark) and LiO₆ (light) octahedra (O atoms small) and La atoms (large).

References: [1] Hyooma H., Hayashi K. (1988), Mater. Res. Bull. 23, 1399-1407.

199
cI200

Li₂Ca₃Be₃[SiO₄]₃F₂

cI200

(199) *I*2₁3 – c⁶b²a⁴

Li₁₆Ca₂₄Be₂₄Si₂₄O₉₆F₁₆ [1], hsianghualite, zeolite ANA(Be)-Ca (LiF)

Structural features: BeO₄ and SiO₄ tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; LiF units in non-intersecting channels along <111>, Ca near the centers of 8-rings.

Rastsvetaeva R.K. et al. (1991) [1]

Be₃Ca₃F₂Li₂O₁₂Si₃

a = 1.2864 nm, *V* = 2.1288 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>c</i>	1	0.0427	0.133	0.3176		non-colinear SiBe
Si2	24 <i>c</i>	1	0.0797	0.3761	0.3447		tetrahedron O ₄
O3	24 <i>c</i>	1	0.1034	0.1066	0.5121		non-colinear BeSi
O4	24 <i>c</i>	1	0.1176	0.2923	0.4326		non-colinear BeSi
Be5	24 <i>c</i>	1	0.1292	0.1704	0.4065		tetrahedron O ₄
O6	24 <i>c</i>	1	0.1416	0.3505	0.238		non-colinear BeSi
Ca7	12 <i>b</i>	2..	0.1555	0	¹ / ₄		square antiprism F ₂ O ₆
Ca8	12 <i>b</i>	2..	0.5863	0	¹ / ₄		square antiprism F ₂ O ₆
Li9	8 <i>a</i>	.3.	0.0231	0.0231	0.0231		tetrahedron FO ₃
F10	8 <i>a</i>	.3.	0.1046	0.1046	0.1046		single atom Li
Li11	8 <i>a</i>	.3.	0.2704	0.2704	0.2704		tetrahedron FO ₃
F12	8 <i>a</i>	.3.	0.3546	0.3546	0.3546		single atom Li

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

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

Remarks: Natural specimen from China. 34.6 wt.% CaO, 25.66 wt.% SiO₂, 15.78 wt.% BeO, 5.85 wt.% Li₂O, and 7.81 wt.% F from chemical analysis.

References: [1] Rastsvetaeva R.K., Rekhlova O.Y., Andrianov V.I., Malinovskii Y.A. (1991), Dokl. Akad. Nauk SSSR 316, 624-628.

199
cI280

$\text{Na}_4[\text{UO}_2]_3\text{Te}_5\text{O}_{15}$	<i>cI280</i>	(199) $I2_13 - c^{10}b^2a^2$
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$\text{Na}_8[(\text{UO}_2)_6(\text{TeO}_3)_{10}]$ [1]

Structural features: UO_7 pentagonal bipyramids share vertices with $:\text{TeO}_3$ ψ -tetrahedra to form a 3D-framework.

Almond P.M. et al. (2002) [1]

$\text{Na}_4\text{O}_{21}\text{Te}_5\text{U}_3$

$a = 1.68969 \text{ nm}$, $V = 4.8242 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.0005	0.0955	0.463		single atom Te
O2	24c	1	0.0066	0.3553	0.3105		single atom Te
O3	24c	1	0.0449	0.3389	0.1256		single atom U
Na4	24c	1	0.0498	0.3074	0.5656	0.333	non-coplanar triangle O_2Na
O5	24c	1	0.0758	0.5007	0.1571		single atom Te
O6	24c	1	0.1017	0.2319	0.4405		single atom U
Te7	24c	1	0.10329	0.39142	0.34665		non-coplanar triangle O_3
U8	24c	1	0.11411	0.14061	0.38788		7-vertex polyhedron O_7
O9	24c	1	0.1381	0.2106	0.2741		single atom Te
O10	24c	1	0.1595	0.3855	0.2501		non-colinear TeU
Na11	12b	2..	0.0271	0	$1/4$		octahedron O_6
Na12	12b	2..	0.2264	0	$1/4$		octahedron O_6
Te13	8a	.3.	0.01209	0.01209	0.01209		non-coplanar triangle O_3
Te14	8a	.3.	0.23957	0.23957	0.23957		non-coplanar triangle O_3

Transformation from published data: $1/4-y, 1/4-x, 1/4-z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.018$, $T = 193 \text{ K}$

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

References: [1] Almond P.M., McKee M.L., Albrecht Schmitt T.E. (2002), Angew. Chem. Int. Ed. 41, 3426-3429.

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cI392

$\text{K}_6\text{Ga}_6[\text{GeO}_4]_6[\text{H}_2\text{O}]_7$	<i>cI392</i>	(199) $I2_13 - c^{14}b^2a^4$
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$(\text{KGaGeO}_4)_6 \cdot 7\text{H}_2\text{O}$ [1]

Structural features: GaO_4 and GeO_4 tetrahedra share vertices to form helical ribbons which are interconnected into two 3D-frameworks (built from left- and right-handed helical ribbons, respectively); K and H_2O in two independent sets of cross-linked helical channels.

Gier T.E. et al. (1998) [1]

$\text{Ga}_6\text{Ge}_6\text{H}_{14}\text{K}_6\text{O}_{31}$

$a = 1.86766 \text{ nm}$, $V = 6.5147 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24c	1	0.0061	0.5486	0.1293		non-colinear GeGa
Ge2	24c	1	0.0095	0.1365	0.4014		tetrahedron O_4

K3	24c	1	0.0314	0.1577	0.193	square pyramid O ₂ (OH ₂) ₃
O4	24c	1	0.0492	0.1375	0.4845	non-colinear GeGa
O5	24c	1	0.059	0.1781	0.3345	non-colinear GeGa
O6	24c	1	0.0722	0.3177	0.4145	non-colinear GeGa
O7	24c	1	0.084	0.4261	0.1859	non-colinear GeGa
Ga8	24c	1	0.0981	0.5093	0.1367	tetrahedron O ₄
Ga9	24c	1	0.1133	0.2597	0.3483	tetrahedron O ₄
O10	24c	1	0.1276	0.2957	0.2593	non-colinear GeGa
Ge11	24c	1	0.1525	0.3863	0.2404	tetrahedron O ₄
K12	24c	1	0.1558	0.3029	0.531	8-vertex polyhedron O ₄ (OH ₂) ₄
O13	24c	1	0.1636	0.4315	0.3209	non-colinear GeGa
O14	24c	1	0.1997	0.239	0.3912	non-colinear GeGa
(OH ₂)15	12b	2..	0.0773	0	¹ / ₄	tetrahedron K ₂ O ₂
(OH ₂)16	12b	2..	0.5737	0	¹ / ₄	trigonal prism O ₂ K ₄
(OH ₂)17	8a	.3.	0.0702	0.0702	0.0702	octahedron O ₃ K ₃
(OH ₂)18	8a	.3.	0.1817	0.1817	0.1817	trigonal prism O ₃ K ₃
(OH ₂)19	8a	.3.	0.3204	0.3204	0.3204	octahedron K ₃ O ₃
(OH ₂)20	8a	.3.	0.4272	0.4272	0.4272	octahedron K ₃ O ₃

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: single crystal, diffractometer, X-rays, R = 0.038, T = 293 K

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

References: [1] Gier T.E., Bu X., Feng P., Stucky G.D. (1998), Nature (London) 395, 154-157.