

Space group (210) $F4_132$ 210
 $cF224$

$H_6[TeO_6]$	$cF224$	(210) $F4_132 - h^2e$
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Te(OH)₆ cubic [1]

Structural features: Te(OH)₆ octahedra (3 longer and 3 shorter bonds) are loosely interconnected via hydrogen bonding.

Mullica D.F. et al. (1980) [1]

H_6O_6Te

$a = 1.5699 \text{ nm}$, $V = 3.8692 \text{ nm}^3$, $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96h	1	0.0194	0.0793	0.3503		single atom Te
O2	96h	1	0.0928	0.2607	0.1616		single atom Te
Te3	32e	.3.	0.3771	0.3771	0.3771		octahedron O ₆
H4	96h	1	0.0157	0.2009	0.1224	0.5	
H5	96h	1	0.0287	0.1425	0.5068	0.5	
H6	96h	1	0.0949	0.2596	0.2225	0.5	
H7	96h	1	0.1117	0.1785	0.5224	0.5	

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

Experimental: single crystal, diffractometer, neutrons, wR = 0.093

Remarks: Space group (228) $Fd-3c$ was tested and rejected. Supersedes a report on cubic Te(OH)₆ with space group (225) $Fm-3m$ and $\frac{1}{8}$ cell volume in [2], and different structure proposals in space group (228) $Fd-3c$ ([3], [4], [5], [6]). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Mullica D.F., Korp J.D., Milligan W.O., Beall G.W., Bernal I. (1980), Acta Crystallogr. B 36, 2565-2570. [2] Gossner B., Kraus O. (1934), Z. Kristallogr. 88, 298-303. [3] Kirkpatrick L.M., Pauling L. (1926), Z. Kristallogr. 63, 502-506. [4] Avinens C., Petit H. (1968), C. R. Seances Acad. Sci., Ser. C 266, 981-983. [5] Falck L., Lindqvist O. (1978), Acta Crystallogr. B 34, 3145-3146. [6] Cohen Addad C. (1971), Bull. Soc. Fr. Mineral. Cristallogr. 94, 172-174.

210
 $cF264$

$Ca_6Mg_2[BO_3]_4[CO_3]_2[H_2O]_{0.25}$	$cF264$	(210) $F4_132 - hgfedca$
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Ca₃Mg(BO₃)₂CO₃·xH₂O [1], sakhaite

Structural features: MgO₆ octahedra and BO₃ trigonal units share vertices to form a 3D-framework; (OH₂)Ca₆ octahedra (in part vacant) and CO₃ trigonal units in voids. See Fig. II.35.

Chichagov A.V. et al. (1974) [1]

$B_4C_2Ca_6H_{0.50}Mg_2O_{18.25}$

$a = 1.469 \text{ nm}$, $V = 3.1700 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96h	1	0.116	0.124	0.264		single atom B
O2	48g	..2	$\frac{1}{8}$	0.436	0.814		single atom C
Ca3	48f	2..	0.239	0	0		square antiprism O ₈
B4	32e	.3.	0.341	0.341	0.341		coplanar triangle O ₃

C5	16 <i>d</i>	.32	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$		coplanar triangle O ₃
Mg6	16 <i>c</i>	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		octahedron O ₆
(OH ₂)7	8 <i>a</i>	23.	0	0	0	0.25	tetrahedron B ₄

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

Experimental: single crystal, diffractometer, X-rays, R = 0.069

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

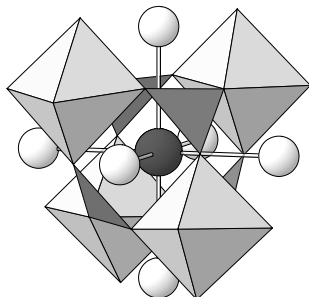
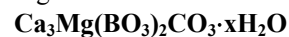


Fig. II.35.



Arrangement of MgO₆ octahedra (light), BO₃ triangles (dark) and Ca atoms (light) around a central H₂O molecule (O atom dark).

References: [1] Chichagov A.V., Simonov M.A., Belov N.V. (1974), Dokl. Akad. Nauk SSSR 218, 576-579.

210
cF328

Ca ₆ Mg ₂ [BO ₃] ₄ [CO ₃] ₂ [H ₂ O] _{0.72}	cF328	(210) F4 ₁ 32 – h ² fe ² da
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Ca₃Mg(BO₃)₂CO₃·0.36H₂O [1], sakhaite

Structural features: MgO₆ octahedra and BO₃ trigonal units share vertices to form a 3D-framework; (OH₂)Ca₆ octahedra (in part vacant) and CO₃ trigonal units (orientational disorder) in voids.

Iakubovich O.V. et al. (1978) [1]

B₄C₂Ca₆H_{1.50}Mg₂O_{18.75}

a = 1.4685 nm, *V* = 3.1668 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.015	0.123	0.368		single atom B
O2	96 <i>h</i>	1	0.045	0.134	0.157	0.5	single atom O
Ca3	48 <i>f</i>	2..	0.2511	0	0		non-collinear O ₂
C4	32 <i>e</i>	.3.	0.114	0.114	0.114	0.5	
B5	32 <i>e</i>	.3.	0.399	0.399	0.399		non-coplanar triangle O ₃
Mg6	16 <i>d</i>	.32	$\frac{5}{8}$	$\frac{5}{8}$	$\frac{5}{8}$		octahedron O ₆
(OH ₂)7	8 <i>a</i>	23.	0	0	0	0.75	tetrahedron C ₄

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

Experimental: single crystal, diffractometer, X-rays, R = 0.075

Remarks: Natural specimen from Solongo. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (227) *Fd-3m* was tested and rejected.

References: [1] Iakubovich O.V., Egorov Tismenko I.K., Simonov M.A., Belov N.V. (1978), Dokl. Akad. Nauk SSSR 239, 1103-1106.

210
cF336

$\text{H}_2\text{Ta}_3\text{Cl}_6[\text{CN}]_3[\text{H}_2\text{O}]_6$	<i>cF336</i>	(210) $F4_132 - h^2f^3$
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$\text{H}_4\text{Ta}_6\text{Cl}_{12}(\text{CN})_6 \cdot 12\text{H}_2\text{O}$ [1]

Structural features: $\text{Ta}_6\text{Cl}_{12}(\text{CN})_6$ clusters (a Ta_6 octahedron surrounded by a Cl_{12} cuboctahedron and a large $(\text{CN})_6$ octahedron); H_2O between the units.

Basson S.S., Leipoldt J.G. (1982) [1]

$\text{C}_3\text{Cl}_6\text{H}_{12}\text{N}_3\text{O}_6\text{Ta}_3$

$a = 1.991 \text{ nm}$, $V = 7.8925 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH ₂)1	96 <i>h</i>	1	0.017	0.095	0.364		single atom N
Cl2	96 <i>h</i>	1	0.1281	0.2512	0.1287		non-colinear Ta ₂
Ta3	48 <i>f</i>	2..	0.10415	0	0		5-vertex polyhedron CCl ₄
C4	48 <i>f</i>	2..	0.215	0	0		single atom N
N5	48 <i>f</i>	2..	0.274	0	0		single atom C

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

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

References: [1] Basson S.S., Leipoldt J.G. (1982), Transition Met. Chem. London 7, 207-209.