

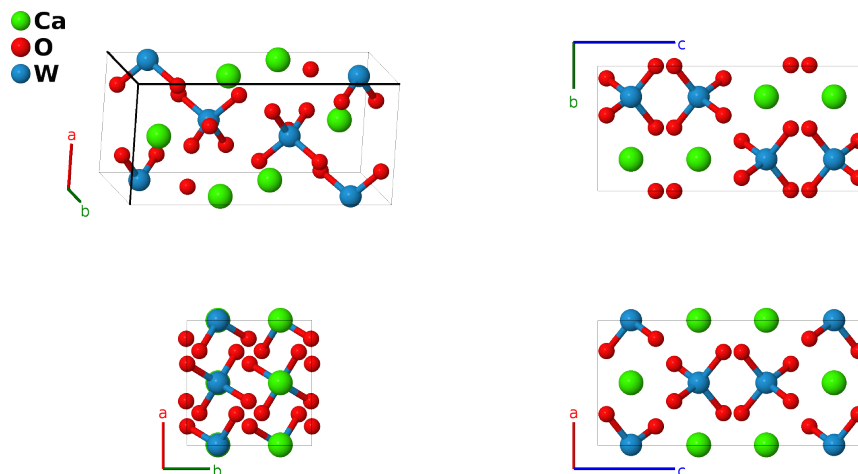
Scheelite (CaWO_4 , $H0_4$) Structure: AB4C_tI24_88_a_f_b-003

This structure originally had the label AB4C_tI24_88_b_f_a. Calls to that address will be redirected here.

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<https://afLOW.org/p/Y9T0>

https://afLOW.org/p/AB4C_tI24_88_a_f_b-003



Prototype	CaO_4W
AFLOW prototype label	AB4C_tI24_88_a_f_b-003
<i>Strukturbericht</i> designation	$H0_4$
Mineral name	scheelite
ICSD	60547
Pearson symbol	tI24
Space group number	88
Space group symbol	$I4_1/a$
AFLOW prototype command	<code>afLOW --proto=AB4C_tI24_88_a_f_b-003 --params=a, c/a, x3, y3, z3</code>

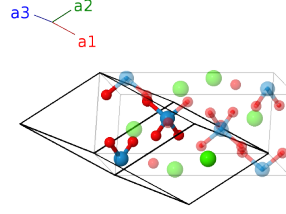
Other compounds with this structure

ZrSiO_4 , LaNbO_4 , YTao_4 , YNbO_4 , $(\text{Y, RE})\text{NbO}_4$ (fergusonite), YVO_4 , BiVO_4 , BaWO_4 , PbWO_4 (wulfenite), SrWO_4 , EuWO_4 , PbMoO_4 (stolzite), SrMoO_4 , CaMoO_4 (powellite), CdMoO_4 , KReO_4 , TlReO_4 , AgReO_4 , NaAlH_4

- (Ewald, 1931) originally gave this structure the *Strukturbericht* designation $H4$, but this was changed to $H0_4$ in (Gottfried, 1937).

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{3}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(4a)	Ca I
\mathbf{B}_2	$= \frac{5}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(4a)	Ca I
\mathbf{B}_3	$= \frac{7}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + \frac{5}{8}c \hat{\mathbf{z}}$	(4b)	W I
\mathbf{B}_4	$= \frac{1}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - \frac{1}{8}c \hat{\mathbf{z}}$	(4b)	W I
\mathbf{B}_5	$= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16f)	O I
\mathbf{B}_6	$= (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16f)	O I
\mathbf{B}_7	$= (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$-a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	O I
\mathbf{B}_8	$= (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	O I
\mathbf{B}_9	$= -(y_3 + z_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16f)	O I
\mathbf{B}_{10}	$= (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(16f)	O I
\mathbf{B}_{11}	$= -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	O I
\mathbf{B}_{12}	$= (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	O I

References

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- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).
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Found in

- [1] Y. Zhang, N. A. W. Holzwarth, and R. T. Williams, *Electronic band structures of the scheelite materials CaMoO_4 , CaWO_4 , PbMoO_4 , and PbWO_4* , Phys. Rev. B **57**, 12738–12750 (1988), doi:10.1103/PhysRevB.57.12738.