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

This structure previously used the label(s) `AB4C_tI24_88_b_f_a`. Calls to these addresses will be redirected here.

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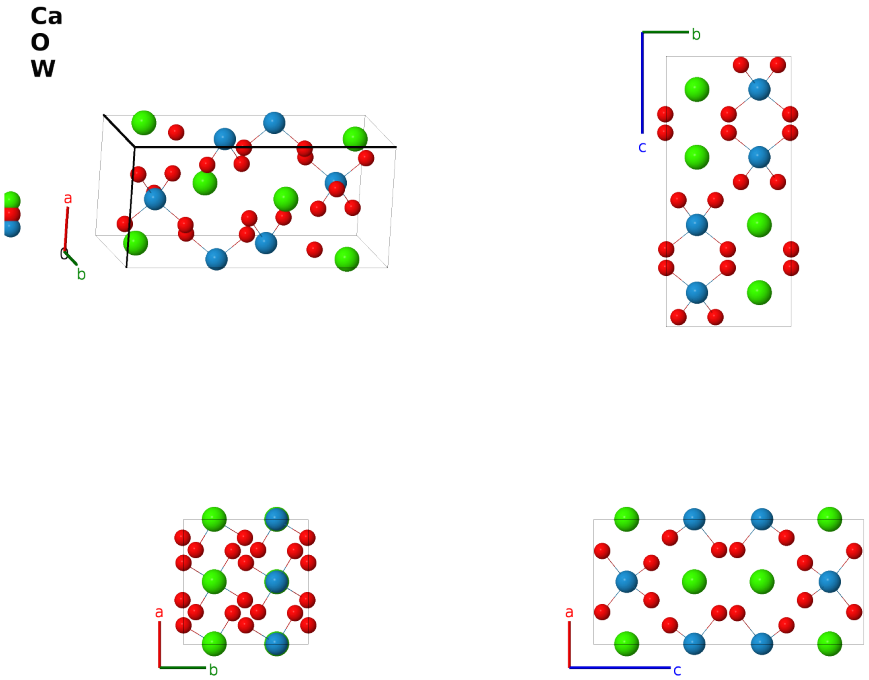
https://aflow.org/prototype-encyclopedia/Y9T0

https://aflow.org/prototype-encyclopedia/AB4C_tI24_88_a_f_b-003



Prototype	CaO_4W
AFLOW prototype label	AB4C_tI24_88_a_f_b-003
***Strukturbericht* designation**	$H0_4$
Mineral name	scheelite
ICSD	60547
CCDC	1624142
Pearson symbol	tI24
Space group number	88
Space group symbol	$I4_1/a$

AFLOW prototype command `aflow --proto=AB4C_tI24_88_a_f_b-003 --params=`$a, c/a, x_3, y_3, z_3$

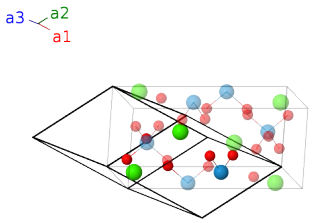
Other compounds with this structure

(Y, RE)NbO_4 (fergusonite), $AgReO_4$, $BaLiF_4$, $BaMoO_4$, $BaWO_4$, $BiVO_4$, $CaMoO_4$ (powellite), $CaSeO_4$, $CdMoO_4$, $CsAlH_4$, $CsBrO_4$, $CsRuO_4$, $CsTcO_4$, $DyNbO_4$, $ErCrO_4$, $ErVO_4$, $EuMoO_4$, $EuWO_4$, $GeUO_4$, $HfGeO_4$, $HoCrO_4$, $HoVO_4$, KIO_4, $KOsO_4$, $KReO_4$, $KRuO_4$, $KTcO_4$, $KTlO_4$, $LaAsO_4$, $LaNbO_4$, $LiScO_4$, $LiYF_4$, $LiYbF_4$, LuP_4, LuV_4, $NaAlH_4$, $NaIO_4$, $NaReO_4$, $NaTcO_4$, $NdNbO_4$, $NdTaO_4$, $PbCrO_4$, $PbMoO_4$ (stolzite), $PbWO_4$ (wulfenite), $PrAsO_4$, $RbIO_4$, $RbOsO_4$, $RbReO_4$, $RbRuO_4$, $RbTcO_4$, $SmAsO_4$, $SmVO_4$, $SrCrO_4$, $SrMoO_4$, $SrWO_4$, $SrZnCl_4$, $SrZnF_4$, $TbCrO_4$, $ThGeO_4$, $TlIO_4$, $TlReO_4$, $TlTlO_4$, $TmVO_4$, $YAsO_4$, $YCrO_4$, $YliF_4$, $YMoO_4$, $YNbO_4$, $YTaO_4$, YVO_4, $YbMoO_4$, $YbPO_4$, $ZrGeO_4$, $ZrSiO_4$

- (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

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_6}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16f)	O I
$\mathbf{B_7}$	=	$\left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (y_3 - z_3)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16f)	O I
$\mathbf{B_8}$	=	$\left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$\left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_3 - z_3)\,\mathbf{a}_2 + \left(x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16f)	O I
$\mathbf{B_{11}}$	=	$-\left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16f)	O I

$\mathbf{B_{12}}$ = $\left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 - y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ = $-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$ (16f) O I

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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

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First cited in

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