Th_3P_4 ($D7_3$) Structure: A4B3_cI28_220_c_a-001

This structure originally had the label `A4B3_cI28_220_c_a`. Calls to that address will be redirected here.

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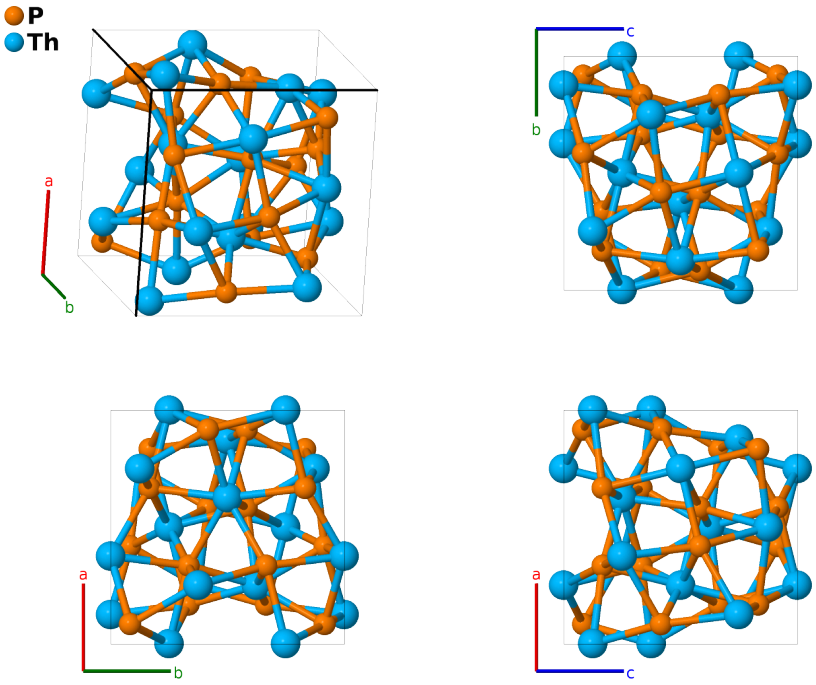
https://aflow.org/p/JM9C

https://aflow.org/p/A4B3_cI28_220_c_a-001



Prototype	P_4Th_3
AFLOW prototype label	A4B3_cI28_220_c_a-001
***Strukturbericht* designation**	$D7_3$
ICSD	648207
Pearson symbol	cI28
Space group number	220
Space group symbol	$I\bar{4}3d$
AFLOW prototype command	`aflow --proto=A4B3_cI28_220_c_a-001 --params=`a, x_2

Other compounds with this structure

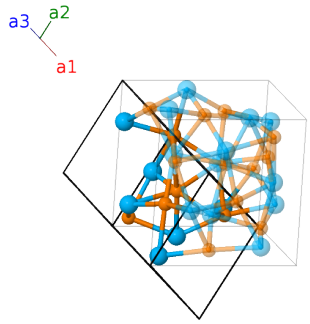
Bi_3Yb_4, Ce_3S_4, Ce_3Se_4, Ce_3Te_4, Eu_3S_4, La_3S_4, La_3Se_4, La_3Te_4, N_3P_4, Nd_3S_4, Nd_3Se_4, Nd_3Te_4, Pa_3As_4, Pa_3P_4, Pa_3Sb_4, Pr_3S_4, Pr_3Se_4, Pr_3Te_4, Sm_3S_4, Sm_3Se_4, Sm_3Te_4, Th_3As_4, Th_3As_4, Th_3Bi_4, Th_3P_4, Th_3Sb_4, U_3As_4, U_3Bi_4, U_3P_4, U_3Sb_4, U_3Te_4, $BaCe_2S_4$, $BaCe_2Se_4$, $BaLa_2S_4$, $BaLa_2Se_4$, $BaNd_2S_4$, $BaNd_2Se_4$, $BaPr_2S_4$, $BaPr_2Se_4$, $CaCe_2S_4$, $CaDy_2S_4$, $CaGd_2S_4$, $CaLa_2S_4$, $CaNd_2S_4$, $CaPr_2S_4$, $CaSm_2S_4$, $CaTb_2S_4$, $SrCe_2S_4$, $SrCe_2Se_4$, $SrGd_2S_4$, $SrGd_2Se_4$, $SrLa_2S_4$, $SrLa_2Se_4$, $SrNd_2S_4$, $SrNd_2Se_4$,

$SrPr_2S_4$, $SrPr_2Se_4$, $SrSm_2S_4$, $SrSm_2Se_4$, Ac_2S_3, Am_2S_3, Ce_2S_3, Ce_2Te_3, Gd_2S_3, La_2S_3, La_2Te_3, Nd_2S_3, Nd_2Te_3, Pr_2S_3, Pr_2Te_3, Sm_2S_3, Sm_2Te_3, Tb_2S_3

- The Th_3P_4 structure allows a large degree of disorder in the thorium (12a) site. Compounds of the form AB_2C_4 have the A and B atoms mixed on the (12a) site (Flahaut, 1965). Compounds of the form A_2B_3 should more properly be listed as $A_{3-x}B_4$, with x in the range [0,1/3] and a corresponding number of vacancies distributed statistically on the (12a) site (Zachariasen, 1949).

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12a)	Th I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(12a)	Th I
$\mathbf{B_3}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}}$	(12a)	Th I
$\mathbf{B_4}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}}$	(12a)	Th I
$\mathbf{B_5}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12a)	Th I
$\mathbf{B_6}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12a)	Th I
$\mathbf{B_7}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16c)	P I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16c)	P I
$\mathbf{B_9}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16c)	P I
$\mathbf{B_{10}}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16c)	P I
$\mathbf{B_{11}}$	=	$\left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	P I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_3$	=	$-a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	P I
$\mathbf{B_{13}}$	=	$-2x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	P I
$\mathbf{B_{14}}$	=	$-2x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	P I

References

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