$Sr_4Ti_3O_{10}$ Structure: A10B4C3_tI34_139_c2eg_2e_ae-001

This structure originally had the label `A10B4C3_tI34_139_c2eg_2e_ae`. Calls to that address will be redirected here.

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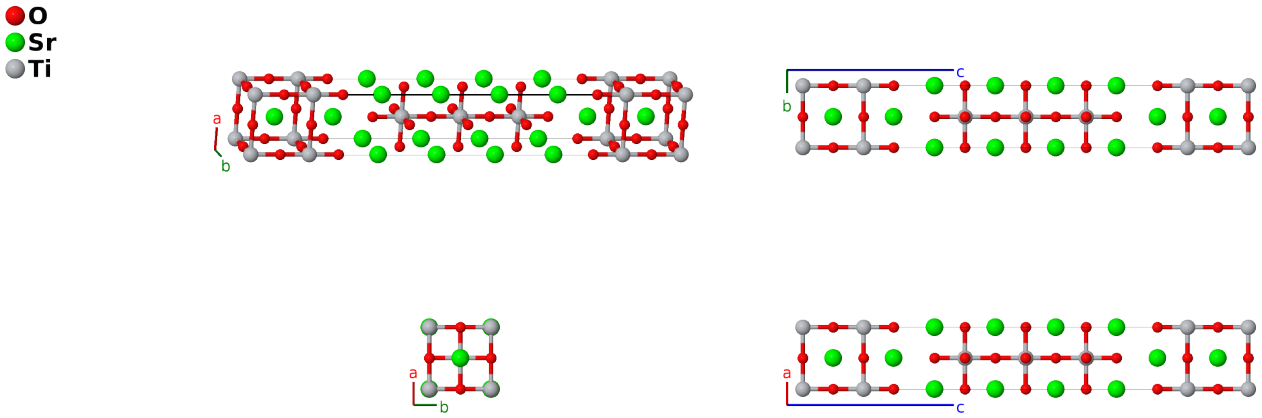
https://aflow.org/p/TJ17

https://aflow.org/p/A10B4C3_tI34_139_c2eg_2e_ae-001



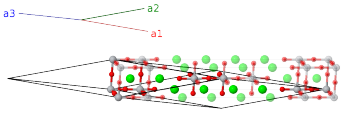
Prototype	$O_{10}Sr_4Ti_3$
AFLOW prototype label	A10B4C3_tI34_139_c2eg_2e_ae-001
ICSD	34630
Pearson symbol	tI34
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A10B4C3_tI34_139_c2eg_2e_ae-001 --params=`$a, c/a, z_3, z_4, z_5, z_6, z_7, z_8$

Other compounds with this structure

$La_4Ni_3O_{10}$, $Sr_4V_3O_{10}$, $K_2La_2Ti_3O_{10}$, $Li_2Eu_2Ti_3O_{10}$, $Na_2Eu_2Ti_3O_{10}$, $Na_2Sr_2Nb_2MnO_{10}$

Body-centered Tetragonal primitive vectors

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



Basis vectors

Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type

$\mathbf{B_1}$	=	0	=	0	(2a)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$	=	$cz_5\,\hat{\mathbf{z}}$	(4e)	Sr I
$\mathbf{B_9}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$	=	$-cz_5\,\hat{\mathbf{z}}$	(4e)	Sr I
$\mathbf{B_{10}}$	=	$z_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2$	=	$cz_6\,\hat{\mathbf{z}}$	(4e)	Sr II
$\mathbf{B_{11}}$	=	$-z_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2$	=	$-cz_6\,\hat{\mathbf{z}}$	(4e)	Sr II
$\mathbf{B_{12}}$	=	$z_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2$	=	$cz_7\,\hat{\mathbf{z}}$	(4e)	Ti II
$\mathbf{B_{13}}$	=	$-z_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2$	=	$-cz_7\,\hat{\mathbf{z}}$	(4e)	Ti II
$\mathbf{B_{14}}$	=	$\left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8g)	O IV
$\mathbf{B_{15}}$	=	$z_8\,\mathbf{a}_1 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(8g)	O IV
$\mathbf{B_{16}}$	=	$-\left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8g)	O IV
$\mathbf{B_{17}}$	=	$-z_8\,\mathbf{a}_1 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(8g)	O IV

References

[1] S. N. Ruddlesden and P. Popper, *The compound $Sr_3Ti_2O_7$ and its structure*, Acta Cryst. **11**, 54–55 (1958), doi:10.1107/S0365110X58000128.

Found in

[1] Wikipedia, *Ruddlesden-Popper phase*. $A_3B_2X_7$ series.