

Sr₄Ti₃O₁₀ Structure:

A10B4C3_tI34_139_c2eg_2e_ae-001

This structure previously used the label(s) **A10B4C3_tI34_139_c2eg_2e_ae**. Calls to these addresses will be redirected here.

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<https://afLOW.org/prototype-encyclopedia/TJ17>

https://afLOW.org/prototype-encyclopedia/A10B4C3_tI34_139_c2eg_2e_ae-001

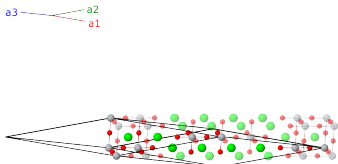
Prototype	O ₁₀ Sr ₄ Ti ₃
AFLOW prototype label	A10B4C3_tI34_139_c2eg_2e_ae-001
ICSD	34630
CCDC	1607010
Pearson symbol	tI34
Space group number	139
Space group symbol	<i>I</i> 4/ <i>mmm</i>
AFLOW prototype command	<code>afLOW --proto=A10B4C3_tI34_139_c2eg_2e_ae-001</code> <code>--params=a,c/a,z₃,z₄,z₅,z₆,z₇,z₈</code>

Other compounds with this structure

La₄Ni₃O₁₀, Sr₄V₃O₁₀, K₂La₂Ti₃O₁₀, Li₂Eu₂Ti₃O₁₀, Na₂Eu₂Ti₃O₁₀, Na₂Sr₂Nb₂MnO₁₀

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
B₁	=	0	=	0	(2a) Ti I
B₂	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}}$	(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 $\text{Sr}_3\text{Ti}_2\text{O}_7$ and its structure*, Acta Cryst. **11**, 54–55 (1958), doi:10.1107/S0365110X58000128.

Found in

- [1] Wikipedia, *Ruddlesden-Popper phase*. $\text{A}_3\text{B}_2\text{X}_7$ series.

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O
Sr
Ti

