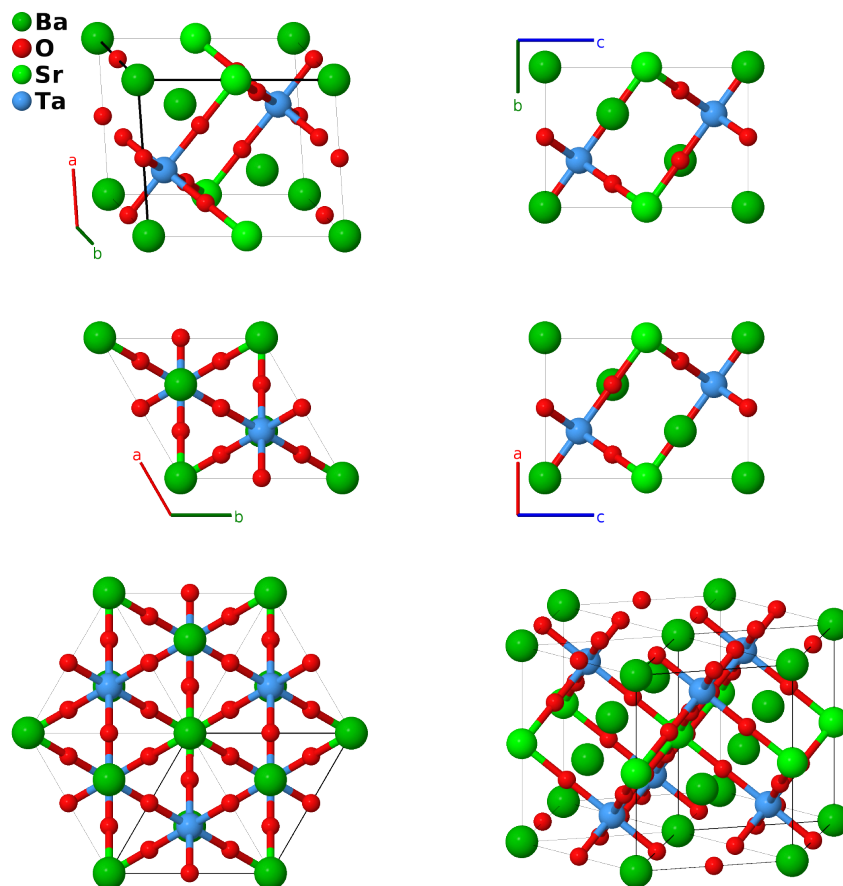


# Ba<sub>3</sub>SrTa<sub>2</sub>O<sub>9</sub> Structure: A3B9CD2\_hP15\_164\_ad\_ei\_b\_d-001

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<https://aflow.org/p/4LGS>

[https://aflow.org/p/A3B9CD2\\_hP15\\_164\\_ad\\_ei\\_b\\_d-001](https://aflow.org/p/A3B9CD2_hP15_164_ad_ei_b_d-001)



Prototype	Ba <sub>3</sub> O <sub>9</sub> SrTa <sub>2</sub>
AFLOW prototype label	A3B9CD2_hP15_164_ad_ei_b_d-001
ICSD	27496
Pearson symbol	hP15
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	<code>aflow --proto=A3B9CD2_hP15_164_ad_ei_b_d-001 --params=a, c/a, z<sub>3</sub>, z<sub>4</sub>, x<sub>6</sub>, z<sub>6</sub></code>

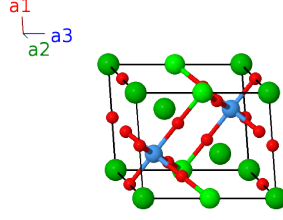
**Other compounds with this structure**  
Ba<sub>3</sub>CoNb<sub>2</sub>O<sub>9</sub>

- Despite its hexagonal unit cell, this is closely related to cubic perovskite,  $E2_1$ , as can be seen by looking at the nearly perfect cubes formed by the strontium and tantalum atoms.

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### Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$0$	$=$	$0$	(1a)	Ba I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Sr I
$\mathbf{B}_3$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2d)	Ba II
$\mathbf{B}_4$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2d)	Ba II
$\mathbf{B}_5$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2d)	Ta I
$\mathbf{B}_6$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2d)	Ta I
$\mathbf{B}_7$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3e)	O I
$\mathbf{B}_8$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3e)	O I
$\mathbf{B}_9$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(3e)	O I
$\mathbf{B}_{10}$	$x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B}_{12}$	$-2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B}_{13}$	$-x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\sqrt{3}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B}_{14}$	$2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B}_{15}$	$-x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(6i)	O II

### References

- [1] F. Galasso, J. R. Barrante, and L. Katz, *Alkaline Earth-Tantalum-Oxygen Phases Including the Crystal Structure of an Ordered Perovskite Compound,  $Ba_3SrTa_2O_9$* , J. Am. Chem. Soc. **83**, 2830–2832 (1961), doi:10.1021/ja01474a010.

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