SrCoO:
ABC_hP6_194_a_b_c-001

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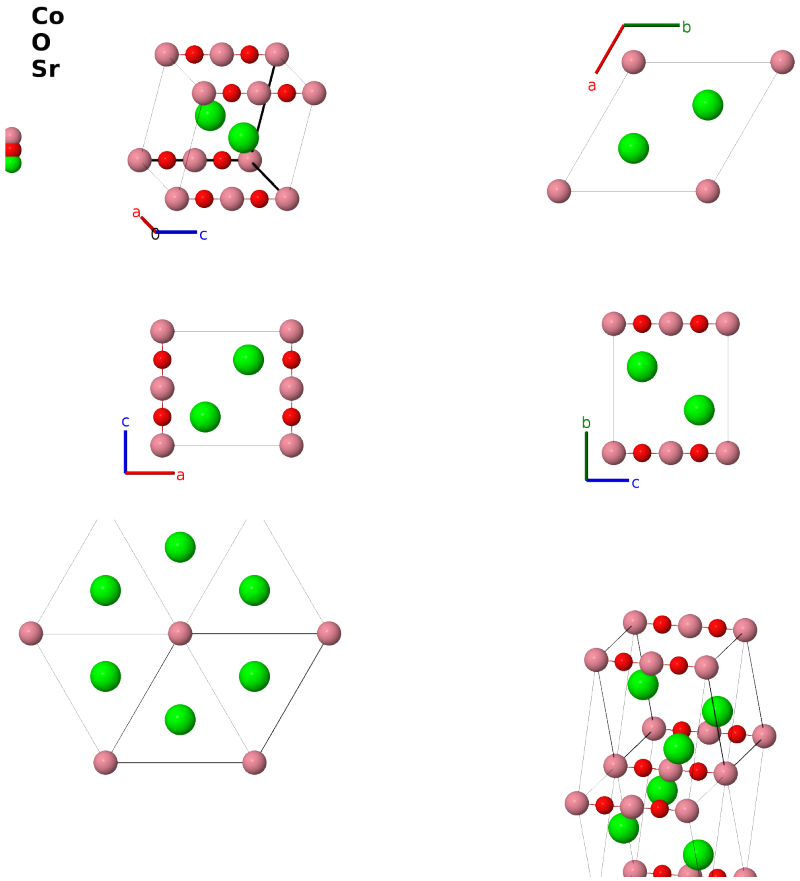
https://aflow.org/prototype-encyclopedia/047D

https://aflow.org/prototype-encyclopedia/ABC_hP6_194_a_b_c-001

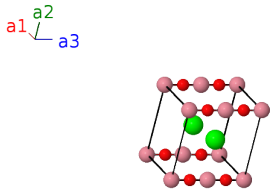


Prototype	CoOSr
AFLOW prototype label	ABC_hP6_194_a_b_c-001
ICSD	78731
CCDC	1639002
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=ABC_hP6_194_a_b_c-001 --params=`$a, c/a$

- We found this in the ICSD while looking for compounds in the LiBC structure. This is the only ICSD report of a compound occupying the first three Wyckoff positions of space group $P6_3/mmc$ #194.
- (Gaoke, 2006) refer to this as $SrCoO_x$, but the reported structure is stochiometric SrCoO. The Co-O distance is only 1.05Å, so this structure may not be entirely correct.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Co I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Sr I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Sr I

References

[1] Z. Gaoke, L. Ying, Y. Xia, W. Yanping, O. Shixi, and L. Hangxing, *Comparison of synthesis methods, crystal structure and characterization of strontium cobaltite powders*, Mater. Chem. Phys. **99**, 88–95 (2006), doi:10.1016/j.matchemphys.2005.09.078.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 78731 [CoOS].

First cited in

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