

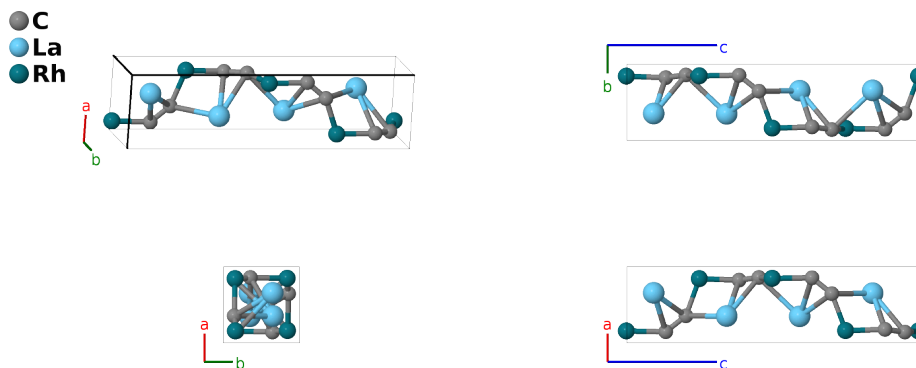
# LaRhC<sub>2</sub> Structure: A2BC\_tP16\_76\_2a\_a\_a-001

This structure originally had the label A2BC\_tP16\_76\_2a\_a\_a. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/5CQR>

[https://aflow.org/p/A2BC\\_tP16\\_76\\_2a\\_a\\_a-001](https://aflow.org/p/A2BC_tP16_76_2a_a_a-001)



Prototype	C <sub>2</sub> LaRh
AFLOW prototype label	A2BC_tP16_76_2a_a_a-001
ICSD	100986
Pearson symbol	tP16
Space group number	76
Space group symbol	<i>P</i> 4 <sub>1</sub>
AFLOW prototype command	<code>aflow --proto=A2BC_tP16_76_2a_a_a-001 --params=a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></code>

## Other compounds with this structure

CeRhC<sub>2</sub>

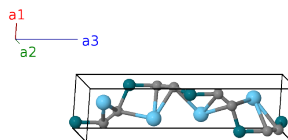
- This structure may also be found in the enantiomorphic space group *P*4<sub>3</sub> #78.

## Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors

	Lattice coordinates	=	Cartesian coordinates	=	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	=	(4a)	C I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	=	(4a)	C I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + (z_1 + \frac{1}{4}) \mathbf{a}_3$	=	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	=	(4a)	C I
$\mathbf{B}_4$	$= y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{3}{4}) \mathbf{a}_3$	=	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{3}{4}) \hat{\mathbf{z}}$	=	(4a)	C I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	=	(4a)	C II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	=	(4a)	C II
$\mathbf{B}_7$	$= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{1}{4}) \mathbf{a}_3$	=	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	=	(4a)	C II
$\mathbf{B}_8$	$= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{3}{4}) \mathbf{a}_3$	=	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{3}{4}) \hat{\mathbf{z}}$	=	(4a)	C II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	=	(4a)	La I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	=	(4a)	La I
$\mathbf{B}_{11}$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{4}) \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	=	(4a)	La I
$\mathbf{B}_{12}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{3}{4}) \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{3}{4}) \hat{\mathbf{z}}$	=	(4a)	La I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	=	(4a)	Rh I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	=	(4a)	Rh I
$\mathbf{B}_{15}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{4}) \mathbf{a}_3$	=	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	=	(4a)	Rh I
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{3}{4}) \mathbf{a}_3$	=	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{3}{4}) \hat{\mathbf{z}}$	=	(4a)	Rh I

## References

- [1] A. O. Tsokol, O. I. Bodak, E. P. Marusin, and V. E. Zavodnik, *X-ray diffraction studies of ternary  $RRhC_2$  ( $R = La, Ce, Pr, Nd, Sm$ ) compounds*, Sov. Phys. Crystallogr. **33**, 202–203 (1988). Translated from Kristallografiya.

## Found in

- [1] P. Villars, *LaRhC<sub>2</sub> Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.