

LaRhC₂ Structure: A2BC_tP16_76_2a_a_a-001

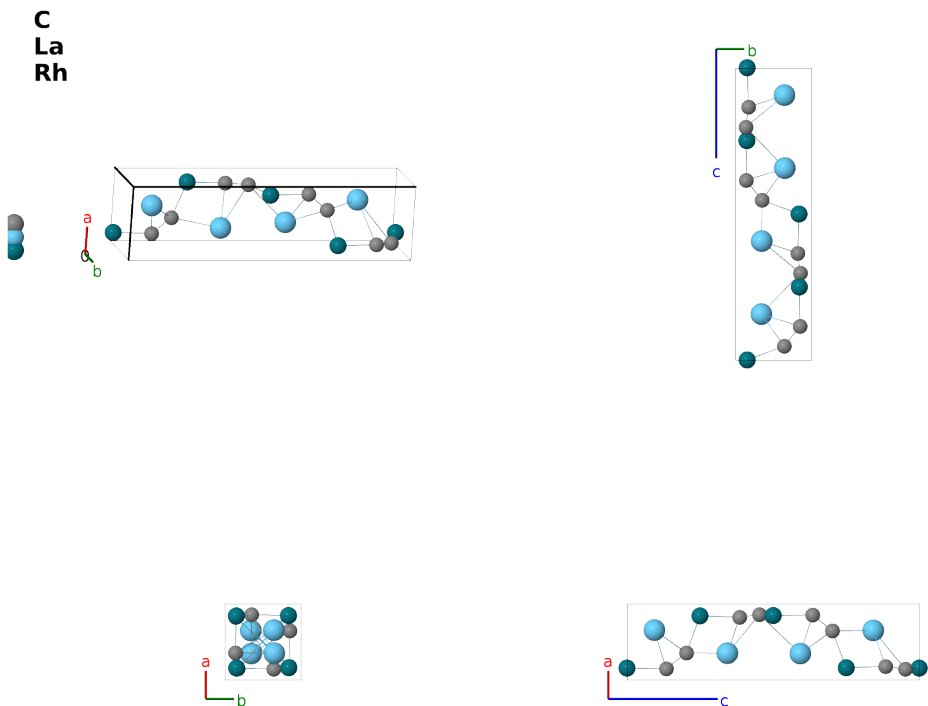
This structure previously used the label(s) **A2BC_tP16_76_2a_a_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/5CQR>

https://aflow.org/prototype-encyclopedia/A2BC_tP16_76_2a_a_a-001



Prototype	C ₂ LaRh
AFLOW prototype label	A2BC_tP16_76_2a_a_a-001
ICSD	100986
CCDC	1626217
Pearson symbol	tP16
Space group number	76
Space group symbol	<i>P</i> 4 ₁

AFLOW prototype command `aflow --proto=A2BC_tP16_76_2a_a_a-001`
 `--params=a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4`

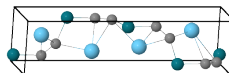
Other compounds with this structure

CeRhC₂

- This structure may also be found in the enantiomorphic space group $P4_3$ #78.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	C I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	C I
$\mathbf{B}_4$	$= y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(z_1 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	C II
$\mathbf{B}_7$	$= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	C II
$\mathbf{B}_8$	$= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	La I
$\mathbf{B}_{11}$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	La I
$\mathbf{B}_{12}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Rh I
$\mathbf{B}_{15}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(4a)	Rh I
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(z_4 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(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, *LaRhC₂ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

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