Hexagonal Hollandite ($BaRu_4Cr_2O_{12}$) Structure: AB2C12D4_tP76_75_2a2b_2d_12d_4d-001

This structure originally had the label `AB2C12D4_tP76_75_2a2b_2d_12d_4d`. Calls to that address will be redirected here.

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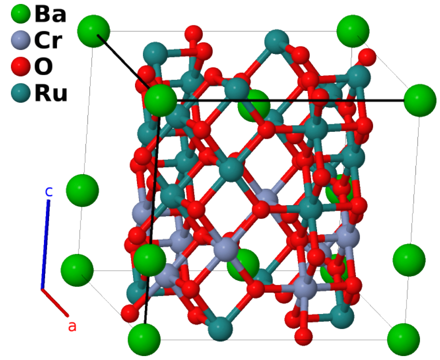
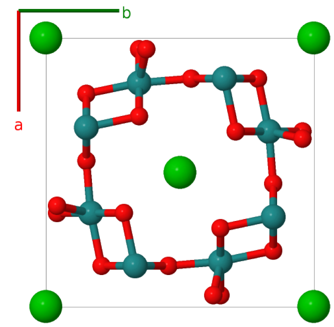
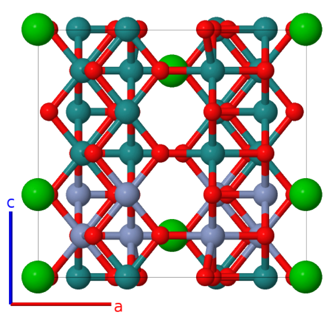
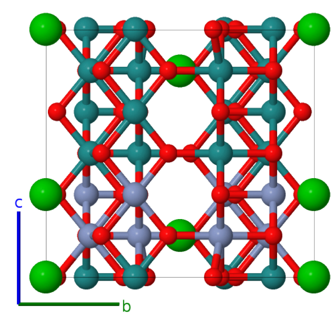
https://aflow.org/p/MXLF

https://aflow.org/p/AB2C12D4_tP76_75_2a2b_2d_12d_4d-001









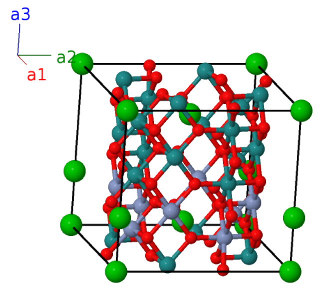
Prototype	$BaCr_2O_{12}Ru_4$
AFLOW prototype label	AB2C12D4_tP76_75_2a2b_2d_12d_4d-001
Mineral name	hollandite
ICSD	100578
Pearson symbol	tP76
Space group number	75
Space group symbol	$P4$
AFLOW prototype command	`aflow --proto=AB2C12D4_tP76_75_2a2b_2d_12d_4d-001` `--params=`$a, c/a, z_1, z_2, z_3, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}$

- This is a superstructure of conventional hollandite.

- (Cadé, 1979) and the ICSD entry omit the coordinates for the O-VI atom. We have used the values provided by (Villars, 2016).
- Space group $P4$ #74 allows for an arbitrary origin of the z-axis. We follow (Villars, 2016) and set $z_1 = 0$ for the Ba-I atom. This is a shift of $c/2$ from the origin used by (Cadé, 1979).

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Ba I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(1a)	Ba II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(1b)	Ba III
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(1b)	Ba IV
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B_6}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B_7}$	=	$-y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B_8}$	=	$y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	Cr I
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B_{11}}$	=	$-y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B_{12}}$	=	$y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4d)	Cr II
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B_{15}}$	=	$-y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B_{16}}$	=	$y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B_{17}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_{18}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_{19}}$	=	$-y_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_{20}}$	=	$y_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_{21}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_{22}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_{23}}$	=	$-y_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-ay_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_{24}}$	=	$y_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ay_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_{25}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	O IV

$\mathbf{B_{26}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_{27}}$	=	$-y_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ay_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_{28}}$	=	$y_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ay_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	O IV
$\mathbf{B_{29}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_{30}}$	=	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} - ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_{31}}$	=	$-y_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-ay_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_{32}}$	=	$y_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$ay_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4d)	O V
$\mathbf{B_{33}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}} + ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B_{34}}$	=	$-x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}} - ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B_{35}}$	=	$-y_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$-ay_{12}\,\hat{\mathbf{x}} + ax_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B_{36}}$	=	$y_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$ay_{12}\,\hat{\mathbf{x}} - ax_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4d)	O VI
$\mathbf{B_{37}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}} + ay_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4d)	O VII
$\mathbf{B_{38}}$	=	$-x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} - ay_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4d)	O VII
$\mathbf{B_{39}}$	=	$-y_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$-ay_{13}\,\hat{\mathbf{x}} + ax_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4d)	O VII
$\mathbf{B_{40}}$	=	$y_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$ay_{13}\,\hat{\mathbf{x}} - ax_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4d)	O VII
$\mathbf{B_{41}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}} + ay_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$	(4d)	O VIII
$\mathbf{B_{42}}$	=	$-x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}} - ay_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$	(4d)	O VIII
$\mathbf{B_{43}}$	=	$-y_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$-ay_{14}\,\hat{\mathbf{x}} + ax_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$	(4d)	O VIII
$\mathbf{B_{44}}$	=	$y_{14}\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$ay_{14}\,\hat{\mathbf{x}} - ax_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$	(4d)	O VIII
$\mathbf{B_{45}}$	=	$x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$ax_{15}\,\hat{\mathbf{x}} + ay_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(4d)	O IX
$\mathbf{B_{46}}$	=	$-x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$-ax_{15}\,\hat{\mathbf{x}} - ay_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(4d)	O IX
$\mathbf{B_{47}}$	=	$-y_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$-ay_{15}\,\hat{\mathbf{x}} + ax_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(4d)	O IX
$\mathbf{B_{48}}$	=	$y_{15}\,\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$ay_{15}\,\hat{\mathbf{x}} - ax_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(4d)	O IX
$\mathbf{B_{49}}$	=	$x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$ax_{16}\,\hat{\mathbf{x}} + ay_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}}$	(4d)	O X
$\mathbf{B_{50}}$	=	$-x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$-ax_{16}\,\hat{\mathbf{x}} - ay_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}}$	(4d)	O X
$\mathbf{B_{51}}$	=	$-y_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$-ay_{16}\,\hat{\mathbf{x}} + ax_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}}$	(4d)	O X
$\mathbf{B_{52}}$	=	$y_{16}\,\mathbf{a}_1 - x_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$ay_{16}\,\hat{\mathbf{x}} - ax_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}}$	(4d)	O X
$\mathbf{B_{53}}$	=	$x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$ax_{17}\,\hat{\mathbf{x}} + ay_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}}$	(4d)	O XI
$\mathbf{B_{54}}$	=	$-x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$-ax_{17}\,\hat{\mathbf{x}} - ay_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}}$	(4d)	O XI
$\mathbf{B_{55}}$	=	$-y_{17}\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$-ay_{17}\,\hat{\mathbf{x}} + ax_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}}$	(4d)	O XI
$\mathbf{B_{56}}$	=	$y_{17}\,\mathbf{a}_1 - x_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$ay_{17}\,\hat{\mathbf{x}} - ax_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}}$	(4d)	O XI
$\mathbf{B_{57}}$	=	$x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$ax_{18}\,\hat{\mathbf{x}} + ay_{18}\,\hat{\mathbf{y}} + cz_{18}\,\hat{\mathbf{z}}$	(4d)	O XII
$\mathbf{B_{58}}$	=	$-x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$-ax_{18}\,\hat{\mathbf{x}} - ay_{18}\,\hat{\mathbf{y}} + cz_{18}\,\hat{\mathbf{z}}$	(4d)	O XII
$\mathbf{B_{59}}$	=	$-y_{18}\,\mathbf{a}_1 + x_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$-ay_{18}\,\hat{\mathbf{x}} + ax_{18}\,\hat{\mathbf{y}} + cz_{18}\,\hat{\mathbf{z}}$	(4d)	O XII
$\mathbf{B_{60}}$	=	$y_{18}\,\mathbf{a}_1 - x_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$ay_{18}\,\hat{\mathbf{x}} - ax_{18}\,\hat{\mathbf{y}} + cz_{18}\,\hat{\mathbf{z}}$	(4d)	O XII
$\mathbf{B_{61}}$	=	$x_{19}\,\mathbf{a}_1 + y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	=	$ax_{19}\,\hat{\mathbf{x}} + ay_{19}\,\hat{\mathbf{y}} + cz_{19}\,\hat{\mathbf{z}}$	(4d)	Ru I
$\mathbf{B_{62}}$	=	$-x_{19}\,\mathbf{a}_1 - y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	=	$-ax_{19}\,\hat{\mathbf{x}} - ay_{19}\,\hat{\mathbf{y}} + cz_{19}\,\hat{\mathbf{z}}$	(4d)	Ru I
$\mathbf{B_{63}}$	=	$-y_{19}\,\mathbf{a}_1 + x_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	=	$-ay_{19}\,\hat{\mathbf{x}} + ax_{19}\,\hat{\mathbf{y}} + cz_{19}\,\hat{\mathbf{z}}$	(4d)	Ru I
$\mathbf{B_{64}}$	=	$y_{19}\,\mathbf{a}_1 - x_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	=	$ay_{19}\,\hat{\mathbf{x}} - ax_{19}\,\hat{\mathbf{y}} + cz_{19}\,\hat{\mathbf{z}}$	(4d)	Ru I
$\mathbf{B_{65}}$	=	$x_{20}\,\mathbf{a}_1 + y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	=	$ax_{20}\,\hat{\mathbf{x}} + ay_{20}\,\hat{\mathbf{y}} + cz_{20}\,\hat{\mathbf{z}}$	(4d)	Ru II
$\mathbf{B_{66}}$	=	$-x_{20}\,\mathbf{a}_1 - y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	=	$-ax_{20}\,\hat{\mathbf{x}} - ay_{20}\,\hat{\mathbf{y}} + cz_{20}\,\hat{\mathbf{z}}$	(4d)	Ru II

$\mathbf{B_{67}}$	=	$-y_{20}\,\mathbf{a}_1 + x_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	=	$-ay_{20}\,\hat{\mathbf{x}} + ax_{20}\,\hat{\mathbf{y}} + cz_{20}\,\hat{\mathbf{z}}$	(4d)	Ru II
$\mathbf{B_{68}}$	=	$y_{20}\,\mathbf{a}_1 - x_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	=	$ay_{20}\,\hat{\mathbf{x}} - ax_{20}\,\hat{\mathbf{y}} + cz_{20}\,\hat{\mathbf{z}}$	(4d)	Ru II
$\mathbf{B_{69}}$	=	$x_{21}\,\mathbf{a}_1 + y_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	=	$ax_{21}\,\hat{\mathbf{x}} + ay_{21}\,\hat{\mathbf{y}} + cz_{21}\,\hat{\mathbf{z}}$	(4d)	Ru III
$\mathbf{B_{70}}$	=	$-x_{21}\,\mathbf{a}_1 - y_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	=	$-ax_{21}\,\hat{\mathbf{x}} - ay_{21}\,\hat{\mathbf{y}} + cz_{21}\,\hat{\mathbf{z}}$	(4d)	Ru III
$\mathbf{B_{71}}$	=	$-y_{21}\,\mathbf{a}_1 + x_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	=	$-ay_{21}\,\hat{\mathbf{x}} + ax_{21}\,\hat{\mathbf{y}} + cz_{21}\,\hat{\mathbf{z}}$	(4d)	Ru III
$\mathbf{B_{72}}$	=	$y_{21}\,\mathbf{a}_1 - x_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	=	$ay_{21}\,\hat{\mathbf{x}} - ax_{21}\,\hat{\mathbf{y}} + cz_{21}\,\hat{\mathbf{z}}$	(4d)	Ru III
$\mathbf{B_{73}}$	=	$x_{22}\,\mathbf{a}_1 + y_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	=	$ax_{22}\,\hat{\mathbf{x}} + ay_{22}\,\hat{\mathbf{y}} + cz_{22}\,\hat{\mathbf{z}}$	(4d)	Ru IV
$\mathbf{B_{74}}$	=	$-x_{22}\,\mathbf{a}_1 - y_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	=	$-ax_{22}\,\hat{\mathbf{x}} - ay_{22}\,\hat{\mathbf{y}} + cz_{22}\,\hat{\mathbf{z}}$	(4d)	Ru IV
$\mathbf{B_{75}}$	=	$-y_{22}\,\mathbf{a}_1 + x_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	=	$-ay_{22}\,\hat{\mathbf{x}} + ax_{22}\,\hat{\mathbf{y}} + cz_{22}\,\hat{\mathbf{z}}$	(4d)	Ru IV
$\mathbf{B_{76}}$	=	$y_{22}\,\mathbf{a}_1 - x_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	=	$ay_{22}\,\hat{\mathbf{x}} - ax_{22}\,\hat{\mathbf{y}} + cz_{22}\,\hat{\mathbf{z}}$	(4d)	Ru IV

References

[1] M. C. Cadée and A. Proden, *Tripling of the short axis in the hollandite structure*, Mater. Res. Bull. **14**, 613–618 (1979), doi:10.1016/0025-5408(79)90043-6.

Found in

[1] P. Villars, *Ba0.65Ru2.7Cr1.3O8 (BaCr2Ru4O12) Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.