

KW₃Br₇ Structure:

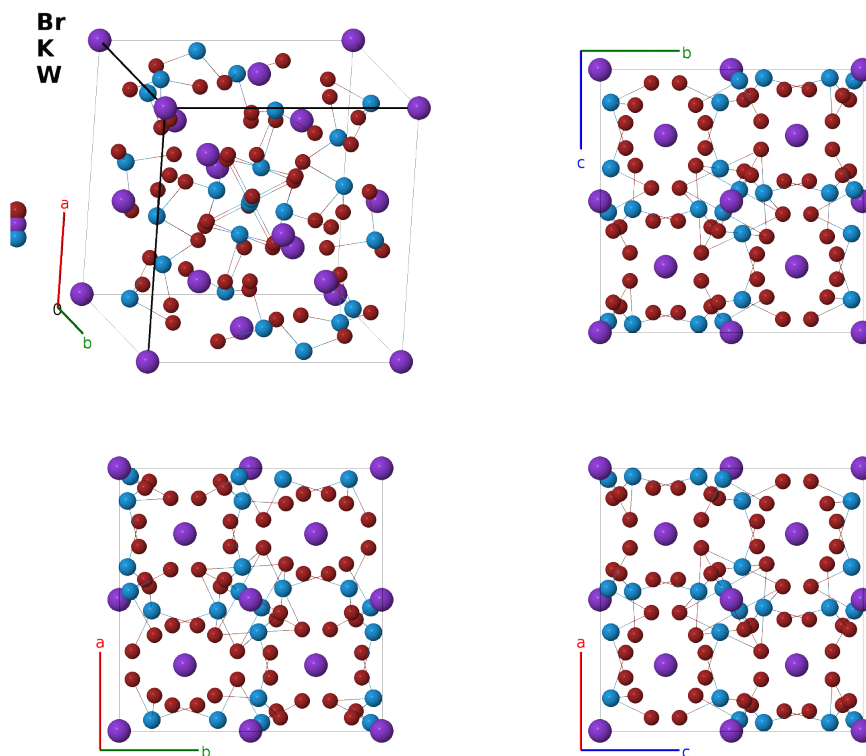
A28B5C12_cP90_201_e2h_bd_h-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/RMGB>

https://aflow.org/prototype-encyclopedia/A28B5C12_cP90_201_e2h_bd_h-001



Prototype	Br ₇ KW ₃
AFLOW prototype label	A28B5C12_cP90_201_e2h_bd_h-001
ICSD	390027
CCDC	1724187
Pearson symbol	cP90
Space group number	201
Space group symbol	$Pn\bar{3}$
AFLOW prototype command	<pre>aflow --proto=A28B5C12_cP90_201_e2h_bd_h-001 --params=a, x₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆</pre>

Other compounds with this structure

KMo₃Br₇, TlW₃Br₇

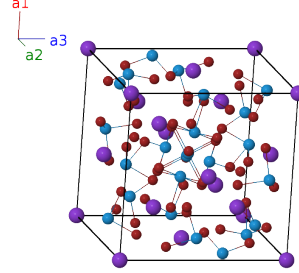
- Only two-thirds of the K-II (6d) sites are occupied.

Simple Cubic primitive vectors

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(4b)	K I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4b)	K I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b)	K I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	K II
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	K II
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	K II
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	K II
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	K II
$\mathbf{B}_{10}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	K II
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + a x_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{12}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a x_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{13}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{14}$	$= x_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - a x_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{16}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a x_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{17}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{18}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}} + a z_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{20}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a z_4 \hat{\mathbf{z}}$	(24h)	Br II

$\mathbf{B}_{21} =$	$-\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 -$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
	$\left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{22} =$	$x_4 \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{23} =$	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{24} =$	$z_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{25} =$	$-\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(24h)	Br II
	$y_4 \mathbf{a}_3$				
$\mathbf{B}_{26} =$	$-\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 -$	$=$	$-a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
	$\left(y_4 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{27} =$	$y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{28} =$	$-\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 -$	$=$	$-a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
	$\left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{29} =$	$y_4 \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{30} =$	$-\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(24h)	Br II
	$x_4 \mathbf{a}_3$				
$\mathbf{B}_{31} =$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{32} =$	$\left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{33} =$	$\left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{34} =$	$-x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-ax_4 \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
	$\left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{35} =$	$-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{36} =$	$-z_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-az_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
	$\left(y_4 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{37} =$	$\left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{38} =$	$\left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{39} =$	$-y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{40} =$	$\left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{41} =$	$-y_4 \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-ay_4 \hat{\mathbf{x}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
	$\left(x_4 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{42} =$	$\left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{43} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + az_5 \$		

$\mathbf{B}_{52} =$	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 + z_5 \mathbf{a}_2 -$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
	$(x_5 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{53} =$	$y_5 \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{54} =$	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(24h)	Br III
	$x_5 \mathbf{a}_3$				
$\mathbf{B}_{55} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{56} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{57} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{58} =$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
	$(z_5 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{59} =$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{60} =$	$-z_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-az_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
	$(y_5 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{61} =$	$(z_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$a(z_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{62} =$	$(z_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (y_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(z_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{63} =$	$-y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{64} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 - z_5 \mathbf{a}_2 + (x_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{65} =$	$-y_5 \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-ay_5 \hat{\mathbf{x}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Br III
	$(x_5 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{66} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(24h)	Br III
$\mathbf{B}_{67} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{68} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(24h)	W I
	$z_6 \mathbf{a}_3$				
$\mathbf{B}_{69} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 -$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
	$(z_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{70} =$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{71} =$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{72} =$	$z_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (y_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{73} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(z_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(24h)	W I
	$y_6 \mathbf{a}_3$				
$\mathbf{B}_{74} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 -$	$=$	$-a(z_6 - \frac{1}{2}) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
	$(y_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{75} =$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{76} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + z_6 \mathbf{a}_2 -$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
	$(x_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{77} =$	$y_6 \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{78} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(24h)	W I
	$x_6 \mathbf{a}_3$				
$\mathbf{B}_{79} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{80} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{81} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
$\mathbf{B}_{82} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	W I
	$(z_6 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{83} =$	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(24h)	W I

$$\begin{aligned}
\mathbf{B}_{84} &= -z_6 \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 = -az_6 \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24h) & \text{W I} \\
\mathbf{B}_{85} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 - y_6 \mathbf{a}_3 = a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (24h) & \text{W I} \\
\mathbf{B}_{86} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 = a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24h) & \text{W I} \\
\mathbf{B}_{87} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 = -ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (24h) & \text{W I} \\
\mathbf{B}_{88} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 - z_6 \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 = a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24h) & \text{W I} \\
\mathbf{B}_{89} &= -y_6 \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 = -ay_6 \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24h) & \text{W I} \\
\mathbf{B}_{90} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 - x_6 \mathbf{a}_3 = a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (24h) & \text{W I}
\end{aligned}$$

References

- [1] Y.-Q. Zheng, K. Peters, Y. Grin, and H. G. von Schnering, *Syntheses and Crystal Structures of the Cluster Compounds* $A_2[(W_6Br_8^i)Br_6^a]$ with $A=K, Rb, Cs$, Z. Anorganische und Allgemeine Chemie **624**, 506–512 (1998), doi:10.1002/(SICI)1521-3749(199806)624:6<959::AID-ZAAC959>3.0.CO;2-U.

Found in

- [1] W. Xu, P. Wang, and Y.-Q. Zheng, *Crystal structure of dipotassium octakis(μ_3 -bromo)hexabromo-octahedro-hexamolybdenate*, $K_2[Mo_6Br_{14}]$, Z. Kristallogr. NCS **221**, 107–108 (2006).

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.