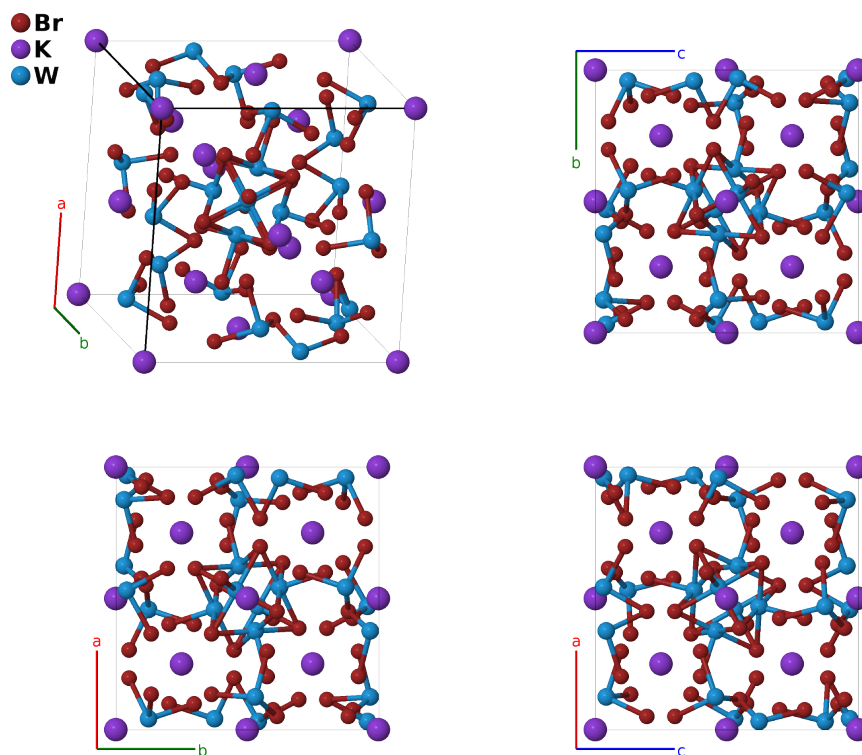


# KW<sub>3</sub>Br<sub>7</sub> Structure: A28B5C12\_cP90\_201\_e2h\_bd\_h-001

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<https://aflow.org/p/RMGB>

[https://aflow.org/p/A28B5C12\\_cP90\\_201\\_e2h\\_bd\\_h-001](https://aflow.org/p/A28B5C12_cP90_201_e2h_bd_h-001)



Prototype	Br <sub>7</sub> KW <sub>3</sub>
AFLOW prototype label	A28B5C12_cP90_201_e2h_bd_h-001
ICSD	390027
Pearson symbol	cP90
Space group number	201
Space group symbol	$Pn\bar{3}$
AFLOW prototype command	<code>aflow --proto=A28B5C12_cP90_201_e2h_bd_h-001 --params=a, x<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></code>

## Other compounds with this structure

KMo<sub>3</sub>Br<sub>7</sub>, TiW<sub>3</sub>Br<sub>7</sub>

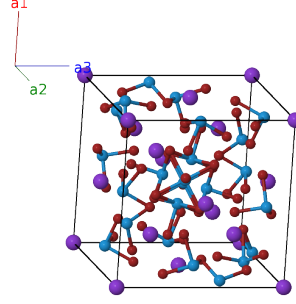
- Only two-thirds of the K-II (6d) sites are occupied.

## 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
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{12}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{13}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{14}$	$= x_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{16}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{17}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{18}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Br I
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{20}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{21}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24h)	Br II
$\mathbf{B}_{22}$	$= x_4 \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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





$$\mathbf{B}_{89} = \begin{matrix} -y_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_6 \hat{\mathbf{x}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{z}} \quad (24h) \quad \text{W I}$$

$$\mathbf{B}_{90} = (y_6 + \frac{1}{2}) \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 - x_6 \mathbf{a}_3 = a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} \quad (24h) \quad \text{W I}$$

## References

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- [1] W. Xu, P. Wang, and Y.-Q. Zheng, *Crystal structure of dipotassium octakis( $\mu_3$ -bromo)hexabromo-octahedro-hexamolybdenate,  $K_2[Mo_6Br_{14}]$* , *Z. Kristallogr. NCS* **221**, 107–108 (2006).