Rhombohedral Al_5Mo Structure: A5B_hR12_167_ce_b-001

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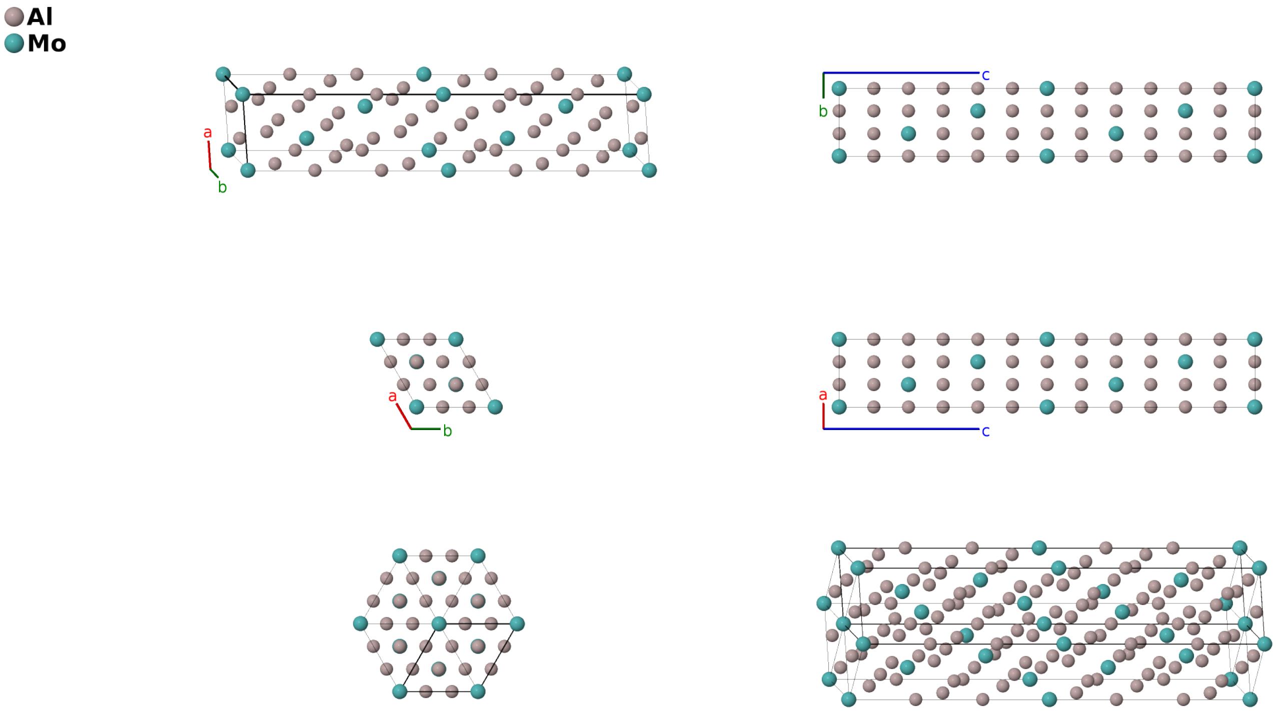
https://aflow.org/p/584Z

https://aflow.org/p/A5B_hR12_167_ce_b-001



Prototype	Al_5Mo
AFLOW prototype label	A5B_hR12_167_ce_b-001
ICSD	105520
Pearson symbol	hR12
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=A5B_hR12_167_ce_b-001` `--params=`$a, c/a, x_2, x_3$

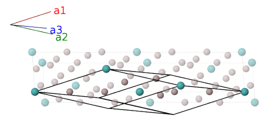
- Al_5Mo is known to have three phases (Schuster, 1991):
  - Below 650K it is in a rhombohedral structure, Al_5Mo(r) (this structure).
  - Between 650K and 750-800K it is in a trigonal structure, Al_5Mo(h').
  - Above 750-800K up to 846K it is in the Al_5W structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	Mo I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Mo I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Al II
$\mathbf{B_8}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Al II
$\mathbf{B_9}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Al II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_3 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Al II
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_3 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Al II
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Al II

References

[1] J. C. Schuster and H. Ipser, *The Al-Al$_8$Mo$_3$ section of the binary system aluminum-molybdenum*, Metall. Trans. A **22**, 1729–1736 (1991), doi:10.1007/BF02646496.