β-Mo_2N_{1-x} Structure: A2B_tI12_141_e_a-003

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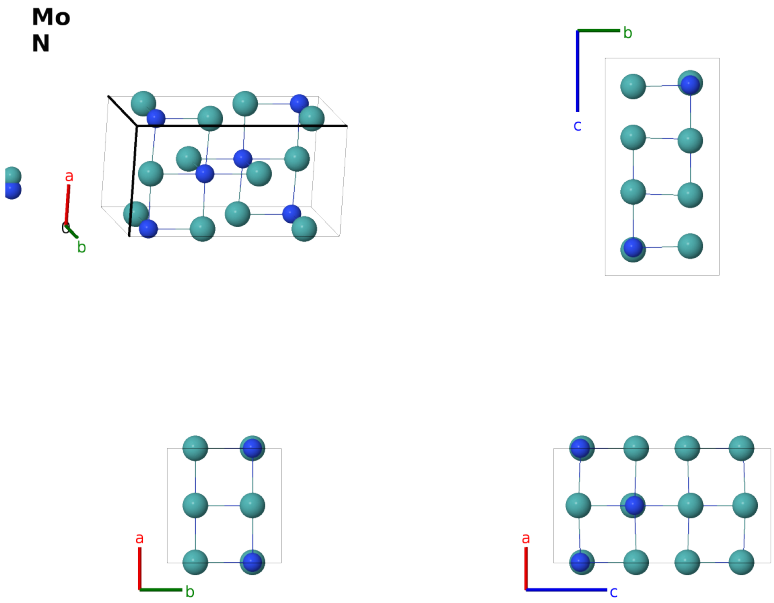
https://aflow.org/prototype-encyclopedia/KT13

https://aflow.org/prototype-encyclopedia/A2B_tI12_141_e_a-003



Prototype	Mo_2N
AFLOW prototype label	A2B_tI12_141_e_a-003
ICSD	30593
CCDC	1604846
Pearson symbol	tI12
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A2B_tI12_141_e_a-003 --params=`$a, c/a, z_2$

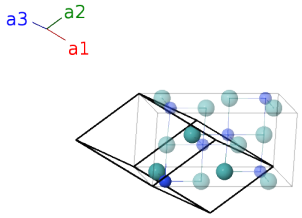
- Mo_2N_{1-x} is found in three forms (Jehn, 1978; Jauberteau, 2015):
  - In α-Mo_2N_{1-x} the molybdenum atoms retain their body-centered cubic (bcc) structure with nitrogen absorbed on random sites.

  - The ground state β-Mo_2N_{1-x} is this tetragonal structure, and
  - γ-$Mo_2N_{1\pm x}$ or Mo_2N_{2-x} is in the rock salt ($B1$) structure with the nitrogen atoms randomly distributed.

- The transition temperature between the β and γ structures is about 850°C when x = 0.286 and drops to about 400°C when x = 0.34 (Ettmayer, 1970).
- In β-Mo_2N_{1-x} the nitrogen atoms randomly occupy the (4a) Wyckoff sites.
- (Ettmayer, 1970) gives the atomic positions in setting 1 of space group $I4_1/amd$ #141. AFLOW transforms this to the standard setting 2.
- Anatase TiO_2 ($C5$), α-$ThSi_2$ (C_c), and β-Mo_2N share the same AFLOW prototype label, A2B_tI12_141_e_a. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B_2}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B_3}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	Mo I
$\mathbf{B_4}$	=	$z_2\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Mo I
$\mathbf{B_5}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	Mo I
$\mathbf{B_6}$	=	$-z_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Mo I

References

[1] P. Ettmayer, *Das System Molybdän - Stickstoff*, Monatsh. Chem. **101**, 127–140 (1970), doi:10.1007/BF00907533.

[2] D. A. Evans and K. H. Jack, *The $\gamma \leftrightarrow \beta$ phase transformation in the Mo-N system*, Acta Cryst. **10**, 833–834 (1957), doi:10.1107/S0365110X57002649. Abstract 13.5.

[3] H. Jehn and P. Ettmayer, *The Molybdenum-Nitrogen Phase Diagram*, J. Less-Common Met. **58**, 85–98 (1978), doi:10.1016/0022-5088(78)90073-5.

[4] I. Jauberteau, A. Bessaudou, R. Mayet, J. Cornette, J. L. Jauberteau, P. Carles, and T. Merle-Méjean, *Molybdenum Nitride Films: Crystal Structures, Synthesis, Mechanical, Electrical and Some Other Properties*, Coatings **5**, 656–687 (2015), doi:10.3390/coatings5040656.

Found in

[1] *AFLOW Database*, https://aflow.org. Mo_2N, ICSD entry 30593.

First cited in

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