CMo Structure: AB_hP12_194_af_bf-001

This structure originally had the label `AB_hP12_194_af_bf`. Calls to that address will be redirected here.

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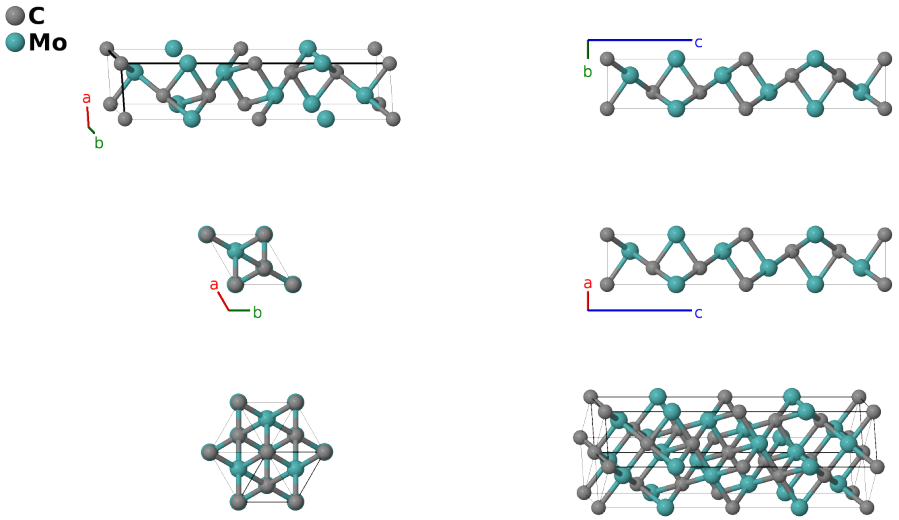
https://aflow.org/p/Q5G8

https://aflow.org/p/AB_hP12_194_af_bf-001



Prototype	CMo
AFLOW prototype label	AB_hP12_194_af_bf-001
ICSD	44987
Pearson symbol	hP12
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB_hP12_194_af_bf-001 --params=`$a, c/a, z_3, z_4$

Other compounds with this structure
CRe, BaGaGe, CaGaGe, CaGaSn, CeNiP, DyNiP, GaGeSr, GdNiP, HoNiP, LiNiP, LuNiP, LuNiP, NdNiP, NiPPr, NiPTb, NiPTm, NiPY, C_2GeTi_3, C_2SiTi_3, C_2AlTi_3

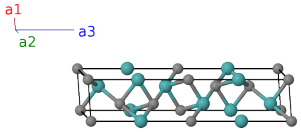
- Note that all of the atoms sit on close packed <0001> planes. The stacking sequence may be written:

Atom	Mo-II	C-II	C-I	C-II	Mo-II	Mo-I	Mo-II	C-II	C-I	C-II	Mo-II	Mo-I
Position	B	C	A	B	C	A	C	B	A	C	B	A

- Thus the Mo-II atoms and all of the C atoms are always in an fcc-like local environment, while the Mo-I atoms are in an hcp-like local environment. Like AlN_3Ti_4, this is a MAX phase. For more information, see (Radovic, 2013).

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	C I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	Mo I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	Mo I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	C II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	C II
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	C II
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	C II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4f)	Mo II
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mo II
$\mathbf{B_{11}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4f)	Mo II
$\mathbf{B_{12}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mo II

References

[1] H. Nowotny, R. Parthé, and F. Benesovsky, *Das Dreistotfsystem: Molybdän–Silizium–K0hlenstoff*, Monatsh. Chem. Verw. Tl. **85**, 255–272 (1954).

[2] M. Radovic and M. W. Barsoum, *MAX phases: Bridging the gap between metals and ceramics*, American Ceramic Society Bulletin **92**, 20–27 (2013).