# CMo Structure: AB_hP12_194_af_bf-001

This structure previously used the label(s) `AB_hP12_194_af_bf`. Calls to these addresses will be redirected here.

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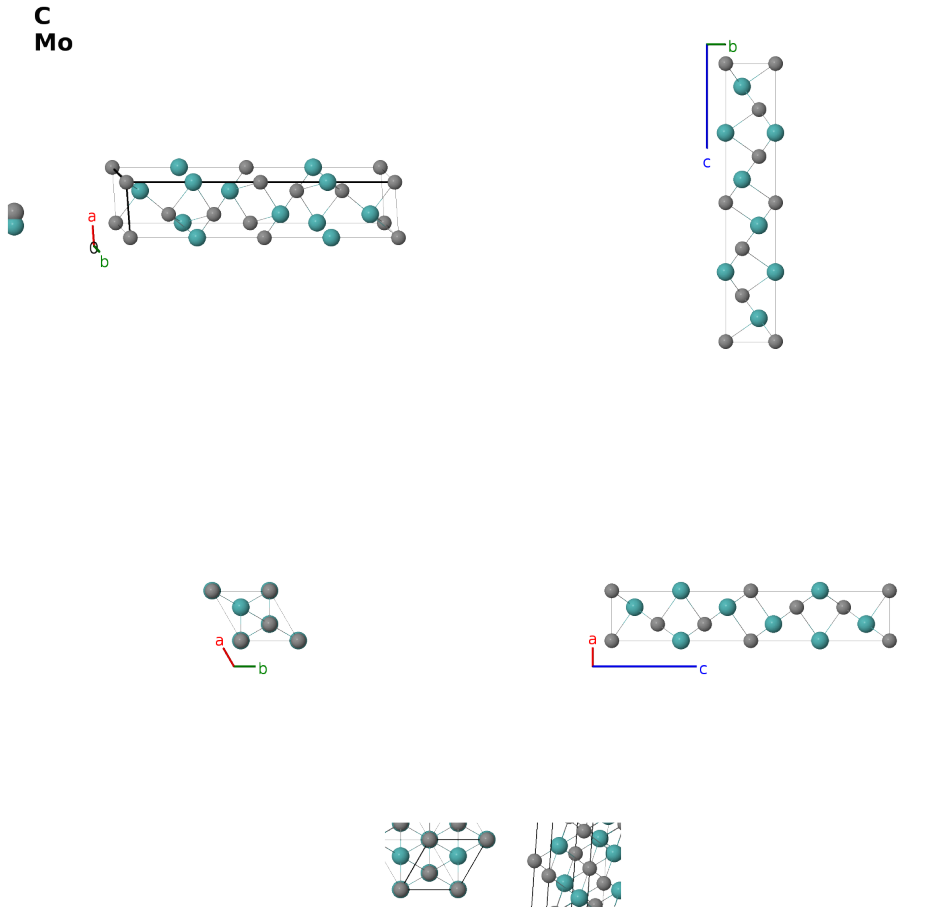
https://aflow.org/prototype-encyclopedia/Q5G8

https://aflow.org/prototype-encyclopedia/AB_hP12_194_af_bf-001




| | |
|---|---|
| **Prototype** | CMo |
| **AFLOW prototype label** | AB_hP12_194_af_bf-001 |
| **ICSD** | 44987 |
| **CCDC** | 1614303 |
| **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=`$a, c/a, z_3, z_4$

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**Other compounds with this structure**

CRe, BaGaGe, CaGaGe, CaGaSn, CeNiP, DyNiP, GaGeSr, GdNiP, HoNiP, LiNiP, LuNiP, LuNiP, NdNiP, NiPPr, NiPTb, NiPTm, NiPY, $C_2GeTi_3$, $C_2SiTi_3$, $C_2AlTi_3$

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- 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).

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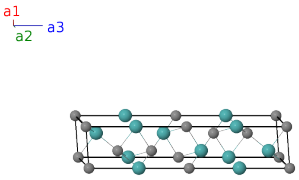
**Hexagonal primitive vectors**

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

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**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).

**First cited in**

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