# $Al_2Mo_3C$ Structure: A2BC3_cP24_213_c_a_d-001

This structure originally had the label `A2BC3_cP24_213_c_a_d`. Calls to that address will be redirected here.

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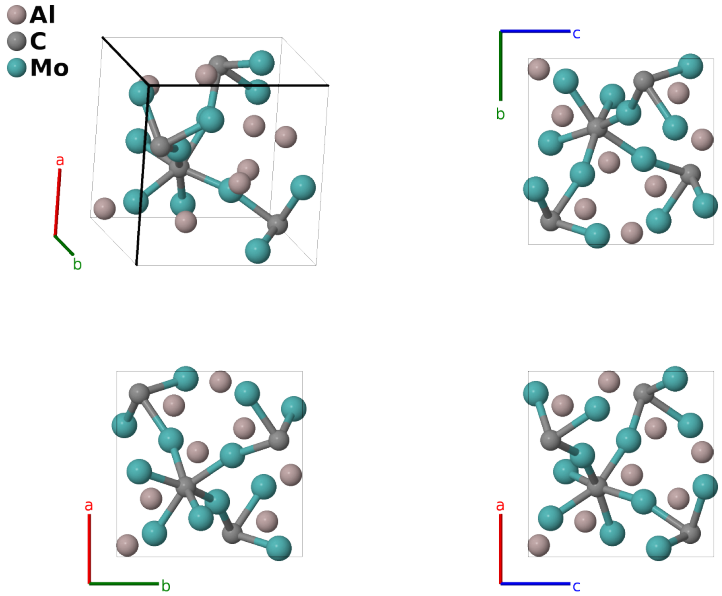
https://aflow.org/p/SRH0

https://aflow.org/p/A2BC3_cP24_213_c_a_d-001




| | |
|---|---|
| **Prototype** | $Al_2CMo_3$ |
| **AFLOW prototype label** | A2BC3_cP24_213_c_a_d-001 |
| **ICSD** | 42917 |
| **Pearson symbol** | cP24 |
| **Space group number** | 213 |
| **Space group symbol** | $P4_132$ |
| **AFLOW prototype command** | `aflow --proto=A2BC3_cP24_213_c_a_d-001 --params=`$a, x_2, y_3$ |

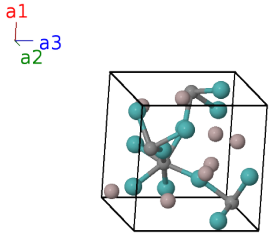
**Other compounds with this structure**

$Ag_2Pd_3Sn$, $Al_2Nb_3C$, $Al_2Nb_3N$, $Al_2Ta_3C$, $Cr_2Re_3B$, $Li_2Pd_3B$, $Li_2Pt_3B$, $Mn_2Rh_3P$, $Ni_2W_3N$, $Re_2W_3C$, $Rh_2Mo_3N$, $(Fe_{2-x}Rh_x)Mo_3N$

- This is a "filled" $\beta$-Mn (A13) structure, with the aluminum and molybdenum atoms almost exactly on the sites of the manganese atoms in A13.
- This structure may also be found in the enantiomorphic space group $P4_332$ #212.

## 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 |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{3}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$ | = | $\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$ | (4a) | C I |
| $\mathbf{B_2}$ | = | $\frac{1}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$ | = | $\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$ | (4a) | C I |
| $\mathbf{B_3}$ | = | $\frac{5}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$ | = | $\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$ | (4a) | C I |
| $\mathbf{B_4}$ | = | $\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$ | = | $\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$ | (4a) | C I |
| $\mathbf{B_5}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_6}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_7}$ | = | $-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_8}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_9}$ | = | $\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_{10}}$ | = | $-\left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_{11}}$ | = | $\left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_{12}}$ | = | $-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (8c) | Al I |
| $\mathbf{B_{13}}$ | = | $\frac{1}{8}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{8}a\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{14}}$ | = | $\frac{3}{8}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{8}a\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + a\left(y_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{15}}$ | = | $\frac{7}{8}\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{7}{8}a\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{16}}$ | = | $\frac{5}{8}\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{5}{8}a\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_3 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{17}}$ | = | $\left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$ | = | $a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{18}}$ | = | $\left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$ | = | $a\left(y_3 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{19}}$ | = | $-\left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{20}}$ | = | $-\left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(y_3 - \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{21}}$ | = | $y_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$ | = | $ay_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{22}}$ | = | $-y_3\,\mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$ | = | $-ay_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$ | (12d) | Mo I |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_{23}}$ | = | $\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-\frac{1}{4}\right)\,\mathbf{a}_2+\frac{7}{8}\,\mathbf{a}_3$ | = | $a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{7}{8}a\,\hat{\mathbf{z}}$ | (12d) | Mo I |
| $\mathbf{B_{24}}$ | = | $-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-\frac{3}{4}\right)\,\mathbf{a}_2+\frac{5}{8}\,\mathbf{a}_3$ | = | $-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_3-\frac{3}{4}\right)\,\hat{\mathbf{y}}+\frac{5}{8}a\,\hat{\mathbf{z}}$ | (12d) | Mo I |

## References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## Found in


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[2] J. Johnston, L. Toth, K. Kennedy, and E. R. Parker, *Superconductivity of $Mo_3Al_2C$*, Solid State Commun. **2**, 123 (1964), doi:10.1016/0038-1098(64)90251-0.