# $BaMo_6S_8$ Structure: AB6C8_hR15_148_a_f_cf-001

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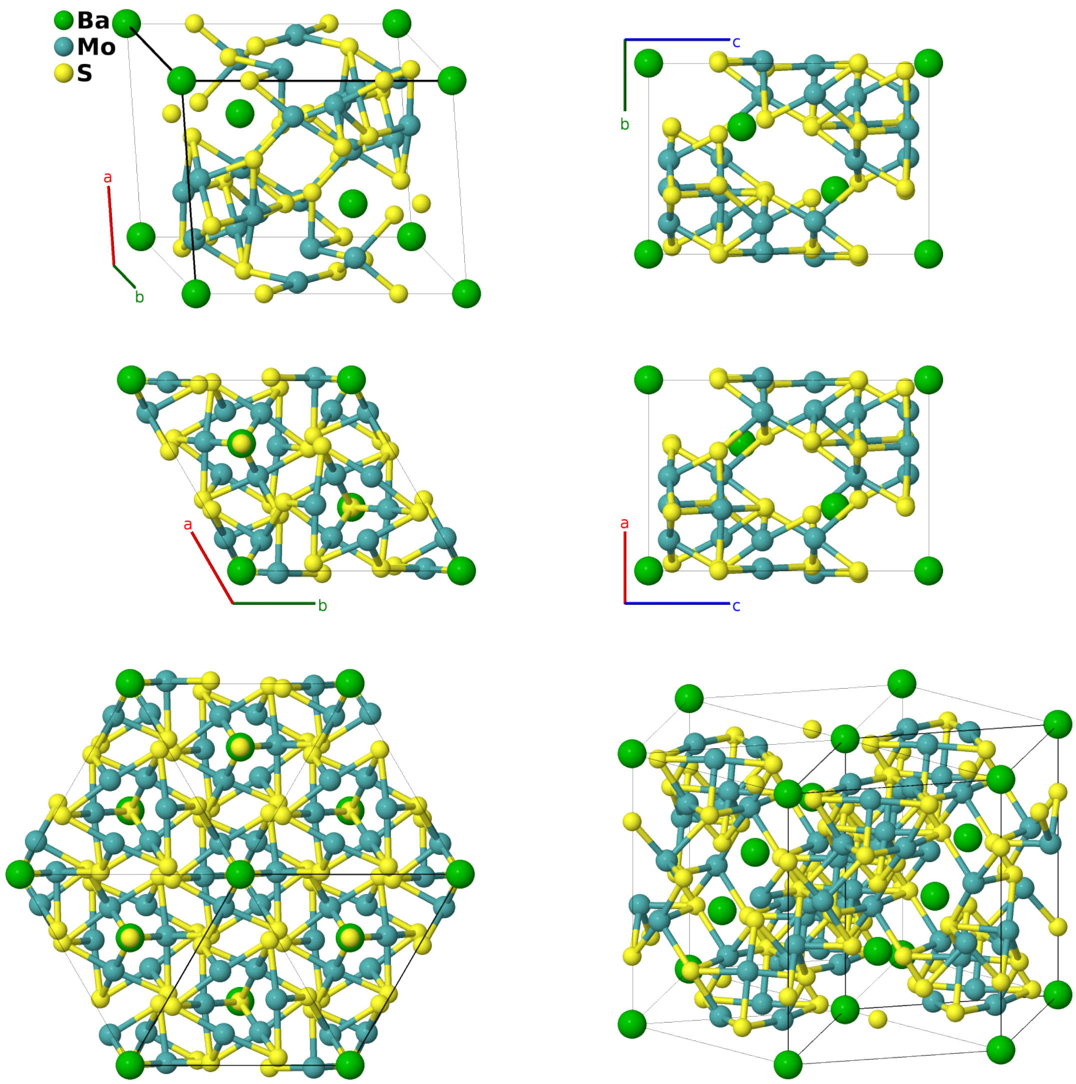
https://aflow.org/p/CY1Y

https://aflow.org/p/AB6C8_hR15_148_a_f_cf-001

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|---|---|
| **Prototype** | $BaMo_6S_8$ |
| **AFLOW prototype label** | AB6C8_hR15_148_a_f_cf-001 |
| **ICSD** | none |
| **Pearson symbol** | hR15 |
| **Space group number** | 148 |
| **Space group symbol** | $R\bar{3}$ |

**AFLOW prototype command** `aflow --proto=AB6C8_hR15_148_a_f_cf-001`
`--params=`$a, c/a, x_2, x_3, y_3, z_3, x_4, y_4, z_4$

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**Other compounds with this structure**

$CaMo_6S_8$, $CeMo_6S_8$, $CeMo_6Se_8$, $EuMo_6S_8$, $LaMo_6S_8$, $LaMo_6Se_8$, $NdMo_6S_8$, $NdMo_6Se_8$, $PbMo_6S_8$, $PrMo_6S_8$, $PrMo_6Se_8$, $SmMo_6S_8$, $SmMo_6Se_8$, $SrMo_6S_8$

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- $BaMo_6S_8$ and other Chevrel phase compounds undergo structural transitions at low temperatures. $BaMo_6S_8$ transforms into a triclinic $P\bar{1}$ structure below 175K. Structural parameters for the low temperature phase can be found in (Kubel, 1990). We use the data for the rhombohedral $R\bar{3}$ structure taken at 177K.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

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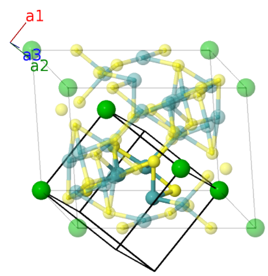
**Rhombohedral primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | Ba I |
| $\mathbf{B_2}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $cx_2\,\hat{\mathbf{z}}$ | (2c) | S I |
| $\mathbf{B_3}$ | = | $-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $-cx_2\,\hat{\mathbf{z}}$ | (2c) | S I |
| $\mathbf{B_4}$ | = | $x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$ | (6f) | Mo I |
| $\mathbf{B_5}$ | = | $z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$ | (6f) | Mo I |
| $\mathbf{B_6}$ | = | $y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$ | (6f) | Mo I |
| $\mathbf{B_7}$ | = | $-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$ | (6f) | Mo I |
| $\mathbf{B_8}$ | = | $-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$ | (6f) | Mo I |
| $\mathbf{B_9}$ | = | $-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$ | (6f) | Mo I |
| $\mathbf{B_{10}}$ | = | $x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$ | (6f) | S II |
| $\mathbf{B_{11}}$ | = | $z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$ | (6f) | S II |
| $\mathbf{B_{12}}$ | = | $y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$ | (6f) | S II |
| $\mathbf{B_{13}}$ | = | $-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$ | (6f) | S II |

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| $\mathbf{B_{14}}$ | = | $-z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(y_4 - z_4)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\;\hat{\mathbf{z}}$ | (6f) | S II |
| $\mathbf{B_{15}}$ | = | $-y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_4 - y_4)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\;\hat{\mathbf{z}}$ | (6f) | S II |

## References


[1] F. Kubel and K. Yvon, *Structural phase transitions in Chevrel phases containing divalent metal cations. II. Structure refinement of triclinic* $EuMo_6S_8$ *and* $BaMo_6S_8$ *at low temperature*, Acta Crystallogr. Sect. C **46**, 181–186 (1990), doi:10.1107/S0108270189005913.


## Found in


[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).