

Magnetoplumbite ($\text{PbFe}_{12}\text{O}_{19}$) Structure: A12B19C_hP64_194_ab2fk_efh2k_c-001

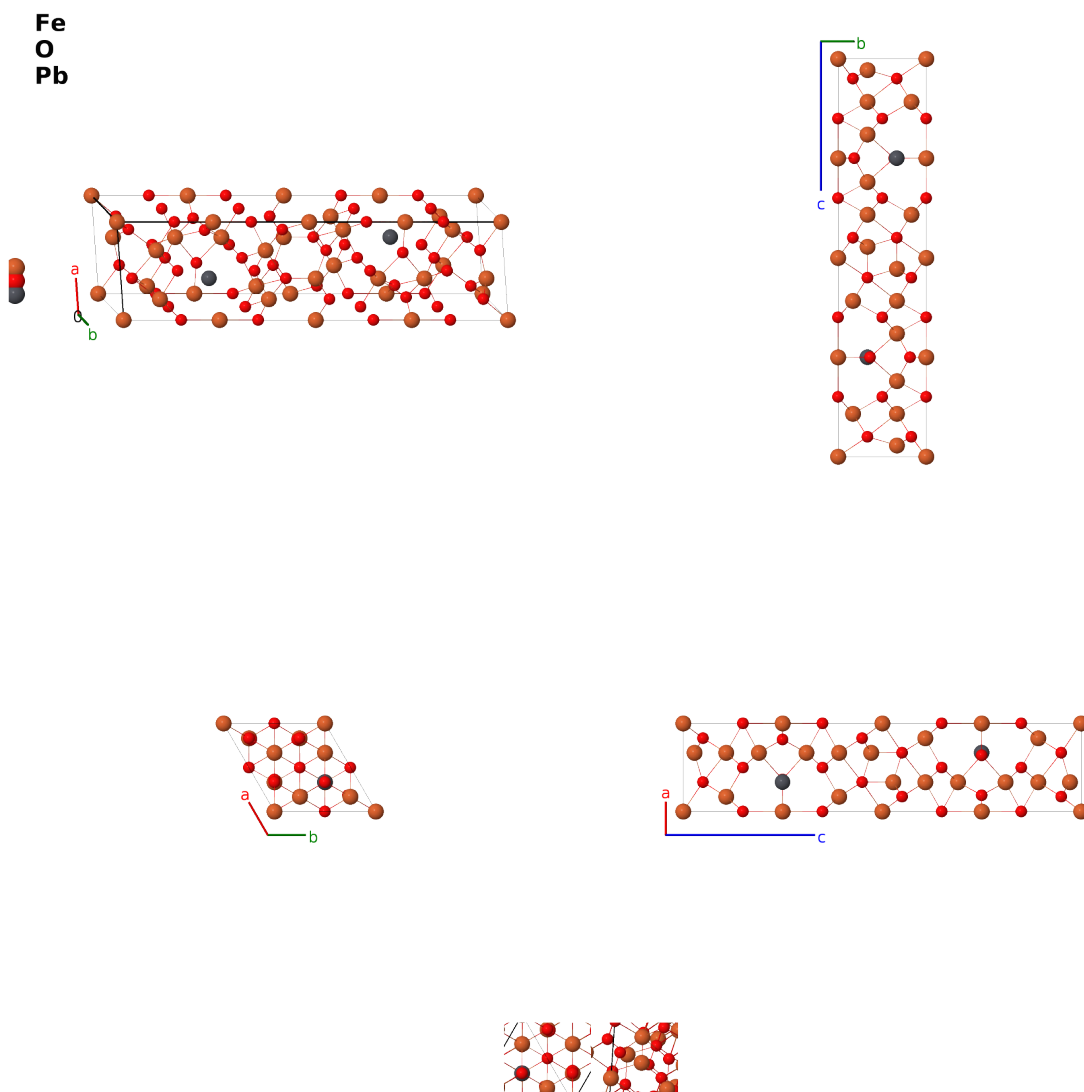
This structure previously used the label(s) **A12B19C_hP64_194_ab2fk_efh2k.d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5L5V>

https://aflow.org/prototype-encyclopedia/A12B19C_hP64_194_ab2fk_efh2k_c-001



Prototype

$\text{Fe}_{12}\text{O}_{19}\text{Pb}$

AFLOW prototype label

A12B19C_hP64_194_ab2fk_efh2k_c-001

Mineral name

magnetoplumbite

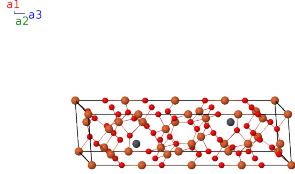
ICSD	36259
CCDC	1608021
Pearson symbol	hP64
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A12B19C_hP64_194_ab2fk_efh2k_c-001</code> <code>--params=a, c/a, z₄, z₅, z₆, z₇, x₈, x₉, z₉, x₁₀, z₁₀, x₁₁, z₁₁</code>

Other compounds with this structure

PbAl₁₂O₁₉, PbGa₁₂O₁₉, PbMn₁₂O₁₉, Pb(Co, Ti)₁₂O₁₉, BaAl₁₂O₁₉, BaFe₁₂O₁₉, BaGa₁₂O₁₉, BaMn₁₂O₁₉, Ba(Co, Ti)₁₂O₁₉, CaAl₁₂O₁₉, CaGa₁₂O₁₉, CaMn₁₂O₁₉, Ca(Co, Ti)₁₂O₁₉, SrAl₁₂O₁₉, SrGa₁₂O₁₉, SrMn₁₂O₁₉, Sr(Co, Ti)₁₂O₁₉

- In addition to the listed compounds, the lead and iron sites may be alloyed with a wide variety of metals and semi-metals resulting in high-entropy phases (Vinnik, 2019).
- We did not find an ICSD or CCDC entry for (Simsa, 1994). We use the ICSD entry from the early work of (Adelskoeld, 1938).

Hexagonal primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Fe I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2b)	Fe II
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2b)	Fe II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Pb I
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Pb I
$\mathbf{B}_7$	$= z_4 \mathbf{a}_3$	$=$	$cz_4 \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_8$	$= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_9$	$= -z_4 \mathbf{a}_3$	$=$	$-cz_4 \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{10}$	$= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B}_{11}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4f)	Fe III
$\mathbf{B}_{12}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4f)	Fe III

$$\begin{aligned}
\mathbf{B}_{54} &= -2x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= -\frac{3}{2}ax_{11} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{55} &= x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= -\sqrt{3}ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{56} &= -x_{11} \mathbf{a}_1 - 2x_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_{11} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{57} &= 2x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_{11} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{58} &= -x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= \sqrt{3}ax_{11} \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{59} &= 2x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= \frac{3}{2}ax_{11} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{60} &= -x_{11} \mathbf{a}_1 - 2x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= -\frac{3}{2}ax_{11} \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{61} &= -x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= \sqrt{3}ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{62} &= -2x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{3}{2}ax_{11} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{63} &= x_{11} \mathbf{a}_1 + 2x_{11} \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{3}{2}ax_{11} \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{O V} \\
\mathbf{B}_{64} &= x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 &= -\sqrt{3}ax_{11} \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} &(12k) & \text{O V}
\end{aligned}$$

References

- [1] R. Gerber, Z. Šimša, and L. Jenšovský, *A note on the magnetoplumbite crystal structure*, Czech. J. Phys. **44**, 937–940 (1994), doi:10.1007/BF01715487.
- [2] D. A. Vinnik, E. A. Trofimov, V. E. Zhivulin, O. V. Zaitseva, S. A. Gudkova, A. Y. Starikov, D. A. Zhrebtssov, A. A. Kirsanova, M. Häßner, and R. Niewa, *High-entropy oxide phases with magnetoplumbite structure*, Ceram. Int. **45**, 12942–12948 (2019), doi:10.1016/j.ceramint.2019.03.221.
- [3] V. Adelskoeld, *X-ray studies on magneto plumbite $PbO(Fe_2O_3)_6$ and other substances resembling β -alumina $Na_2O(Al_2O_3)_{11}$* , Arkiv för Kemi, Mineralogi och Geologi **12**, 1–9 (1938).

First cited in

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