

Th₆Mn₂₃ (*D*8_a) Structure: A23B6_cF116_225_ad2f_e-001

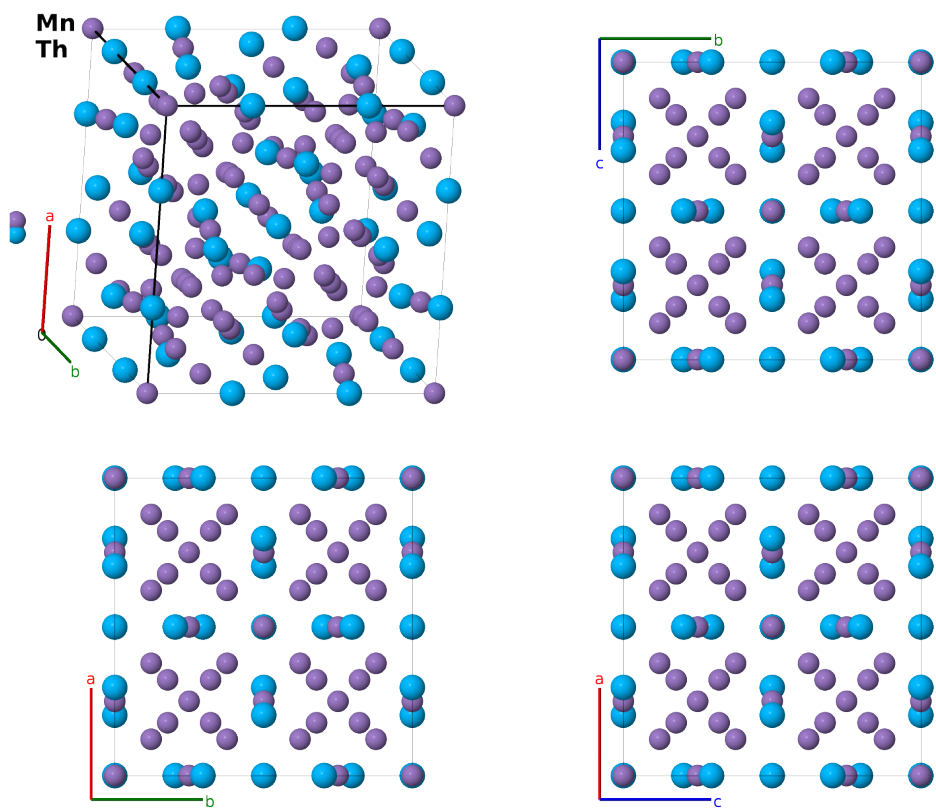
This structure previously used the label(s) **A23B6_cF116_225_bd2f_e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/W8MF>

https://aflow.org/prototype-encyclopedia/A23B6_cF116_225_ad2f_e-001



Prototype	Mn ₂₃ Th ₆
AFLOW prototype label	A23B6_cF116_225_ad2f_e-001
<i>Strukturbericht</i> designation	<i>D</i> 8 _a
ICSD	104987
CCDC	1662886
Pearson symbol	cF116
Space group number	225
Space group symbol	<i>Fm</i> $\bar{3}$ <i>m</i>

AFLOW prototype command `aflow --proto=A23B6_cF116_225_ad2f_e-001`
 `--params=a, x3, x4, x5`

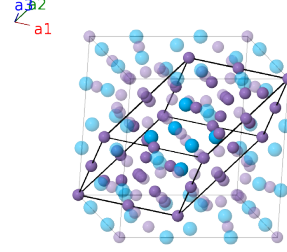
Other compounds with this structure

Co₂₃Zr₆, Fe₂₃Er₆, Fe₂₃Ho₆, Fe₂₃Sm₆, Fe₂₃Tb₆, Li₂₃Sr₆, Mg₂₃Ba₆, Mg₂₃Dy₆, Mg₂₃Er₆, Mg₂₃Gd₆, Mg₂₃Ho₆, Mg₂₃Lu₆, Mg₂₃Nd₆, Mg₂₃Sr₆, Mg₂₃Tb₆, Mg₂₃Th₆, Mg₂₃Tm₆, Mg₂₃Y₆, Mn₂₃Th_{6-x}Y_x, Mn₂₃Th₆, Mn₂₃Y₆, Fe₃Zn, Ge₁₃Fe₁₀Ti₆

- We have moved the ternary compounds with this structure to the Mg₆Si₇Cu₁₆ page.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(4a) Mn I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mn II
$\mathbf{B}_3$	$=$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mn II
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mn II
$\mathbf{B}_5$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d) Mn II
$\mathbf{B}_6$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(24d) Mn II
$\mathbf{B}_7$	$=$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d) Mn II
$\mathbf{B}_8$	$=$	$-x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}}$	(24e) Th I
$\mathbf{B}_9$	$=$	$x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}}$	(24e) Th I
$\mathbf{B}_{10}$	$=$	$x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{y}}$	(24e) Th I
$\mathbf{B}_{11}$	$=$	$-x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{y}}$	(24e) Th I
$\mathbf{B}_{12}$	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{z}}$	(24e) Th I
$\mathbf{B}_{13}$	$=$	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{z}}$	(24e) Th I
$\mathbf{B}_{14}$	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(32f) Mn III
$\mathbf{B}_{15}$	$=$	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - 3x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(32f) Mn III
$\mathbf{B}_{16}$	$=$	$x_4\mathbf{a}_1 - 3x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(32f) Mn III
$\mathbf{B}_{17}$	$=$	$-3x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(32f) Mn III
$\mathbf{B}_{18}$	$=$	$-x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + 3x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(32f) Mn III
$\mathbf{B}_{19}$	$=$	$-x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(32f) Mn III
$\mathbf{B}_{20}$	$=$	$-x_4\mathbf{a}_1 + 3x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(32f) Mn III
$\mathbf{B}_{21}$	$=$	$3x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(32f) Mn III

$\mathbf{B}_{22}$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV
$\mathbf{B}_{23}$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV
$\mathbf{B}_{24}$	$=$	$x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV
$\mathbf{B}_{25}$	$=$	$-3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV
$\mathbf{B}_{26}$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + 3x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV
$\mathbf{B}_{27}$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV
$\mathbf{B}_{28}$	$=$	$-x_5 \mathbf{a}_1 + 3x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV
$\mathbf{B}_{29}$	$=$	$3x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(32f)	Mn IV

References

- [1] J. V. Florio, R. E. Rundle, and A. I. Snow, *Compounds of thorium with transition metals. I. The thorium-manganese system* **5**, 445–457 (1952), doi:10.1107/S0365110X52001337.

Found in

- [1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

First cited in

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