# $Th_6Mn_{23}$ ($D8_a$) Structure: A23B6_cF116_225_ad2f_e-001

This structure originally had the label `A23B6_cF116_225_bd2f_e`. Calls to that address will be redirected here.

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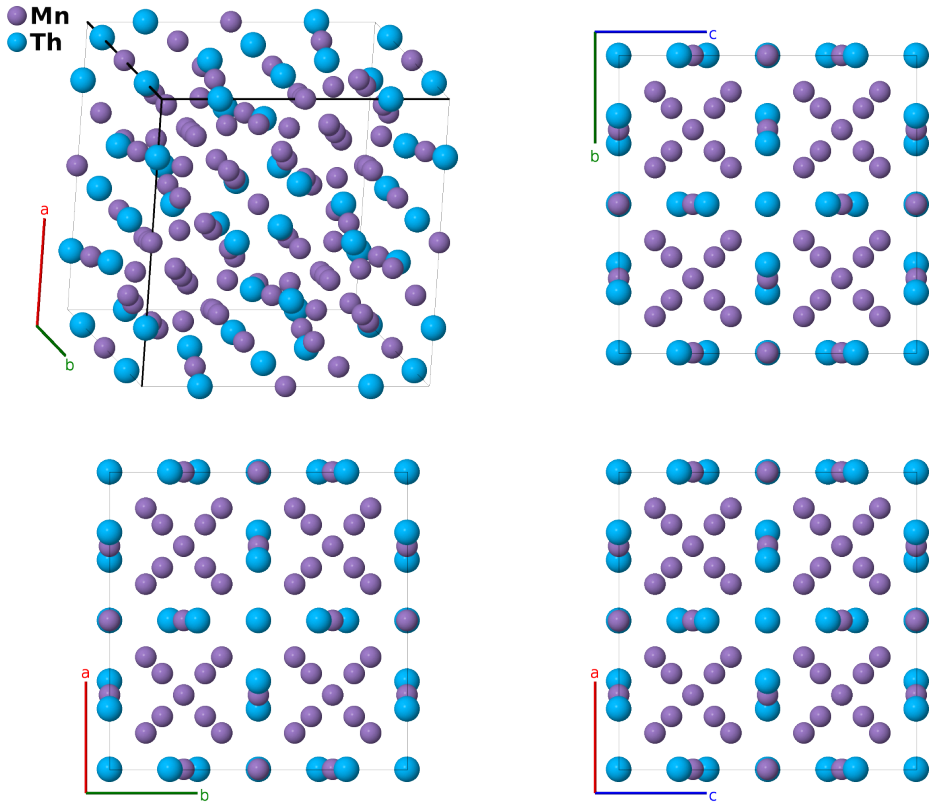
https://aflow.org/p/W8MF

https://aflow.org/p/A23B6_cF116_225_ad2f_e-001




| | |
|---|---|
| **Prototype** | $Mn_{23}Th_6$ |
| **AFLOW prototype label** | A23B6_cF116_225_ad2f_e-001 |
| ***Strukturbericht* designation** | $D8_a$ |
| **ICSD** | 104987 |
| **Pearson symbol** | cF116 |
| **Space group number** | 225 |
| **Space group symbol** | $Fm\overline{3}m$ |
| **AFLOW prototype command** | `aflow --proto=A23B6_cF116_225_ad2f_e-001 --params=`$a, x_3, x_4, x_5$ |

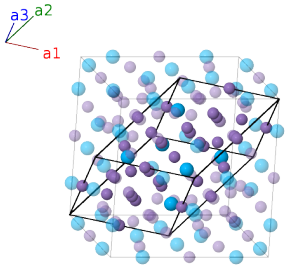
**Other compounds with this structure**

$Co_{23}Zr_6$, $Fe_{23}Er_6$, $Fe_{23}Ho_6$, $Fe_{23}Sm_6$, $Fe_{23}Tb_6$, $Li_{23}Sr_6$, $Mg_{23}Ba_6$, $Mg_{23}Dy_6$, $Mg_{23}Er_6$, $Mg_{23}Gd_6$, $Mg_{23}Ho_6$, $Mg_{23}Lu_6$, $Mg_{23}Nd_6$, $Mg_{23}Sr_6$, $Mg_{23}Tb_6$, $Mg_{23}Th_6$, $Mg_{23}Tm_6$, $Mg_{23}Y_6$, $Mn_{23}Th_{6-x}Y_x$, $Mn_{23}Th_6$, $Mn_{23}Y_6$, $Fe_3Zn$, $Ge_{13}Fe_{10}Ti_6$

- We have moved the ternary compounds with this structure to the $Mg_6Si_7Cu_{16}$ page.

**Face-centered Cubic primitive vectors**

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\ \mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}\end{aligned}$$




**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 |

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|---|---|---|---|---|---|---|
| $\mathbf{B_{24}}$ | = | $x_5\,\mathbf{a}_1 - 3x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$ | (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, Frankfort, 1958), 1964 reprint with corrections edn.