

# Cr<sub>23</sub>C<sub>6</sub> (*D*8<sub>4</sub>) Structure: A6B23\_cF116\_225\_e\_acfh-001

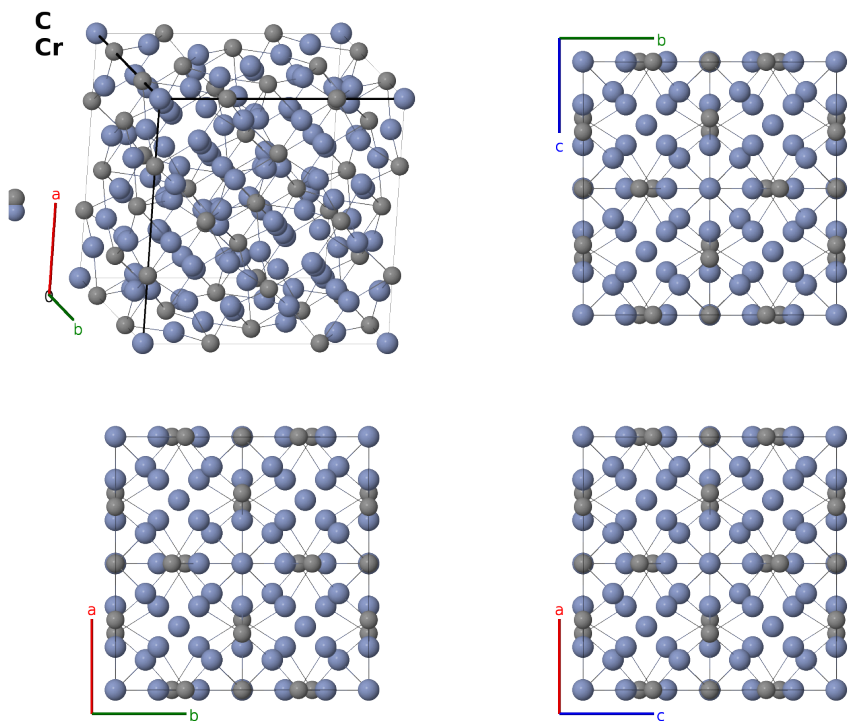
This structure previously used the label(s) **A6B23\_cF116\_225\_e\_acfh**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/EY4X>

[https://aflow.org/prototype-encyclopedia/A6B23\\_cF116\\_225\\_e\\_acfh-001](https://aflow.org/prototype-encyclopedia/A6B23_cF116_225_e_acfh-001)



|                                    |                                                                                                                                                           |
|------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype                          | C <sub>6</sub> Cr <sub>23</sub>                                                                                                                           |
| AFLOW prototype label              | A6B23_cF116_225_e_acfh-001                                                                                                                                |
| <i>Strukturbericht</i> designation | <i>D</i> 8 <sub>4</sub>                                                                                                                                   |
| ICSD                               | 2837                                                                                                                                                      |
| CCDC                               | 1592638                                                                                                                                                   |
| Pearson symbol                     | cF116                                                                                                                                                     |
| Space group number                 | 225                                                                                                                                                       |
| Space group symbol                 | <i>Fm</i> $\bar{3}$ <i>m</i>                                                                                                                              |
| AFLOW prototype command            | <code>aflow --proto=A6B23_cF116_225_e_acfh-001</code><br><code>--params=<i>a</i>, <i>x</i><sub>3</sub>, <i>x</i><sub>4</sub>, <i>y</i><sub>5</sub></code> |

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### Other compounds with this structure

Mn<sub>23</sub>C<sub>6</sub>, Co<sub>21</sub>Sn<sub>2</sub>B<sub>6</sub>, Fe<sub>21</sub>Mo<sub>2</sub>C<sub>6</sub>, Fe<sub>21</sub>W<sub>2</sub>C<sub>6</sub>, Ni<sub>20</sub>Mg<sub>3</sub>B<sub>6</sub>, Ni<sub>21</sub>In<sub>2</sub>B<sub>6</sub>, Ni<sub>21</sub>Sn<sub>2</sub>B<sub>6</sub>

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### Face-centered Cubic primitive vectors




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### Basis vectors

|                   | Lattice<br>coordinates |                                                                                  | Cartesian<br>coordinates | Wyckoff<br>position                                                                             | Atom<br>type |
|-------------------|------------------------|----------------------------------------------------------------------------------|--------------------------|-------------------------------------------------------------------------------------------------|--------------|
| $\mathbf{B}_1$    | =                      | 0                                                                                | =                        | 0                                                                                               | (4a) Cr I    |
| $\mathbf{B}_2$    | =                      | $\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$ | =                        | $\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$ | (8c) Cr II   |
| $\mathbf{B}_3$    | =                      | $\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$ | =                        | $\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$ | (8c) Cr II   |
| $\mathbf{B}_4$    | =                      | $-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                        | =                        | $ax_3 \hat{\mathbf{x}}$                                                                         | (24e) C I    |
| $\mathbf{B}_5$    | =                      | $x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$                         | =                        | $-ax_3 \hat{\mathbf{x}}$                                                                        | (24e) C I    |
| $\mathbf{B}_6$    | =                      | $x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                         | =                        | $ax_3 \hat{\mathbf{y}}$                                                                         | (24e) C I    |
| $\mathbf{B}_7$    | =                      | $-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$                        | =                        | $-ax_3 \hat{\mathbf{y}}$                                                                        | (24e) C I    |
| $\mathbf{B}_8$    | =                      | $x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$                         | =                        | $ax_3 \hat{\mathbf{z}}$                                                                         | (24e) C I    |
| $\mathbf{B}_9$    | =                      | $-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                        | =                        | $-ax_3 \hat{\mathbf{z}}$                                                                        | (24e) C I    |
| $\mathbf{B}_{10}$ | =                      | $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$                         | =                        | $ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$                         | (32f) Cr III |
| $\mathbf{B}_{11}$ | =                      | $x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$                        | =                        | $-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$                        | (32f) Cr III |
| $\mathbf{B}_{12}$ | =                      | $x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$                        | =                        | $-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                        | (32f) Cr III |
| $\mathbf{B}_{13}$ | =                      | $-3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$                       | =                        | $ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                         | (32f) Cr III |
| $\mathbf{B}_{14}$ | =                      | $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + 3x_4 \mathbf{a}_3$                       | =                        | $ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                         | (32f) Cr III |
| $\mathbf{B}_{15}$ | =                      | $-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$                        | =                        | $-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                        | (32f) Cr 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) Cr 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) Cr III |
| $\mathbf{B}_{18}$ | =                      | $2y_5 \mathbf{a}_1$                                                              | =                        | $ay_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$                                                 | (48h) Cr IV  |
| $\mathbf{B}_{19}$ | =                      | $2y_5 \mathbf{a}_2 - 2y_5 \mathbf{a}_3$                                          | =                        | $-ay_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$                                                | (48h) Cr IV  |
| $\mathbf{B}_{20}$ | =                      | $-2y_5 \mathbf{a}_2 + 2y_5 \mathbf{a}_3$                                         | =                        | $ay_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$                                                 | (48h) Cr IV  |
| $\mathbf{B}_{21}$ | =                      | $-2y_5 \mathbf{a}_1$                                                             | =                        | $-ay_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$                                                | (48h) Cr IV  |
| $\mathbf{B}_{22}$ | =                      | $2y_5 \mathbf{a}_2$                                                              | =                        | $ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$                                                 | (48h) Cr IV  |
| $\mathbf{B}_{23}$ | =                      | $-2y_5 \mathbf{a}_1 + 2y_5 \mathbf{a}_3$                                         | =                        | $ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$                                                 | (48h) Cr IV  |
| $\mathbf{B}_{24}$ | =                      | $2y_5 \mathbf{a}_1 - 2y_5 \mathbf{a}_3$                                          | =                        | $-ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{z}}$                                                | (48h) Cr IV  |
| $\mathbf{B}_{25}$ | =                      | $-2y_5 \mathbf{a}_2$                                                             | =                        | $-ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{z}}$                                                | (48h) Cr IV  |
| $\mathbf{B}_{26}$ | =                      | $2y_5 \mathbf{a}_3$                                                              | =                        | $ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}}$                                                 | (48h) Cr IV  |

$$\begin{array}{llllll}
\mathbf{B}_{27} & = & 2y_5 \mathbf{a}_1 - 2y_5 \mathbf{a}_2 & = & -ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} & (48h) \quad \text{Cr IV} \\
\mathbf{B}_{28} & = & -2y_5 \mathbf{a}_1 + 2y_5 \mathbf{a}_2 & = & ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} & (48h) \quad \text{Cr IV} \\
\mathbf{B}_{29} & = & -2y_5 \mathbf{a}_3 & = & -ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} & (48h) \quad \text{Cr IV}
\end{array}$$

## References

- [1] A. L. Bowman, G. P. Arnold, E. K. Storms, and N. G. Nereson, *The crystal structure of  $\text{Cr}_{23}\text{C}_6$* , Acta Crystallogr. Sect. B **28**, 3102–3103 (1972), doi:10.1107/S0567740872007526.

## First cited in

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