

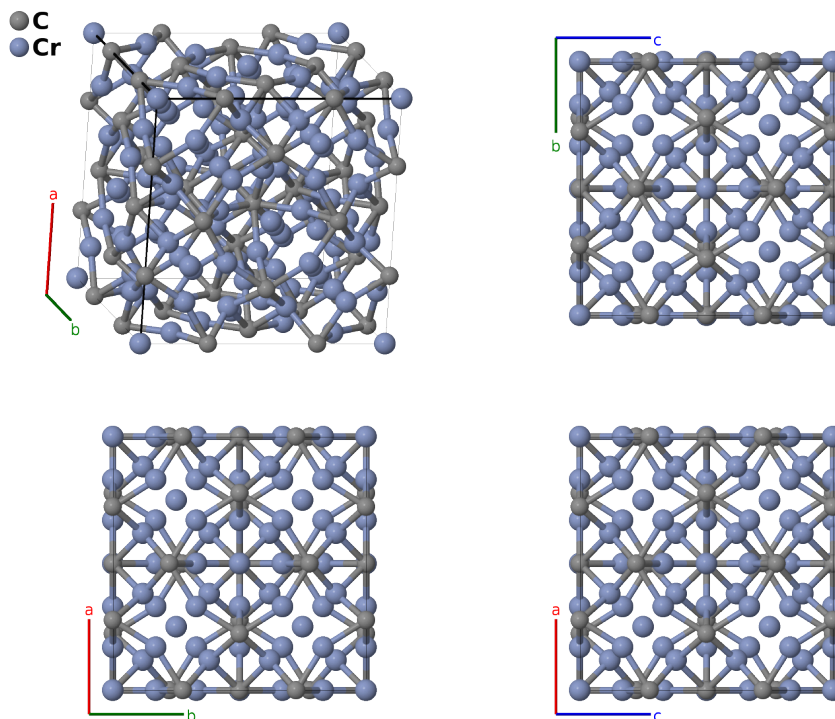
# Cr<sub>23</sub>C<sub>6</sub> (*D*8<sub>4</sub>) Structure: A6B23\_cF116\_225\_e\_acfh-001

This structure originally had the label A6B23\_cF116\_225\_e\_acfh. Calls to that address will be redirected here.

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<https://aflow.org/p/EY4X>

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



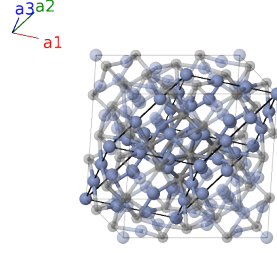
Prototype	C <sub>6</sub> Cr <sub>23</sub>
AFLOW prototype label	A6B23_cF116_225_e_acfh-001
<i>Strukturbericht</i> designation	<i>D</i> 8 <sub>4</sub>
ICSD	2837
Pearson symbol	cF116
Space group number	225
Space group symbol	<i>Fm</i> $\bar{3}$ <i>m</i>
AFLOW prototype command	<code>aflow --proto=A6B23_cF116_225_e_acfh-001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

## 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>

## 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)	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
$\mathbf{B}_{27}$	$2y_5 \mathbf{a}_1 - 2y_5 \mathbf{a}_2$	$=$	$-ay_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}}$	(48h)	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)	Cr IV
$\mathbf{B}_{29}$	$-2y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}}$	(48h)	Cr IV

## References

- [1] A. L. Bowman, G. P. Arnold, E. K. Storms, and N. G. Nereson, *The crystal structure of  $Cr_{23}C_6$* , Acta Crystallogr. Sect. B **28**, 3102–3103 (1972), doi:10.1107/S0567740872007526.