

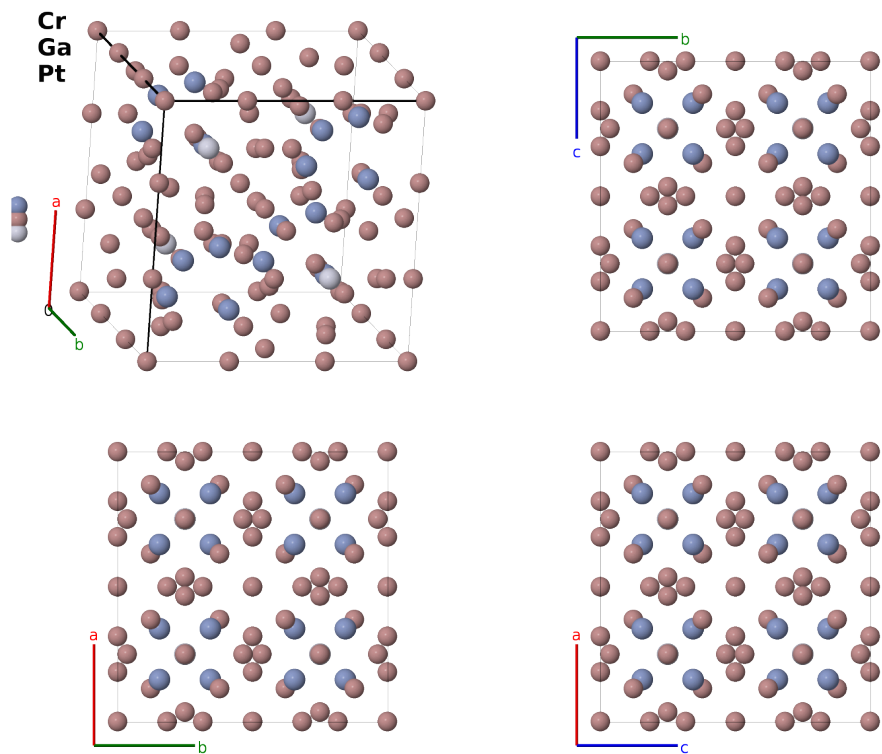
Cubic Cr₄PtGa₁₇ Structure: A4B17C_cF88_216_e_aefg_c-001

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<https://aflow.org/prototype-encyclopedia/9Q9K>

https://aflow.org/prototype-encyclopedia/A4B17C_cF88_216_e_aefg_c-001

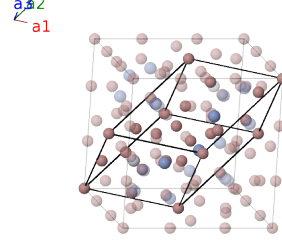


Prototype	Cr ₄ Ga ₁₇ Pt
AFLOW prototype label	A4B17C_cF88_216_e_aefg_c-001
ICSD	36836
CCDC	2093835
Pearson symbol	cF88
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A4B17C_cF88_216_e_aefg_c-001</code> <code>--params=a, x₃, x₄, x₅, x₆</code>

- (Gui, 2021) describe this compound as a rhombohedral structure in space group $R3m$ #160, a distortion of the half-Heusler ($C1_b$) structure. Uncertainty in the atomic positions leads to this cubic structure, which we use as the prototype.

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) Ga I
$\mathbf{B}_2$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(4c) Pt I
$\mathbf{B}_3$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16e) Cr I
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16e) Cr I
$\mathbf{B}_5$	$=$	$x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16e) Cr I
$\mathbf{B}_6$	$=$	$-3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16e) Cr I
$\mathbf{B}_7$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(16e) Ga II
$\mathbf{B}_8$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(16e) Ga II
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(16e) Ga II
$\mathbf{B}_{10}$	$=$	$-3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(16e) Ga II
$\mathbf{B}_{11}$	$=$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}}$	(24f) Ga III
$\mathbf{B}_{12}$	$=$	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}}$	(24f) Ga III
$\mathbf{B}_{13}$	$=$	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{y}}$	(24f) Ga III
$\mathbf{B}_{14}$	$=$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{y}}$	(24f) Ga III
$\mathbf{B}_{15}$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{z}}$	(24f) Ga III
$\mathbf{B}_{16}$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{z}}$	(24f) Ga III
$\mathbf{B}_{17}$	$=$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Ga IV
$\mathbf{B}_{18}$	$=$	$x_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Ga IV
$\mathbf{B}_{19}$	$=$	$x_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Ga IV
$\mathbf{B}_{20}$	$=$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Ga IV
$\mathbf{B}_{21}$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(24g) Ga IV
$\mathbf{B}_{22}$	$=$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24g) Ga IV

References

- [1] X. Gui, E. Feng, H. Cao, and R. J. Cava, *Ferromagnetic $\text{Cr}_4\text{PtGa}_{17}$: A Novel Half-Heusler-Type Compound with a Breathing Pyrochlore Lattice*, J. Am. Chem. Soc. **143**, 14342–14351 (2021), doi:10.1021/jacs.1c06667.

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