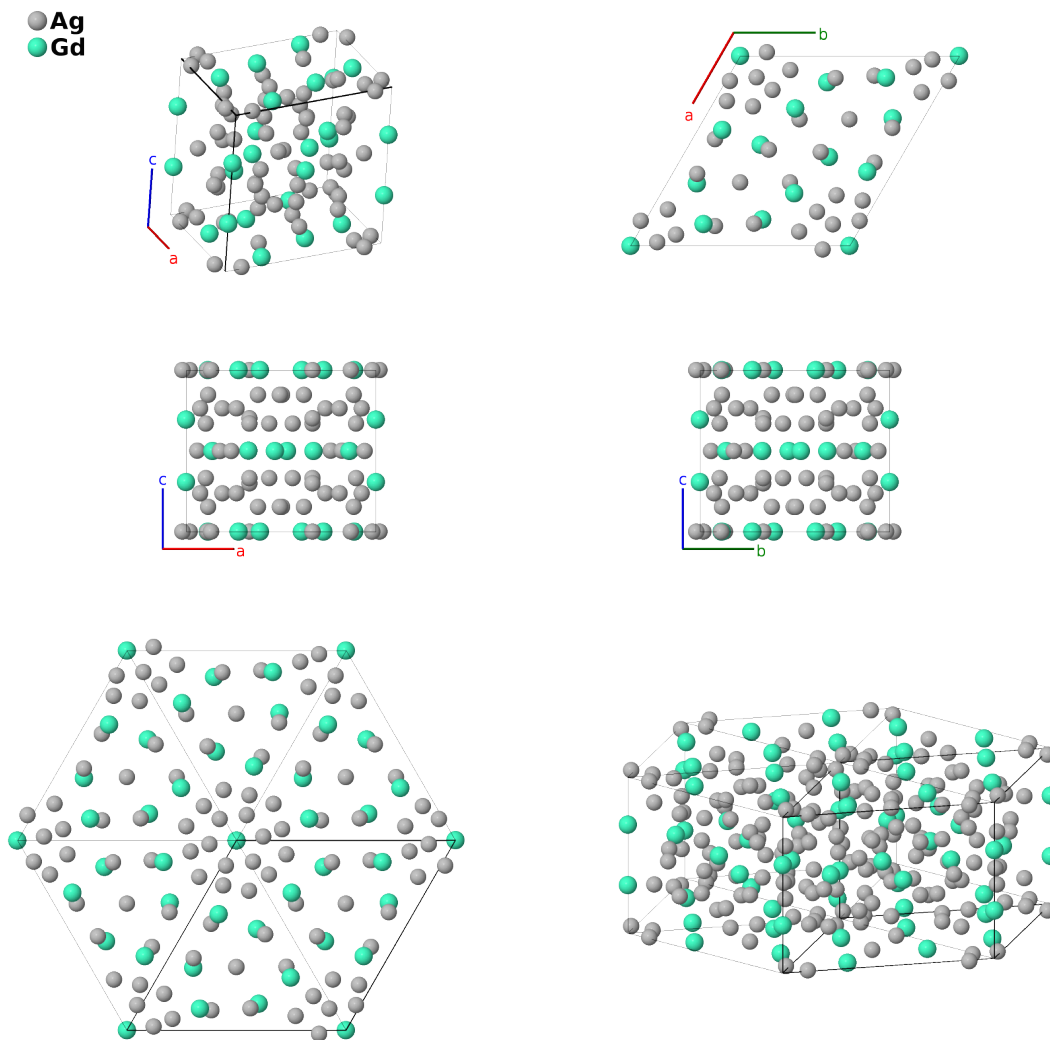


Ag₅₁Gd₁₄ Structure: A27B7_hP68_175_chjk3l_ejk-001

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<https://aflow.org/p/V9AH>

https://aflow.org/p/A27B7_hP68_175_chjk3l_ejk-001



Prototype	Ag ₅₁ Gd ₁₄
AFLOW prototype label	A27B7_hP68_175_chjk3l_ejk-001
ICSD	9085
Pearson symbol	hP68
Space group number	175
Space group symbol	<i>P6/m</i>
AFLOW prototype command	<code>aflow --proto=A27B7_hP68_175_chjk3l_ejk-001 --params=a, c/a, z₂, z₃, x₄, y₄, x₅, y₅, x₆, y₆, x₇, y₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀</code>

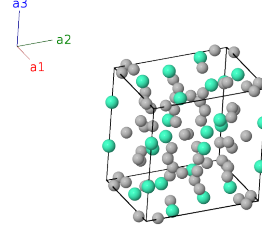
Other compounds with this structure

Ag₅₁Ce₁₄, Ag₅₁Dy₁₄, Ag₅₁Er₁₄, Ag₅₁Ho₁₄, Ag₅₁La₁₄, Ag₅₁Nd₁₄, Ag₅₁Pr₁₄, Ag₅₁Pu₁₄, Ag₅₁Sm₁₄, Ag₅₁Tb₁₄, Ag₅₁Th₁₄, Ag₅₁Y₁₄, Au₅₁Ce₁₄, Au₅₁Dy₁₄, Au₅₁Gd₁₄, Au₅₁Ho₁₄, Au₅₁La₁₄, Au₅₁Pd₁₄, Au₅₁Pr₁₄, Au₅₁Sm₁₄, Au₅₁Tb₁₄, Au₅₁Th₁₄, Au₅₁U₁₄, Au₅₁Y₁₄, Cd₅₁Cu₁₄, Cd₅₁Eu₁₄, Cd₅₁Hg₁₄, Cd₅₁Th₁₄, Cd₅₁Yb₁₄, Cu₅₁Hf₁₄, Cu₅₁Th₁₄, Cu₅₁Zr₁₄, Hg₅₁Eu₁₄, Hg₅₁Sr₁₄, Hg₅₁Yb₁₄, Ag₉Au₄₂U₁₄, Au₄₂Cu₉U₁₄, Au₅₁Th₇U₇, Cu₉Au₄₂U₁₄, Cu₃₈Ga₁₃Lu₁₄, Cu₄₆Ga₅U₁₄, Cu₄₀Ga₁₁Er₁₄

- This is often referred to as Ag_{3.6}Gd. Sources such as (Wang, 2008) list this as Ag₅₁Gd₁₄, but the exact stoichiometry depends on the occupation of the Ag-III (6j) site. If this site is half-filled we get the preferred stoichiometry. The Al (6j) sites are quite close together, forming a hexagon of side 1.57Å with second neighbors at 2.72Å. When the site is half filled it is likely that the three silver atoms form a triangle with side 2.57Å in one of the two allowed orientations.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Ag I
\mathbf{B}_2	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(2c)	Ag I
\mathbf{B}_3	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2e)	Gd I
\mathbf{B}_4	$= -z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(2e)	Gd I
\mathbf{B}_5	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4h)	Ag II
\mathbf{B}_6	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4h)	Ag II
\mathbf{B}_7	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4h)	Ag II
\mathbf{B}_8	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4h)	Ag II
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}}$	(6j)	Ag III
\mathbf{B}_{10}	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6j)	Ag III
\mathbf{B}_{11}	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}}$	(6j)	Ag III
\mathbf{B}_{12}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}}$	(6j)	Ag III
\mathbf{B}_{13}	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6j)	Ag III
\mathbf{B}_{14}	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}}$	(6j)	Ag III
\mathbf{B}_{15}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}}$	(6j)	Gd II
\mathbf{B}_{16}	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}}$	(6j)	Gd II
\mathbf{B}_{17}	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}}$	(6j)	Gd II
\mathbf{B}_{18}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}}$	(6j)	Gd II
\mathbf{B}_{19}	$= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2$	$=$	$\frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}}$	(6j)	Gd II
\mathbf{B}_{20}	$= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2$	$=$	$\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}}$	(6j)	Gd II
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)	Ag IV
\mathbf{B}_{22}	$= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6k)	Ag IV

$$\begin{aligned}
\mathbf{B}_{63} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(121) & \text{Ag VII} \\
\mathbf{B}_{64} &= y_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= \frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(121) & \text{Ag VII} \\
\mathbf{B}_{65} &= (x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= \frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(121) & \text{Ag VII} \\
\mathbf{B}_{66} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= \frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(121) & \text{Ag VII} \\
\mathbf{B}_{67} &= -y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= \frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(121) & \text{Ag VII} \\
\mathbf{B}_{68} &= -(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(121) & \text{Ag VII}
\end{aligned}$$

References

- [1] D. M. Bailey and G. R. Klein, *The Crystal Structure of GdAg_{3,6}*, Acta Crystallogr. Sect. B **27**, 650–653 (1971), doi:10.1107/S0567740871002711.

Found in

- [1] H. Wang, L. G. Zhang, W. J. Zhu, H. S. Liu, and Z. P. Jin, *Thermodynamic assessment of the Ag–Gd binary system*, J. Alloys Compd. **466**, 165–168 (2008), doi:10.1016/j.jallcom.2007.11.049.