# $Ag_{51}Gd_{14}$ Structure: A27B7_hP68_175_chjk3l_ejk-001

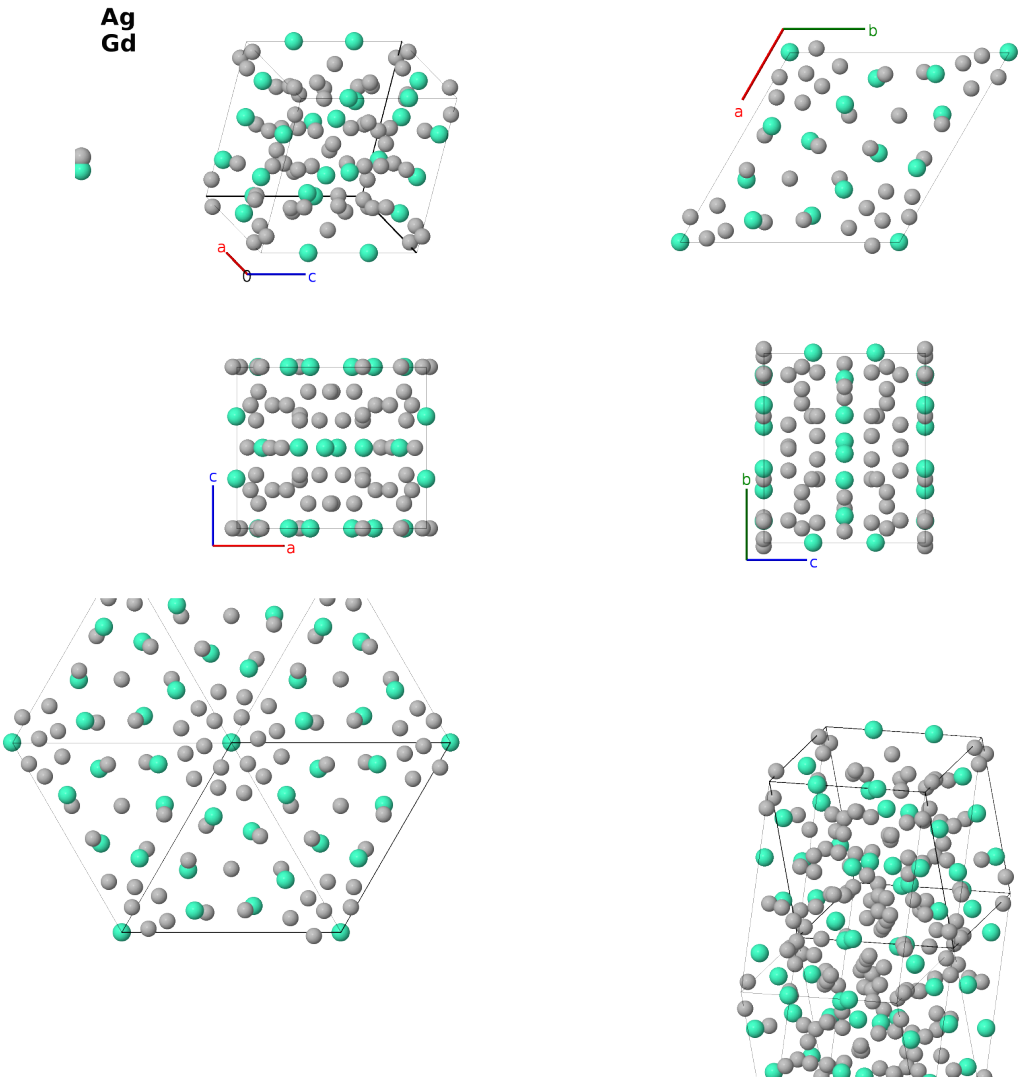
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/V9AH

https://aflow.org/prototype-encyclopedia/A27B7_hP68_175_chjk3l_ejk-001




| | |
|---|---|
| **Prototype** | $Ag_{51}Gd_{14}$ |
| **AFLOW prototype label** | A27B7_hP68_175_chjk3l_ejk-001 |
| **ICSD** | 9085 |
| **CCDC** | 1594139 |
| **Pearson symbol** | hP68 |

| | |
|---|---|
| **Space group number** | 175 |
| **Space group symbol** | $P6/m$ |
| **AFLOW prototype command** | `aflow --proto=A27B7_hP68_175_chjk3l_ejk-001 --params=`$a, c/a, z_2, z_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$ |

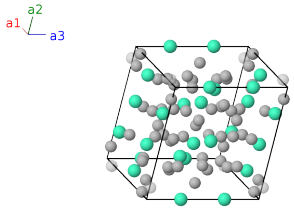
**Other compounds with this structure**

$Ag_{51}Ce_{14}$, $Ag_{51}Dy_{14}$, $Ag_{51}Er_{14}$, $Ag_{51}Ho_{14}$, $Ag_{51}La_{14}$, $Ag_{51}Nd_{14}$, $Ag_{51}Pr_{14}$, $Ag_{51}Pu_{14}$, $Ag_{51}Sm_{14}$, $Ag_{51}Tb_{14}$, $Ag_{51}Th_{14}$, $Ag_{51}Y_{14}$, $Au_{51}Ce_{14}$, $Au_{51}Dy_{14}$, $Au_{51}Gd_{14}$, $Au_{51}Ho_{14}$, $Au_{51}La_{14}$, $Au_{51}Pd_{14}$, $Au_{51}Pr_{14}$, $Au_{51}Sm_{14}$, $Au_{51}Tb_{14}$, $Au_{51}Th_{14}$, $Au_{51}U_{14}$, $Au_{51}Y_{14}$, $Cd_{51}Cu_{14}$, $Cd_{51}Eu_{14}$, $Cd_{51}Hg_{14}$, $Cd_{51}Th_{14}$, $Cd_{51}Yb_{14}$, $Cu_{51}Hf_{14}$, $Cu_{51}Th_{14}$, $Cu_{51}Zr_{14}$, $Hg_{51}Eu_{14}$, $Hg_{51}Sr_{14}$, $Hg_{51}Yb_{14}$, $Ag_9Au_{42}U_{14}$, $Au_{42}Cu_9U_{14}$, $Au_{51}Th_7U_7$, $Cu_9Au_{42}U_{14}$, $Cu_{38}Ga_{13}Lu_{14}$, $Cu_{46}Ga_5U_{14}$, $Cu_{40}Ga_{11}Er_{14}$

- This is often referred to as $Ag_{3.6}Gd$. Sources such as (Wang, 2008) list this as $Ag_{51}Gd_{14}$, 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 allow orientations.

**Hexagonal primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




**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 |
| $\mathbf{B_{23}}$ | $=$ | $-(x_6-y_6)\;\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Ag IV |
| $\mathbf{B_{24}}$ | $=$ | $-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Ag IV |
| $\mathbf{B_{25}}$ | $=$ | $y_6\,\mathbf{a}_1 - (x_6-y_6)\;\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(-x_6+2y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Ag IV |
| $\mathbf{B_{26}}$ | $=$ | $(x_6-y_6)\;\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Ag IV |
| $\mathbf{B_{27}}$ | $=$ | $x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Gd III |
| $\mathbf{B_{28}}$ | $=$ | $-y_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Gd III |
| $\mathbf{B_{29}}$ | $=$ | $-(x_7-y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Gd III |
| $\mathbf{B_{30}}$ | $=$ | $-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Gd III |
| $\mathbf{B_{31}}$ | $=$ | $y_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Gd III |
| $\mathbf{B_{32}}$ | $=$ | $(x_7-y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\;\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6k) | Gd III |
| $\mathbf{B_{33}}$ | $=$ | $x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{34}}$ | $=$ | $-y_8\,\mathbf{a}_1 + (x_8-y_8)\;\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_8-2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{35}}$ | $=$ | $-(x_8-y_8)\;\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{36}}$ | $=$ | $-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{37}}$ | $=$ | $y_8\,\mathbf{a}_1 - (x_8-y_8)\;\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(-x_8+2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{38}}$ | $=$ | $(x_8-y_8)\;\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{39}}$ | $=$ | $-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{40}}$ | $=$ | $y_8\,\mathbf{a}_1 - (x_8-y_8)\;\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(-x_8+2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{41}}$ | $=$ | $(x_8-y_8)\;\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{42}}$ | $=$ | $x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{43}}$ | $=$ | $-y_8\,\mathbf{a}_1 + (x_8-y_8)\;\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_8-2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{44}}$ | $=$ | $-(x_8-y_8)\;\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$ | (12l) | Ag V |
| $\mathbf{B_{45}}$ | $=$ | $x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{46}}$ | $=$ | $-y_9\,\mathbf{a}_1 + (x_9-y_9)\;\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_9-2y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{47}}$ | $=$ | $-(x_9-y_9)\;\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{48}}$ | $=$ | $-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{49}}$ | $=$ | $y_9\,\mathbf{a}_1 - (x_9-y_9)\;\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(-x_9+2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{50}}$ | $=$ | $(x_9-y_9)\;\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{51}}$ | $=$ | $-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{52}}$ | $=$ | $y_9\,\mathbf{a}_1 - (x_9-y_9)\;\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(-x_9+2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{53}}$ | $=$ | $(x_9-y_9)\;\mathbf{a}_1 + x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{54}}$ | $=$ | $x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{55}}$ | $=$ | $-y_9\,\mathbf{a}_1 + (x_9-y_9)\;\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_9-2y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{56}}$ | $=$ | $-(x_9-y_9)\;\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$ | (12l) | Ag VI |
| $\mathbf{B_{57}}$ | $=$ | $x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_{10}+y_{10})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{10}-y_{10})\;\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$ | (12l) | Ag VII |

$$\mathbf{B_{58}} = -y_{10}\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10} - 2y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{59}} = -(x_{10} - y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{60}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{61}} = y_{10}\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{10} + 2y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{62}} = (x_{10} - y_{10})\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{63}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{64}} = y_{10}\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_{10} + 2y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{65}} = (x_{10} - y_{10})\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{66}} = x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{67}} = -y_{10}\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10} - 2y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

$$\mathbf{B_{68}} = -(x_{10} - y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad (12l) \quad \text{Ag VII}$$

## 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.


## First cited in


H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.