# Ca$_5$Pb$_3$ Structure:
# A5B3_hP48_186_3cd_3c-001

https://aflow.org/p/XPM6

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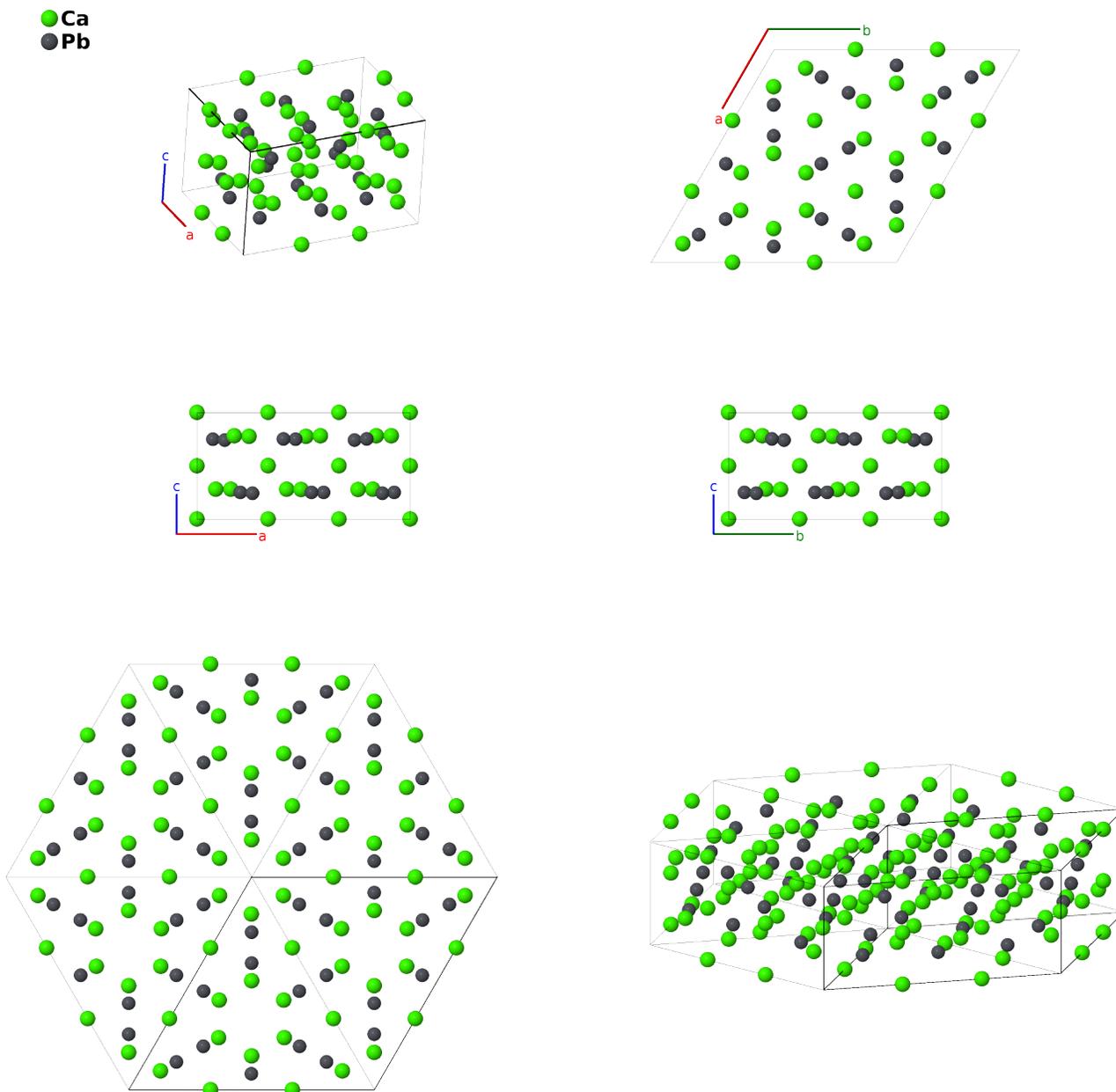


| Prototype | Ca$_5$Pb$_3$ |
|---|---|
| **AFLOW prototype label** | A5B3_hP48_186_3cd_3c-001 |
| **ICSD** | 58922 |

| | | Pearson symbol | | hP48 |
|---|---|---|---|---|

**Pearson symbol**  hP48

**Space group number**  186

**Space group symbol**  $P6_3mc$

**AFLOW prototype command**  `aflow --proto=A5B3_hP48_186_3cd_3c-001`
`--params=`$a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, y_7, z_7$

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**Hexagonal primitive vectors**

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



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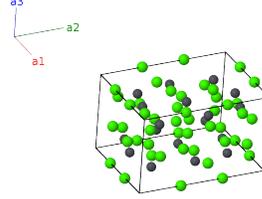
**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $x_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$ | = | $-\sqrt{3}ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (6c) | Ca I |
| $\mathbf{B_2}$ | = | $x_1\,\mathbf{a_1} + 2x_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_1\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (6c) | Ca I |
| $\mathbf{B_3}$ | = | $-2x_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_1\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (6c) | Ca I |
| $\mathbf{B_4}$ | = | $-x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + \left(z_1 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\sqrt{3}ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca I |
| $\mathbf{B_5}$ | = | $-x_1\,\mathbf{a_1} - 2x_1\,\mathbf{a_2} + \left(z_1 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_1\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca I |
| $\mathbf{B_6}$ | = | $2x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + \left(z_1 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_1\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca I |
| $\mathbf{B_7}$ | = | $x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$ | = | $-\sqrt{3}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (6c) | Ca II |
| $\mathbf{B_8}$ | = | $x_2\,\mathbf{a_1} + 2x_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (6c) | Ca II |
| $\mathbf{B_9}$ | = | $-2x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (6c) | Ca II |
| $\mathbf{B_{10}}$ | = | $-x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\sqrt{3}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca II |
| $\mathbf{B_{11}}$ | = | $-x_2\,\mathbf{a_1} - 2x_2\,\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca II |
| $\mathbf{B_{12}}$ | = | $2x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca II |
| $\mathbf{B_{13}}$ | = | $x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$ | = | $-\sqrt{3}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (6c) | Ca III |
| $\mathbf{B_{14}}$ | = | $x_3\,\mathbf{a_1} + 2x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (6c) | Ca III |
| $\mathbf{B_{15}}$ | = | $-2x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (6c) | Ca III |
| $\mathbf{B_{16}}$ | = | $-x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\sqrt{3}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca III |
| $\mathbf{B_{17}}$ | = | $-x_3\,\mathbf{a_1} - 2x_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca III |
| $\mathbf{B_{18}}$ | = | $2x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Ca III |
| $\mathbf{B_{19}}$ | = | $x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$ | = | $-\sqrt{3}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (6c) | Pb I |
| $\mathbf{B_{20}}$ | = | $x_4\,\mathbf{a_1} + 2x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (6c) | Pb I |
| $\mathbf{B_{21}}$ | = | $-2x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (6c) | Pb I |
| $\mathbf{B_{22}}$ | = | $-x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\sqrt{3}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Pb I |
| $\mathbf{B_{23}}$ | = | $-x_4\,\mathbf{a_1} - 2x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $-\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Pb I |
| $\mathbf{B_{24}}$ | = | $2x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$ | = | $\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$ | (6c) | Pb I |
| $\mathbf{B_{25}}$ | = | $x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$ | = | $-\sqrt{3}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (6c) | Pb II |

$$\mathbf{B_{26}} = x_5\,\mathbf{a}_1 + 2x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \tfrac{3}{2}ax_5\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb II}$$

$$\mathbf{B_{27}} = -2x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = -\tfrac{3}{2}ax_5\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb II}$$

$$\mathbf{B_{28}} = -x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a}_3 = \sqrt{3}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb II}$$

$$\mathbf{B_{29}} = -x_5\,\mathbf{a}_1 - 2x_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{3}{2}ax_5\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb II}$$

$$\mathbf{B_{30}} = 2x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{3}{2}ax_5\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb II}$$

$$\mathbf{B_{31}} = x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = -\sqrt{3}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb III}$$

$$\mathbf{B_{32}} = x_6\,\mathbf{a}_1 + 2x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{3}{2}ax_6\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb III}$$

$$\mathbf{B_{33}} = -2x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = -\tfrac{3}{2}ax_6\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb III}$$

$$\mathbf{B_{34}} = -x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = \sqrt{3}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb III}$$

$$\mathbf{B_{35}} = -x_6\,\mathbf{a}_1 - 2x_6\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{3}{2}ax_6\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb III}$$

$$\mathbf{B_{36}} = 2x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{3}{2}ax_6\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (6c) \qquad \text{Pb III}$$

$$\mathbf{B_{37}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\left(x_7 + y_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_7 - y_7\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{38}} = -y_7\,\mathbf{a}_1 + \left(x_7 - y_7\right)\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\left(x_7 - 2y_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{39}} = -\left(x_7 - y_7\right)\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\left(2x_7 - y_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{40}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_7 + y_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_7 - y_7\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{41}} = y_7\,\mathbf{a}_1 - \left(x_7 - y_7\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(-x_7 + 2y_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{42}} = \left(x_7 - y_7\right)\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(2x_7 - y_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{43}} = -y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_7 + y_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_7 - y_7\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{44}} = -\left(x_7 - y_7\right)\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\left(-x_7 + 2y_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{45}} = x_7\,\mathbf{a}_1 + \left(x_7 - y_7\right)\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\left(2x_7 - y_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{46}} = y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_7 + y_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_7 - y_7\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{47}} = \left(x_7 - y_7\right)\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_7 - 2y_7\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

$$\mathbf{B_{48}} = -x_7\,\mathbf{a}_1 - \left(x_7 - y_7\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(2x_7 - y_7\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (12d) \qquad \text{Ca IV}$$

## References

[1] O. Helleis, H. Kandler, E. Leicht, W. Quiring, and E. Wölfel, *Die Kristallstrukturen der intermetallischen Phasen Ca₃₃Ge, Ca₇Ge, Ca₃Pb und Ca₅Pb₃*, Z. Anorganische und Allgemeine Chemie **320**, 86–100 (1963), doi:10.1002/zaac.19633200113.

## Found in

[1] G. Bruzzone and F. Merlo, *The equilibrium phase diagram of the calcium-lead system and crystal structures of the compounds CaPb, EuPb and YbPb*, J. Less-Common Met. **48**, 103–109 (1976), doi:10.1016/0022-5088(76)90236-8.