# $CaC_6$ Structure: A6B_hR7_166_f_b-001

This structure previously used the label(s) `A6B_hR7_166_g_a`. Calls to these addresses will be redirected here.

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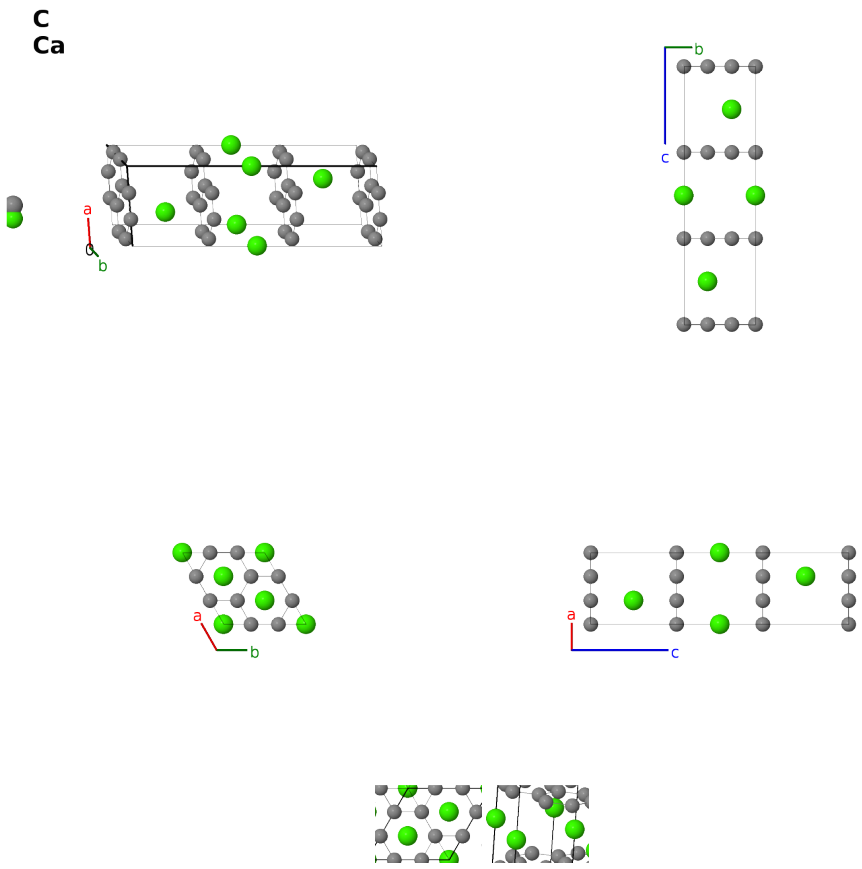
https://aflow.org/prototype-encyclopedia/N45M

https://aflow.org/prototype-encyclopedia/A6B_hR7_166_f_b-001




| | |
|---|---|
| **Prototype** | $CaC_6$ |
| **AFLOW prototype label** | A6B_hR7_166_f_b-001 |
| **Pearson symbol** | hR7 |
| **Space group number** | 166 |
| **Space group symbol** | $R\bar{3}m$ |
| **AFLOW prototype command** | `aflow --proto=A6B_hR7_166_f_b-001 --params=`$a, c/a, x_2$ |

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- Superconducting structure, $T_c = 11.5$K.
- (Emery, 2005) completely described the structure, but and referenced an upcoming paper fully detailing there methods, but we have found no reference to this paper, and ICSD entry, or a CCDC entry.
- Hexagonal settings of rhombohedral structures can be obtained with the option `--hex`.

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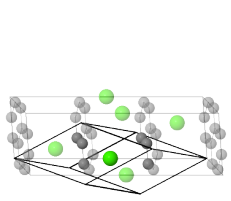
**Rhombohedral primitive vectors**

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (1b) | Ca I |
| $\mathbf{B_2}$ | = | $x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$ | = | $\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$ | (6f) | C I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$ | (6f) | C I |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}}$ | (6f) | C I |
| $\mathbf{B_5}$ | = | $-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$ | = | $-\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$ | (6f) | C I |
| $\mathbf{B_6}$ | = | $-x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $-\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$ | (6f) | C I |
| $\mathbf{B_7}$ | = | $x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}}$ | (6f) | C I |

**References**


[1] N. Emery, C. Hérold, M. d'Astuto, V. Garcia, C. Bellin, J. F. Marêché, P. Lagrange, and G. Loupias, *Superconductivity of Bulk $CaC_6$*, Phys. Rev. Lett. **95**, 087003 (2005), doi:10.1103/PhysRevLett.95.087003.


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