CaC_6 Structure: A6B_hR7_166_f_b-001

This structure originally had the label `A6B_hR7_166_g_a`. Calls to that address will be redirected here.

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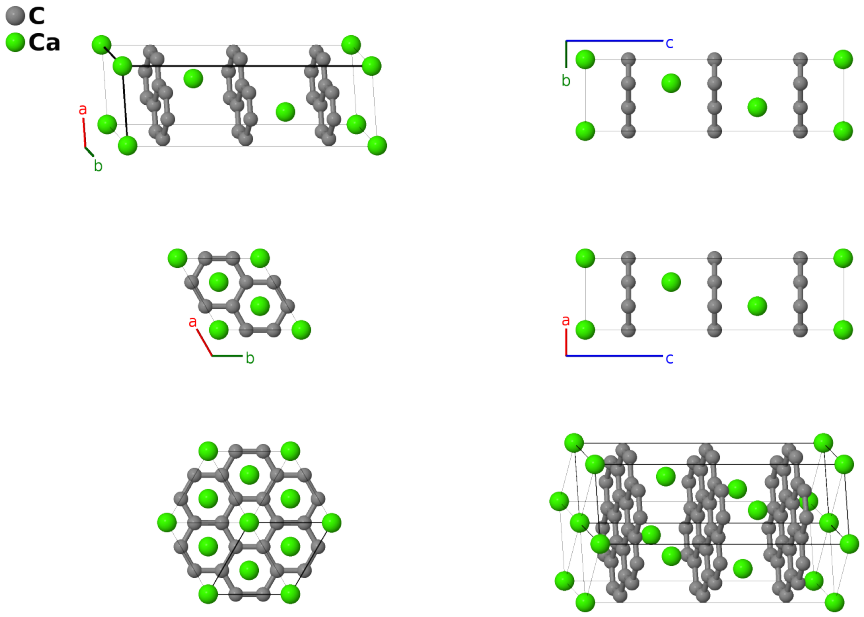
https://aflow.org/p/N45M

https://aflow.org/p/A6B_hR7_166_f_b-001

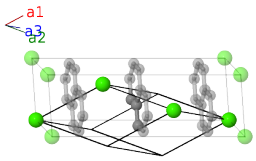


Prototype	CaC_6
AFLOW prototype label	A6B_hR7_166_f_b-001
ICSD	none
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A6B_hR7_166_f_b-001 --params=`$a, c/a, x_2$

- 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`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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.