

$\text{Ba}_{6.7}\text{Ca}_{0.3}\text{Cl}_2\text{F}_{12}$  $hP30$  $(176) P6_3/m - h^4cba$ **Ba<sub>7-x</sub>Ca<sub>x</sub>Cl<sub>2</sub>F<sub>12</sub> [1]**

Structural features: Infinite columns of base-linked Ba(Cl<sub>2</sub>F<sub>4</sub>)F<sub>3</sub> tricapped trigonal prisms (one split F site) share atoms to form a 3D-framework with propeller-like columns; Ca and additional Ba in channels of hexagonal cross-section parallel to [001] (partial disorder).

Frühmann B. et al. (2004) [1]

 $\text{Ba}_{6.70}\text{Ca}_{0.30}\text{Cl}_2\text{F}_{12}$  $a = 1.05381$ ,  $c = 0.42121$  nm,  $c/a = 0.400$ ,  $V = 0.4051$  nm<sup>3</sup>,  $Z = 1$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	6 <i>h</i>	<i>m</i> ..	0.1154	0.2155	<sup>1</sup> / <sub>4</sub>	0.5	
F2	6 <i>h</i>	<i>m</i> ..	0.1498	0.2708	<sup>1</sup> / <sub>4</sub>	0.5	
Ba3	6 <i>h</i>	<i>m</i> ..	0.40311	0.29278	<sup>1</sup> / <sub>4</sub>		
F4	6 <i>h</i>	<i>m</i> ..	0.43346	0.05625	<sup>1</sup> / <sub>4</sub>		tetrahedron Ba <sub>4</sub>
Cl5	2 <i>c</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		
Ca6	2 <i>b</i>	-3..	0	0	0	0.15	
Ba7	2 <i>a</i>	-6..	0	0	<sup>1</sup> / <sub>4</sub>	0.35	

Experimental: single crystal, diffractometer, X-rays, R = 0.025, T = 300 K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Frühmann B., Kubel F., Hagemann H., Bill H. (2004), Z. Anorg. Allg. Chem. 630, 1484-1488.