

Ba <sub>7</sub> Cl <sub>2</sub> F <sub>12</sub>	<i>hP27</i>	(174) <i>P</i> -6 – k <sup>3</sup> j <sup>4</sup> gedba
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**Ba<sub>7</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 share atoms to form a 3D-framework with propeller-like columns; additional Ba in channels of hexagonal cross-section parallel to [001] (partial disorder, splitting of neighboring site). Variant of Zr<sub>2</sub>Rh<sub>12</sub>P<sub>7</sub> antitype.

Kubel F. et al. (1999) [1]

Ba<sub>6.93</sub>Cl<sub>2</sub>F<sub>12</sub>

*a* = 1.06469, *c* = 0.41789 nm, *c/a* = 0.392, *V* = 0.4102 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	3 <i>k</i>	<i>m</i> ..	0.12	0.2717	<sup>1</sup> / <sub>2</sub>		
Ba2	3 <i>k</i>	<i>m</i> ..	0.40796	0.11095	<sup>1</sup> / <sub>2</sub>		
F3	3 <i>k</i>	<i>m</i> ..	0.4305	0.3719	<sup>1</sup> / <sub>2</sub>		
F4	3 <i>j</i>	<i>m</i> ..	0.0537	0.437	0		
F5	3 <i>j</i>	<i>m</i> ..	0.2165	0.1175	0	0.78	
F6	3 <i>j</i>	<i>m</i> ..	0.275	0.151	0	0.22	
Ba7	3 <i>j</i>	<i>m</i> ..	0.29104	0.40365	0		
Ba8	2 <i>g</i>	3..	0	0	0.25	0.043	
Cl9	1 <i>e</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0		
Cl10	1 <i>d</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>2</sub>		23-vertex polyhedron Ba <sub>9</sub> F <sub>12</sub> Cl <sub>2</sub>
Ba11	1 <i>b</i>	-6..	0	0	<sup>1</sup> / <sub>2</sub>	0.627	
Ba12	1 <i>a</i>	-6..	0	0	0	0.22	

Transformation from published data: *y,x,z*

Experimental: single crystal, diffractometer, X-rays, *wR* = 0.018, *T* = 300 K

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

References: [1] Kubel F., Bill H., Hagemann H. (1999), *Z. Naturforsch. B* 54, 515-518.