$Ba_7Cl_2F_{12}$	*hP*28	(176) $P6_3/m$ – h^4ca

$Ba_7Cl_2F_{12}$ disordered [1]; $Ca_2Co_{12}As_7$ [2]
Structural features: Infinite columns of base-linked $Ba(Cl_2F_4)F_3$ tricapped trigonal prisms (one split F site) share atoms to form a 3D-framework with propeller-like prism columns; additional Ba in channels of hexagonal cross-section parallel to [001]. Variant of $Zr_2Rh_{12}P_7$ antitype.

Kubel F. et al. (1999) [1]
$Ba_7Cl_2F_{12}$
a = 1.05955, c = 0.4201 nm, c/a = 0.396, V = 0.4084 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	6*h*	*m*..	0.1183	0.2167	$^1/_4$	0.5	
F2	6*h*	*m*..	0.1542	0.278	$^1/_4$	0.5	
Ba3	6*h*	*m*..	0.40447	0.29356	$^1/_4$		
F4	6*h*	*m*..	0.4332	0.056	$^1/_4$		tetrahedron Ba_4
Cl5	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$		sixcapped hexagonal prism Ba_6F_{12}
Ba6	2*a*	-6..	0	0	$^1/_4$	0.5	

Experimental: single crystal, diffractometer, X-rays, R = 0.026, T = 300 K

Remarks: The structure was studied jointly on powder and single-crystal diffraction data. Short interatomic distances for partly occupied site(s). An ordered model in space group (174) *P*-6 was tested and rejected; crystals with the ordered structure could, however, be obtained by a different crystal growth technique.

References: [1] Kubel F., Bill H., Hagemann H. (1999), Z. Anorg. Allg. Chem. 625, 643-649. [2] Hellmann A., Mewis A. (2001), Z. Anorg. Allg. Chem. 627, 1357-1364.