

$\text{Ba}_3\text{Zn}_{0.5}\text{MnCl}_3\text{F}_6$ $hP28$ $(176) P6_3/m - ih^2cb$ **Ba₆Mn₂ZnCl₆F₁₂** [1]

Structural features: MnF₆ trigonal prisms and ZnCl₆ octahedra (partial occupancy of infinite columns of face-linked octahedra). Filled-up derivative of Pr₃WO₆Cl₃.

Darriet J. et al. (1992) [1]

 $\text{Ba}_3\text{Cl}_3\text{F}_6\text{MnZn}_{0.50}$ $a = 1.0081, c = 0.58476 \text{ nm}, c/a = 0.580, V = 0.5147 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>i</i>	1	0.1615	0.5197	0.0147		single atom Mn
Cl2	6 <i>h</i>	<i>m</i> ..	0.1766	0.2266	$\frac{1}{4}$		non-colinear Zn ₂
Ba3	6 <i>h</i>	<i>m</i> ..	0.4035	0.0915	$\frac{1}{4}$		10-vertex polyhedron F ₆ Cl ₄
Mn4	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism F ₆
Zn5	2 <i>b</i>	-3..	0	0	0	0.5	octahedron Cl ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.022

References: [1] Darriet J., Ducau M., Feist M., Tressaud A. (1992), Eur. J. Solid State Inorg. Chem. 29, 435-443.