

Ba[ClO <sub>4</sub> ] <sub>2</sub> [H <sub>2</sub> O] <sub>3</sub>	<i>hP</i> 28	(176) <i>P</i> 6 <sub>3</sub> / <i>m</i> – <i>ihf</i> <sup>2</sup> <i>b</i>
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**Ba(ClO<sub>4</sub>)<sub>2</sub>·3H<sub>2</sub>O** [2]

Structural features: Slabs containing ClO<sub>4</sub> tetrahedra and Ba atoms (BaCl<sub>2</sub> triangle mesh) alternate with layers containing H<sub>2</sub>O molecules (perpendicular to [001]).

Gallucci J.C., Gerkin R.E. (1988) [1]

BaCl<sub>2</sub>H<sub>6</sub>O<sub>11</sub>

*a* = 0.7277, *c* = 0.9656 nm, *c/a* = 1.327, *V* = 0.4428 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.4592	0.1811	0.0838		single atom Cl
O2	6 <i>h</i>	<i>m</i> ..	0.1686	0.2562	<sup>1</sup> / <sub>4</sub>		10-vertex polyhedron O <sub>8</sub> Ba <sub>2</sub>
O3	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1132		single atom Cl
Cl4	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.53411		tetrahedron O <sub>4</sub>
Ba5	2 <i>b</i>	-3..	0	0	0		icosahedron O <sub>12</sub>
H6	6 <i>h</i>	<i>m</i> ..	0.16	0.361	<sup>1</sup> / <sub>4</sub>		
H7	6 <i>h</i>	<i>m</i> ..	0.326	0.31	<sup>1</sup> / <sub>4</sub>		

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, *R* = 0.023, *T* = 295 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Gallucci J.C., Gerkin R.E. (1988), Acta Crystallogr. C 44, 1873-1876. [2] Mani N.V., Ramaseshan S. (1960), Z. Kristallogr. 114, 200-214.