

Ba ₄ Cl ₆ O	<i>hP22</i>	(186) <i>P6₃mc</i> – <i>c</i> ³ <i>b</i> ²
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Ba₄OCl₆ [1]; Na₆ZnO₄ [2]; K₆HgS₄ [3]; Na₆ZnS₄ [4]

Structural features: Single OBa₄ tetrahedra in a Mg-type (h.c.p.) arrangement in a matrix of Cl atoms. See Fig. IV.24.

Frit B. et al. (1970) [1]

Ba₄Cl₆O

a = 0.997, *c* = 0.749 nm, *c/a* = 0.751, *V* = 0.6448 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	6 <i>c</i>	. <i>m</i> .	0.1456	0.8544	0.044		tetrahedron Ba ₄
Ba2	6 <i>c</i>	. <i>m</i> .	0.1954	0.8045	0.4366		square antiprism OCl ₇
Cl3	6 <i>c</i>	. <i>m</i> .	0.5296	0.47	0.2322		single atom Ba
Ba4	2 <i>b</i>	3 <i>m</i> .	1/3	2/3	0.0		single atom O
O5	2 <i>b</i>	3 <i>m</i> .	1/3	2/3	0.3391		tetrahedron Ba ₄

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.0634

Experimental: single crystal, Weissenberg photographs, X-rays, *R* = 0.052

Remarks: We assume that in table 1 of [2] the *y*-coordinate of former Na2 is misprinted as -0.5374 instead of 0.5370 (agreement with Wyckoff position 6*c*).

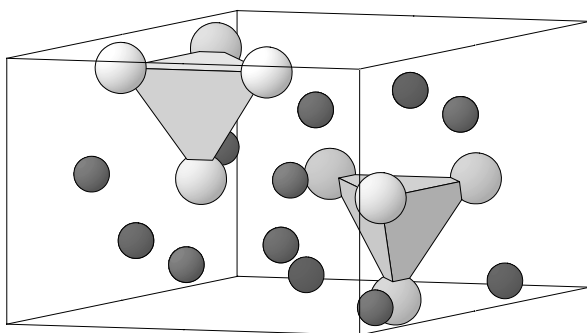


Fig. IV.24. **Ba₄OCl₆**

Arrangement of OBa₄ tetrahedra (Ba atoms large) and Cl atoms (small).

References: [1] Frit B., Holmberg B., Galy J. (1970), Acta Crystallogr. B 26, 16-19. [2] Kastner P., Hoppe R. (1974), Z. Anorg. Allg. Chem. 409, 69-76. [3] Sommer H., Hoppe R., Jansen M. (1976), Naturwissenschaften 63, 194-195. [4] Klepp K.O., Bronger W. (1983), Rev. Chim. Miner. 20, 682-688.