

BCl_3	$hP8$	$(176) P6_3/m - hc$
----------------	-------	---------------------

BCl_3 [2]; BI_3 [3]

Structural features: BCl_3 trigonal units in a Mg-type (h.c.p.) arrangement.

Atoji M., Lipscomb W.N. (1957) [1]

BCl_3

$a = 0.608$, $c = 0.655$ nm, $c/a = 1.077$, $V = 0.2097$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	$6h$	$m..$	0.0455	0.3763	$\frac{1}{4}$		single atom B
B2	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Cl_3

Experimental: single crystal, photographs, X-rays, $R = 0.140$, $T = 108$ K

Remarks: The description in space group $(173) P6_3$ in [1] does not take into consideration all symmetry elements of the proposed structure (space group $(176) P6_3/m$ had been rejected based on a comparison of intensities). BI_3 was reported in space group $(176) P6_3/m$ [3].

References: [1] Atoji M., Lipscomb W.N. (1957), J. Chem. Phys. 27, 195. [2] Rollier M.A., Riva A. (1947), Gazz. Chim. Ital. 77, 361-366. [3] Ring M.A., Donnay J.D.H., Koski W.S. (1962), Inorg. Chem. 1, 109-111.