$Ba_3Cu[P_2O_7]Br_3$	*hP*48	(176) $P6_3/m$ – i^2h^3fa

$Ba_3Cu(P_2O_7)Br_3$ [1]
Structural features: Units of two vertex-linked PO_4 tetrahedra (parallel to [001], split O sites) and $CuBr_3$ trigonal units (perpendicular to [001]).

Etheredge K.M.S. et al. (1996) [1]
$Ba_3Br_3CuO_7P_2$
a = 1.0161, c = 0.7044 nm, c/a = 0.693, V = 0.6298 nm^3, Z = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*i*	1	0.173	0.543	0.015	0.667	
O2	12*i*	1	0.545	0.355	0.076	0.333	
Br3	6*h*	*m*..	0.2417	0.2461	$^1/_4$		single atom Cu
O4	6*h*	*m*..	0.259	0.609	$^1/_4$	0.333	non-colinear O_2
Ba5	6*h*	*m*..	0.39441	0.04523	$^1/_4$		non-colinear O_2
P6	4*f*	3..	$^1/_3$	$^2/_3$	0.0387		
Cu7	2*a*	-6..	0	0	$^1/_4$		coplanar triangle Br_3

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.030, T = 155 K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Etheredge K.M.S., Mackay R., Schimek G.L., Hwu S.J. (1996), Inorg. Chem. 35, 7919-7921.