Crystal structure of tribarium arsenide borate, $\text{Ba}_3\text{As}[\text{BO}_3]$

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Received October 25, 1996, transferred to 1st update of database ICSD in 1998, CSD-No. 402682

Table 1. Parameters used for the X-ray data collection

Crystal:	dark red plate, size 0.12 x 0.16 x 0.25 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	202.72 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	189
Criterion for F_o :	$F_o > 4 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	14
Program:	SHELX-76

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
O	6h	0.522(2)	1.045(3)	1/4	0.019(3)
B	2d	1/3	2/3	3/4	0.021(8)

Source of material: $\text{Ba}_3\text{As}[\text{BO}_3]$ is synthesized from a mixture of Ba_3As_2 and $\text{Ba}_3[\text{BO}_3]_2$ (ratio 1:1.2) in a sealed Nb ampoule at 1550 K.

$\text{Ba}_3\text{As}[\text{BO}_3]$ is isostructural to $\text{Ba}_3\text{P}[\text{BO}_3]$ (see ref. 1). The crystal structure can be described as a space-filling arrangement of distorted cubes Ba_8 and Edshammer polyhedra Ba_{11} which are centered by isolated As atoms and trigonal planar anions $[\text{BO}_3]^{3-}$, respectively ($d(\text{B}-\text{O}) = 1.380(11)$ Å). Note that the U_{33} parameter for Ba2 is significantly larger than that found in ref. 1.

AsBBa_3O_3 , hexagonal, $P6_3/m$ (No. 194), $a = 5.528(1)$ Å, $c = 13.606(2)$ Å, $V = 360.1$ Å³, $Z = 2$, $R(F) = 0.072$, $R_w(F) = 0.069$.

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ba(1)	4f	1/3	2/3	0.0995(2)	0.032(1)	U_{11}	0.033(1)	$U_{11}/2$	0	0
Ba(2)	2b	0	0	1/4	0.012(1)	U_{11}	0.062(2)	$U_{11}/2$	0	0
As	2a	0	0	0	0.037(2)	U_{11}	0.047(4)	$U_{11}/2$	0	0

References

1. Somer, M.; Carrillo-Cabrera, W.; Peters, K.; von Schnering, H.G.: Crystal structure of tribarium phosphide borate, $\text{Ba}_3\text{P}(\text{BO}_3)$. Z. Kristallogr. **210** (1995) 449-450.
2. Sheldrick, G. M.: SHELXL-76, Programs for Crystal Structures Determination. Cambridge, UK 1976.