Crystal structure of indium magnesium tribromide, InMgBr_3

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Fig. 1. [010] view with In as large shaded circles, Mg as small open circles, and Br as medium-sized black circles.

Source of material: Synthesis from molten InBr_3 and elemental magnesium at 723 K for five days in evacuated glass ampoules, followed by slow cooling (2 K/hour).

InMgBr_3 crystallizes in the NH_4CdCl_3 structure type (see ref. 1), as do other ternary transition metal bromides containing univalent indium (see refs. 2, 3). While magnesium is octahedrally coordinated by bromine (262 pm - 273 pm), univalent indium resides in a strongly distorted trigonal prism of bromine, tricapped by additional bromine ions (eight bonds between 330 pm and 353 pm, one distance of 420 pm).

Br_3InMg , orthorhombic, $Pnma$ (No. 62), $a = 9.4395(1) \text{ \AA}$, $b = 3.9538(1) \text{ \AA}$, $c = 15.3744(2) \text{ \AA}$, $V = 573.8 \text{ \AA}^3$, $Z = 4$, $\rho_m = 4.390 \text{ g}\cdot\text{cm}^{-3}$, $R_p = 0.028$, $R_{wp} = 0.036$, $R_{Bragg} = 0.02$, $R_{exp} = 0.028$.

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

Powder:	0.1 mm capillary of powdery, transparent material (ground needles)
Wavelength:	$\text{Cu } K_{\alpha 1}$ radiation (1.54056 $\text{\AA}$)
μ :	249.50 cm^{-1}
Diffractometer:	Stoe STADI powder diffractometer
Sample geometry:	cylinder
Scan mode:	2θ
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	95°
$N(\text{points})_{\text{meas}}$:	8500
$N(\text{param})_{\text{refined}}$:	26
Profile function:	Pseudo Voigt
Background correction:	manual + Fourier filtering
Program:	Rietveld DBW9006

Table 2. Final atomic coordinates and displacement parameters (in $\text{\AA}^2$)

Atom	Site	x	y	z	B_{iso}
In	4c	0.4502(1)	1/4	0.6764(1)	3.01(4)
Mg	4c	0.1619(5)	1/4	0.4457(3)	1.3(1)
Br(1)	4c	0.6738(1)	1/4	0.4979(1)	0.90(4)
Br(2)	4c	0.2755(1)	1/4	0.2905(1)	1.47(5)
Br(3)	4c	0.0228(2)	1/4	0.6008(1)	0.80(4)

References

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