Crystal structure of magnesium iridoboride, MgIrB

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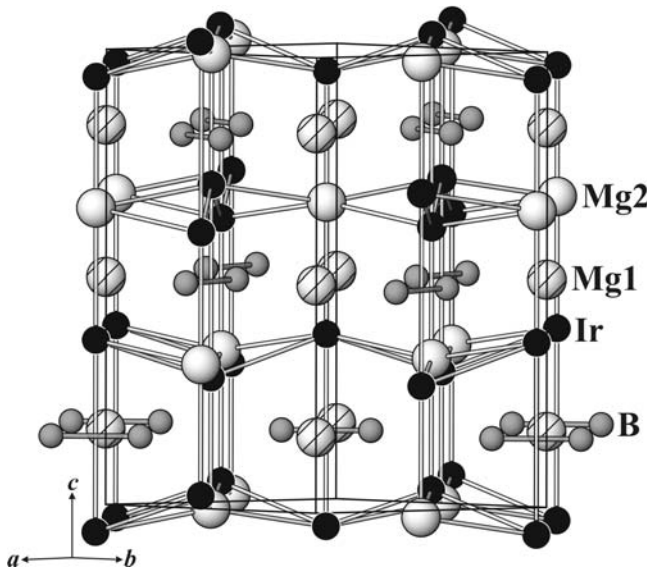

Abstract
BIrMg, hexagonal, $P6_222$ (no. 180), a = 5.2752(7) Å, c = 9.439(2) Å, V = 227.5 Å^3, Z = 6, $R_{gt}(F)$ = 0.017, $wR_{ref}(F)$ = 0.019, T = 295 K.

Source of material
The MgIrB compound was prepared using powders of Mg (99.8 %), Ir (99.9 %) and crystalline B (99.999 %) as starting materials. The elements mixture was ground, pressed into pellets, embedded in Ta ampoules and sealed under argon. The annealing was performed at 1293 K for 14 days and at 1333 K for 15 days with intermediate re-grinding.

Experimental details
The single phase sample was obtained from the sample with nominal composition $Mg_{1.1}IrB_{1.1}$. The X-ray powder diffraction pattern was indexed with a hexagonal unit cell and lattice parameters a = 5.2736(3) Å and c = 9.4358(7) Å. When changing initial mixture compostition to $Mg_{0.96}IrB_{0.94}$ a slight lattice parameters reduction to a = 5.2702(2) Å, c = 9.429(1) Å was observed. The largest lattice parameters (cf. Abstract) were found for the MgIrB single crystal obtained from the sample with nominal composition $Mg_{1.38}IrB_{1.46}$ by annealing at 1273 K for 18 days. Analogously to the Mg_{1-x}RhB phase [1] we assume a small homogeneity range for Mg_{1-x}IrB with the minimum x close to 0 observed in the single crystal used for the structure determination. The Flack parameter value of 0.0 reveals correctness of the absolute structure.

Discussion
The synthesis of numerous ternary magnesium rhodium borides [1-4] initiated us to study the Mg-Ir-B system with iridium as the electron analogue of rhodium with the aim to investigate the platinum metal nature influence on the crystal structure and chemical bonding of ternary borides.
The crystal structure of MgIrB is similar to Mg_{1-x}RhB [1]. It can be described as a framework of the distorted trigonal prisms [$BIr_4(Mg2)_2$], sharing the bases and side edges. The distorted hexagonal channels of the framework directed along c axis are occupied by Mg1 atoms.
Each boron atom forms a short distance of 1.87(1) Å to the next boron atom and, in addition, short distances of 2.203(3) and 2.210(7) Å to the next iridium atoms. On this way a 2D [IrB] network is formed. In Mg_{1-x}RhB [1] the 2D [RhB] network was shown to be anionic. In analogy, we suppose the same character for 2D [IrB]. For the Mg_{1-x}RhB compound the vacancies in Mg1 site were experimentally observed and then interpreted using the results of chemical bonding analysis. The single crystal diffraction data for the MgIrB show the full occupation of the Mg1 positions (99.8(2) %) and yield the composition MgIrB (x = 0). It agrees with the maximum lattice parameters found for the single crystal data.

Table 1. Data collection and handling.

Crystal:	black prism, size 0.050 × 0.020 × 0.020 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	930.5 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC7, φ/ω
$2\theta_{max}$:	63.01°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2830, 244
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 227
$N(param)_{refined}$:	15
Programs:	WinCSD [5], ATOMS [6], SHELXS-97 [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
B	6*j*	0.602(2)	2x–1	½	0.006(2)

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mg(1)	3*b*	0	0	½	0.012(2)	0.011(3)	0.010(2)	½U_{22}	0	0
Mg(2)	3*c*	½	0	0	0.004(2)	0.008(3)	0.008(2)	½U_{22}	0	0
Ir	6*f*	½	0	0.28868(4)	0.0048(2)	0.0033(2)	0.0049(2)	0.0005(2)	0	0

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