Refinement of the crystal structure of triplatinum heptaindium, Pt_3In_7

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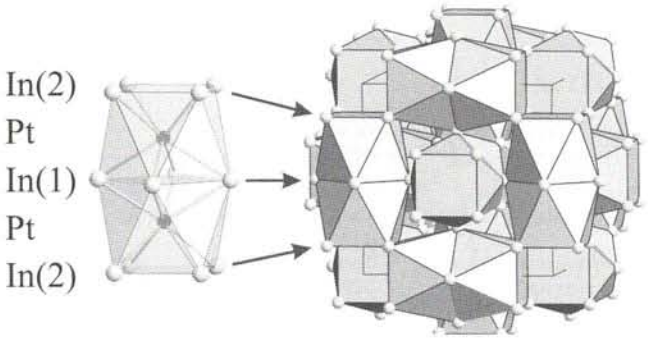

Abstract

In_7Pt_3, cubic, $Im\bar{3}m$ (No. 229), $a = 9.4274(4)$ Å, $V = 837.9$ Å^3, $Z = 4$, $R_{gt}(F) = 0.025$, $wR_{ref}(F^2) = 0.063$, $T = 293$ K.

Source of material

Single crystals of Pt_3In_7 (silver metallic) were grown by heating a melt of indium (99.999%, Alfa, 85 at.%) and platinum (99.95%, Chempur, 15 at.%) to 1273 K followed by cooling with a rate of 8 K/h. The obtained product was treated with concentrated hydrochloric acid for dissolving the excess of indium.

Discussion

Pt_3In_7 was first mentioned in 1947 [1] and based on the analyses of X-ray powder diffraction data assumed to be isotypic to the Ir_3Ge_7 structure [2,3]. Recent investigations of the Pt-In phase diagramm have shown that Pt_3In_7 is the indium richest compound and melts incongruently at about 1173 K [4,5].

The structure refinement based on single crystal X-ray diffraction data given here confirms that Pt_3In_7 crystallizes in the Ir_3Ge_7 type structure. Each Pt atom is surrounded by four In1 and four In2 atoms forming a square antiprism, whose two square faces are rotated by 45°. The Pt—In distances are nearly identical: 2.767(1) Å, (Pt—In1) and 2.774(1) Å (Pt—In2), respectively, whereas the two square faces of an antiprism are of different size with In1—In1 distances of 3.333(1) Å and In2—In2 distances of 3.068(1) Å. Two $PtIn_8$ antiprisms share a common square face (4×In1) forming Pt_2In_{12} units which are joined to a three dimensional framework by sharing common edges of the terminal square faces formed by In2 atoms. A second equivalent framework is generated by the I symmetry of the lattice leading to two interpenetrating frameworks, see also [6]. Between the two frameworks there are very short In2-In2 distances of 2.850(1) Å. The Pt—Pt distance across the common face of two $PtIn_8$ square antiprisms is remarkably short, 277.4(1) Å. However, it can easily shown by band structure calculations that there is no Pt—Pt bonding and that it is just a result of the face sharing of the $PtIn_8$ antiprisms. This is in agreement with the detailed analysis of the electronic situation of this structure type [6].

Table 1. Data collection and handling.

Crystal:	silver metallic block, size 0.2 × 0.3 × 0.4 mm
Wavelength:	Ag K_α radiation (0.56086 Å)
μ:	369.94 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, $\omega/2\theta$
$2\theta_{max}$:	47.86°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1479, 159
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 159
$N(param)_{refined}$:	10
Program:	SHELXL-97 [7]

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Table 2. 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}
Pt(1)	12*e*	0	0.34622(6)	0	0.0034(3)	0.0029(3)	U_{22}	0	0	0
In(1)	12*d*	0	1/2	1/4	0.0103(4)	U11	0.0019(5)	0	0	0
In(2)	16*f*	0.16271(6)	x	x	0.0055(3)	U_{11}	U_{11}	0.0010(2)	U_{12}	U_{12}

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