Refinement of the crystal structure of triplatinum heptaindium, Pt₃In₇

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Abstract

In₇Pt₃, cubic, $Im\bar{3}m$ (No. 229), $a = 9.4274(4)$ Å, $V = 837.9$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.025$, $wR_{\text{ref}}(F^2) = 0.063$, $T = 293$ K.

Source of material

Single crystals of Pt₃In₇ (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

Pt₃In₇ was first mentioned in 1947 [1] and based on the analyses of X-ray powder diffraction data assumed to be isotypic to the Ir₃Ge₇ structure [2,3]. Recent investigations of the Pt-In phase diagram have shown that Pt₃In₇ 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 Pt₃In₇ crystallizes in the Ir₃Ge₇ 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 PtIn₈ antiprisms share a common square face (4×In1) forming Pt₂In₁₂ 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 sym-

metry 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 PtIn₈ 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 PtIn₈ 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, $\omega/2\theta$
$2\theta_{\text{max}}$:	47.86°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	1479, 159
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 159
$N(\text{param})_{\text{refined}}$:	10
Program:	SHELXL-97 [7]

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References

- Hellner, E.; Laves, F.: Kristallchemie des In und Ga in Legierungen mit einigen Übergangsmetallen (Ni, Pd, Pt, Cu, Ag und Au). *Z. Naturforsch.* **2a** (1947) 177–183.
- Schubert, K.; Pfisterer, H.: Zur Kristallchemie der B-Metall-reichsten Phasen in Legierungen von Übergangsmetallen der Eisen- und Platintraden mit Elementen der vierten Nebengruppe. *Z. Metallkunde* **41** (1950) 433–441.
- Nial, O.: X-Ray Studies in Binary Alloys of Tin with Transition Metals. *Svensk Kemisk Tidskrift* **59** (1947) 172–178.
- Jain, K. C.; Bhan, S.: Constitution and structure of platinum-indium alloys. *Trans. Indian Inst. Met.* **25** (1972) 100–118.
- Guex, P.; Feschotte, P.: Les systèmes binaires platine-aluminium, platine-gallium et platine-indium. *J. Less Common Met.* **46** (1976) 101–116.
- Haeussermann, U.; Elding-Pontun, M.; Svensson, C.; Lidin, S.: Compounds with the Ir₃Ge₇ Structure Type: Interpenetrating Frameworks with Flexible Bonding Properties. *Chemistry - A European Journal* **4** (1998) 1007–1015.
- Sheldrick, G. M.: SHELXL-97. Program for crystal structure refinement. University of Göttingen, Germany 1997.

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Pt(1)	12e	0	0.34622(6)	0	0.0034(3)	0.0029(3)	U ₂₂	0	0	0
In(1)	12d	0	1/2	1/4	0.0103(4)	U ₁₁	0.0019(5)	0	0	0
In(2)	16f	0.16271(6)	x	x	0.0055(3)	U ₁₁	U ₁₁	0.0010(2)	U ₁₂	U ₁₂

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