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The Structure of Pu_5Pt_3*

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Abstract. Pu_5Pt_3, $P6_3/mcm$, $Z=2$, $a=8{\cdot}490$ (2), $c=6{\cdot}084$ (2) Å, $\varrho_c=15{\cdot}57$ g cm^{-3}. This structure is of the $D8_8$, Mn_5Si_3 type.

Introduction. The Pu–Pt phase diagram given by Kutaitsev, Chebotarev, Lebedev, Andrianov, Konev & Menshikova (1965) shows five intermetallic compounds: Pu_5Pt_3, PuPt, $PuPt_2$, $PuPt_3$ and $PuPt_5$. The above authors report that PuPt has the CrB, B_f structure, $PuPt_2$ has the Cu_2Mg, $C15$ structure and $PuPt_3$ the $AuCu_3$, $L1_2$ structure. The structure of $PuPt_5$ is unknown. In the present note we report the structure of Pu_5Pt_3. There is at least one additional phase in this system and it is believed to be $Pu_{31}Pt_{20}$ (Cromer & Larson, 1975).

An alloy containing 37 at.% Pt was prepared by arc melting followed by a heat treatment for 73 h at 1100°C. The alloy was crushed and single crystals of two different phases were found. One phase, believed to be $Pu_{31}Pt_{20}$, will be reported later (Cromer & Larson, 1975). Preliminary precession photographs showed the Pu_5Pt_3 phase to be hexagonal, space group $P6_3/mcm$ and probably of the $D8_8$ or Mn_5Si_3 structure type. All hkl reflections were present but $h0l$ reflections were present only for $l=2n$.

Lattice constants [$a=8{\cdot}490$ (2), $c=6{\cdot}084$ (2) Å, Mo $K\alpha$, $\lambda=0{\cdot}70926$ Å] and intensities were measured with graphite-monochromated Mo $K\alpha$ radiation on a Picker automatic diffractometer. The details of data collection are as described by Cromer & Larson (1972). Reflections were measured for $h\geq 0$, and all values of k and l for $2\theta\leq 55°$. Empirical absorption corrections were applied. These corrections were obtained from the variation of intensity as the crystal was rotated about the diffraction vector for several reflections with χ near 90° (Furnas, 1957). In addition, a spherical absorption correction was applied using a mean value of $\mu r=4{\cdot}2$ ($\mu=976$ cm^{-1}) for the irregularly shaped crystal fragment. An index defined as $R_F=\sum_n \sum_i |\bar{F}_n-F_{i,n}|/\sum_n \bar{F}_n$ was 0·079 where $\bar{F}_n=\sum w_i F_i/\sum w_i$ and the summations are over the i equivalent measurements with weight w_i, of the reflection F_n. F_i was considered observed if $(I-B)\geq 2\sigma(I)=2[I+B+(0{\cdot}02\ I)^2]^{1/2}$. Of the 181 unique reflections measured, 167 were observed.

Full-matrix least-squares refinement was begun immediately using the parameters of Mn_5Si_3 as starting values. Relativistic Hartree–Fock scattering factors (Cromer & Waber, 1974) were used along with the anomalous dispersion values of Cromer & Liberman (1970). The assumption of the Mn_5Si_3 structure type was shown to be correct. The final positional and thermal parameters are given in Table 1. For these parameters $R=\sum|\Delta F|/\sum F_o=0{\cdot}0484$ and $R_w=0{\cdot}0594$ $[\sum w(\Delta F)^2/\sum wF_0^2]^{1/2}=0{\cdot}0594$, with unobserved reflections omitted.*

Discussion. This structure type has been discussed in detail recently by Martinez-Ripoll & Brauer (1973). The interatomic distances for the present compound are listed in Table 2. The unit-cell contents and coordination polyhedra for Pu(1) and Pu(2) are shown in Fig. 1. A similar drawing for the Pt atom is in Fig. 2.

The major axes and orientations of the thermal ellipsoids are given in Table 3. The relative values of these axes are compatible with the polyhedra shown in Figs. 1 and 2. Pu(1) has neighbors directly above and below along the c axis and no neighbors in the plane normal to **c**. Pu(2) and Pt on the other hand have no neighbors directly above and below but Pu(2) has five neighbors and Pt has three neighbors in the plane normal to **c**.

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* A listing of the final least-squares cycle, including observed and calculated structure factors, followed by the interatomic distance and thermal-ellipsoid calculations has been deposited with the British Library Lending division as Supplementary Publication No. SUP 30918 (14 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Final least-squares parameters for* Pu_5Pt_3

The anisotropic temperature factor is exp $[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})]$. β values are $\times 10^5$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}
Pu(1)	$\frac{1}{3}$	$\frac{2}{3}$	0	1552 (35)	β_{11}	910 (59)	β_{11}
Pu(2)	0·2435 (4)	0	$\frac{1}{4}$	652 (27)	β_{11}	1389 (48)	730 (49)
Pt	0·6031 (5)	0	$\frac{1}{4}$	634 (30)	β_{11}	4737 (98)	665 (58)

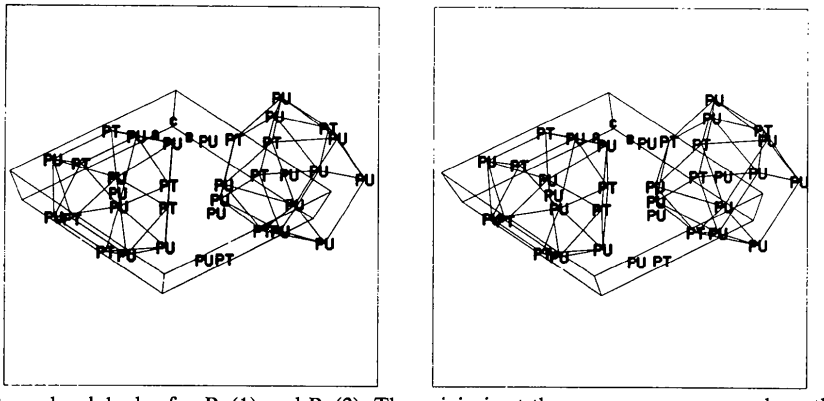

Fig. 1. Unit-cell contents and polyhedra for Pu(1) and Pu(2). The origin is at the upper rear corner where the positive directions of a, b and c are labeled. Pu(1) is at $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ and Pu(2) is at $0,0{\cdot}7565,\frac{3}{4}$.

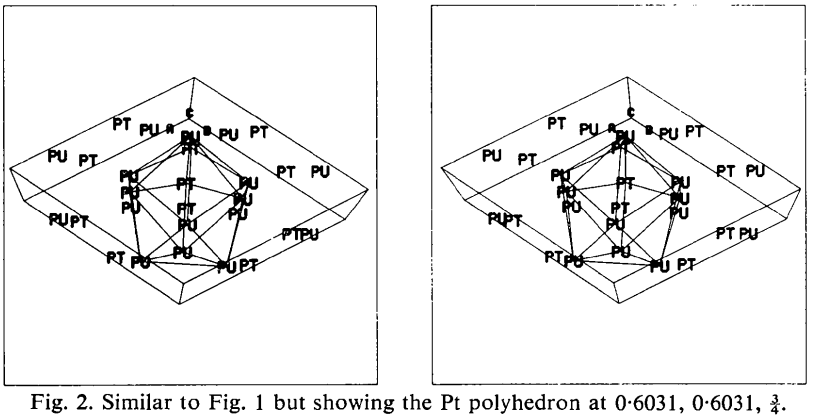

Fig. 2. Similar to Fig. 1 but showing the Pt polyhedron at 0·6031, 0·6031, $\frac{3}{4}$.

Table 2. *Interatomic distances in* Pu_5Pt_3 (Å)

Pu(1)–2Pu(1)	3·042	Pt–4Pu(1)	3·014 (1)
–6Pu(2)	3·615 (1)	–2Pu(2)	2·944 (2)
–6Pt	3·014 (1)	–Pu(2)	3·053 (3)
		–2Pu(2)	3·309 (1)
Pu(2)–4Pu(1)	3·615 (1)	–2Pt	3·509 (2)
–2Pu(2)	3·580 (3)		
–4Pu(2)	3·678 (1)		
–2Pt	2·944 (2)		
–Pt	3·053 (3)		
–2Pt	3·309 (1)		

Table 3. *Thermal ellipsoids in* Pu_5Pt_3

	B_i	Angles (°) relative to direct cell axes		
		α	β	γ
Pu(1)	3·4 (1) Å²	0	120	90
	3·4 (1)	90	30	90
	1·4 (1)	90	90	0
Pu(2)	1·2 (1)	30	150	90
	1·5 (1)	60	60	90
	2·1 (1)	90	90	0
Pt	1·3 (1)	30	150	90
	1·4 (1)	60	60	90
	7·0 (2)	90	90	0

All calculations were made with a CDC 7600 computer using the LASL system of crystallographic programs. We are indebted to V. O. Struebing for preparation of the alloy.

References

CROMER, D. T. & LARSON, A. C. (1972). *Acta Cryst.* B**28**, 2128–2132.

CROMER, D. T. & LARSON, A. C. (1975). To be published.

CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

CROMER, D. T. & WABER, J. T. (1974). In *International Tables for X-ray Crystallography*, Vol. IV. Birmingham: Kynoch Press.

FURNAS, T. C. (1957). *Single Crystal Orienter Instruction Manual.* Milwaukee: General Electric Company.

KUTAITSEV, V. I., CHEBOTAREV, N. T., LEBEDEV, I. G., ANDRIANOV, M. A., KONEV, V. N. & MENSHIKOVA, T. S. (1965). *Plutonium* 1965, pp. 420–449. Edited by A. E. KAY & M. B. WALDRON. London: Chapman & Hall.

MARTINEZ-RIPOLL, M. & BRAUER, G. (1973). *Acta Cryst.* B**29**, 2717–2720.