Table 3. *Selected bond distances and angles in ammonium azide*

Distances and angles marked with an asterisk are involved in hydrogen bonds.

	Uncorrected	Corrected
N(1)–N(2)	1·168 (4) Å	1·186 Å
N(3)–N(4)	1·171 (4)	1·186
N(5)–H(1)*	1·037 (10)	1·067
N(5)–H(2)*	1·001 (9)	1·028
N(5)–N(2)*	2·967 (3)	
N(5)–N(4)*	2·975 (4)	
N(2)–H(1)*	1·930 (9)	
N(4)–H(2)*	1·974 (9)	
H(1)–N(5)–H(1′)	106·0 (1·1)°	
H(1)–N(5)–H(2)	110·3 (0·7)	
H(1)–N(5)–H(2′)	110·3 (0·7)	
H(2)–N(5)–H(2′)	109·6 (1·0)	
N(4)–N(5)–N(2)	109·4 (0·1)	
N(4)–N(5)–N(2′)	108·5 (0·1)	
N(4)–N(5)–N(4′)	112·5 (0·2)	
N(2)–N(5)–N(2′)	108·4 (0·1)	
N(5)–H(1)–N(2)*	177·9 (0·9)	
N(5)–H(2)–N(4)*	177·2 (0·7)	

bonds. The hydrogen bonds are nearly linear. The N–H bond distances within the ammonium group differ by about four times the estimated standard deviation, which is probably significant.

Differences in thermal ellipsoids between constrained and unconstrained models were insignificant, except that the shortest r.m.s. amplitudes for the hydrogen atoms, which were essentially parallel to the N–H bonds in both models, were about 0·02 Å shorter when the ammonium group was held rigid. This would seem to be a reasonable amplitude for an N–H stretching vibration within a strong hydrogen bond.

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Plutonium–Platinum Pu_2Pt*

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Abstract. Orthorhombic, *Pnma*, $Z = 4$, $a = 7{\cdot}046$ (3), $b = 4{\cdot}707$ (2), $c = 8{\cdot}865$ (4) Å, $\rho_c = 15{\cdot}20$ g cm^{-3}, $\mu = 1115$ cm^{-1}, $\lambda = 0{\cdot}70930$ Å. This structure belongs to the *C*23, $PbCl_2$ type.

Introduction. Kutaitsev, Chebotarev, Lebedev, Andrianov, Konev & Menshikova (1965) reported five compounds in the Pu–Pt system: Pu_5Pt_3, PuPt, $PuPt_2$, $PuPt_3$ and $PuPt_5$. They reported that PuPt has the CrB, *C*33 structure, $PuPt_2$ has the $MgCu_2$, *C*15 structure and that $PuPt_3$ has the $AuCu_3$, $L1_2$ structure. Cromer & Larson (1975) reported that Pu_5Pt_3 has the Mn_5Si_3, $D8_8$ structure.

The Pu–Pt system is much more complex than Kutaitsev *et al.* (1965) found. Cromer & Larson (1977) have since reported the existence and structure of $Pu_{31}Pt_{20}$. Land, Peterson & Roof (1978) have reinvestigated this system, particularly the platinum-rich end. They verified the presence of $PuPt_5$ and found that it has the $CaCu_5$, $D2_d$ structure. They also found the compound $PuPt_4$ and proposed an orthorhombic structure based on a distortion of two unit cells of $PuPt_5$ with the twofold Pt atoms removed. In addition, they found two high-temperature forms of $PuPt_3$, one of which appears to be of the Ni_3P, $D0_e$ type. The other $PuPt_3$ phase is poorly characterized.

In the present note the existence and structure of yet another phase, Pu_2Pt, is reported.

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An alloy of stoichiometry Pu_2Pt was prepared by arc melting. It was subsequently heat treated at 550 °C for about two months. During this period, because of a malfunction of the furnace control, the sample was inadvertently heated to 850 °C for a short time. According to the phase diagram given by Kutaitsev *et al.* (1965), this 850 °C temperature lies in the two-phase region of solid Pu_5Pt_3 (0·82 mole fraction) in equilibrium with liquid of composition 15 at.% Pt. This phase diagram is, of course, incorrect in this region as no mention is made of Pu_2Pt. After cooling, a very small amount of metallic mirror was present on the inside of the quartz container, suggesting that a small amount of liquid had been present and had wet the container surface. Whatever the true nature of the phase diagram this liquid would have been richer in Pu and the remaining, solid ingot would have been slightly richer in Pt than the intended Pu_2Pt.

A portion of the ingot was crushed and searched for single crystals. A single crystal was soon found and precession photographs showed it to be orthorhombic, *Pnma*, if centrosymmetric. Reflections $0kl$ were present only if $k + l = 2n$, and reflections $hk0$ were present only if $h = 2n$. The structure determination subsequently confirmed *Pnma*.

Lattice constants were obtained from a least-squares refinement of 12 high-angle reflections measured on an automated Picker diffractometer. Intensity data were collected and processed in the manner described by Cromer & Larson (1977). A complete sphere of reflections was measured. Crystallographic data are given in the *Abstract* and details of data collection are given in Table 1. Empirical absorption corrections were based on the variation of intensities as a function of φ for a few reflections near $\chi = 90°$ (Furnas, 1957). In addition, spherical absorption corrections were applied based on the estimated mean radius of the irregularly shaped crystal.

Table 1. *Data collection and reduction* (*Cromer & Larson*, 1977)

Radiation	Mo $K\alpha$ (graphite monochromated)
$2\theta_{max}$	50°
Take-off angle	3°
Step size	0·05° 2θ
Step time	2 s
Scan range	2° (+$\alpha_1 - \alpha_2$ separation)
T_{min} (threshold parameter)	2·0
Number of reflections	1918
Unique reflections	294
Unique reflections observed	281
Reflections measured twice	11
Reflections measured four times	92
Reflections measured eight times	191
R_F (no corrections)	0·146
R_F (empirical corrections)	0·076
Range of corrective factors	0·020 to 0·138

The space group and axial ratios suggested that the structure might be of the *C*23, $PbCl_2$ type. A structure-factor calculation using the parameters of Ca_2Si gave good qualitative agreement with the precession photographs. A full-matrix least-squares refinement which minimized $\sum w(\Delta F)^2$ was made with anisotropic thermal parameters.[*] Scattering factors were taken from Cromer & Waber (1974) and anomalous dispersion corrections from Cromer & Liberman (1970). Positional parameters are given in Table 2 along with equivalent isotropic thermal parameters.

The stoichiometry was inferred from the structure type. No attempt was made to include occupancy or composition parameters as these two atoms are too close in scattering power to make such a refinement very meaningful.

Discussion. A number of intermetallic compounds have the $PbCl_2$ structure type, but only about 14% of them (Pearson, 1967) contain only truly metallic elements. Most of the compounds of this type contain the elements Si, Ge, Se, P, As or H. Aside from the variable axial ratios of the orthorhombic cell, each of the atoms has variable positional parameters. Consequently the

Table 2. *Final least-squares parameters for* Pu_2Pt

	x	*y*	*z*	Equivalent isotropic *B*
Pu(1)	0·8472 (2)	$\frac{1}{4}$	0·0795 (1)	1·35 Å²
Pu(2)	0·9842 (2)	$\frac{1}{4}$	0·6781 (1)	1·12
Pt	0·2589 (2)	$\frac{1}{4}$	0·1002 (1)	1·49

Table 3. *Interatomic distances* (Å) *in* Pu_2Pt

Pu(1)–Pt	2·907 (2)	Pu(2)–Pt	2·934 (2)
Pu(1)–Pt	2·907 (3)	Pu(2)–2Pt	3·048 (2)
Pu(1)–2Pt	2·938 (1)	Pu(2)–2Pt	3·512 (2)
Pu(1)–Pt	4·149 (3)	Pu(2)–Pt	4·212 (2)
Pu(1)–2Pt(1)	3·487 (1)	Pu(2)–2Pu(1)	3·401 (2)
Pu(1)–2Pu(2)	3·401 (2)	Pu(2)–2Pu(1)	3·429 (2)
Pu(1)–2Pu(2)	3·429 (2)	Pu(2)–Pu(1)	3·429 (2)
Pu(1)–Pu(2)	3·429 (2)	Pu(2)–Pu(1)	3·687 (2)
Pu(1)–Pu(2)	3·687 (2)	Pu(2)–2Pu(2)	3·746 (1)
		Pu(2)–2Pu(2)	3·945 (1)
Pt–Pu(1)	2·907 (2)		
Pt–Pu(1)	2·907 (3)		
Pt–2Pu(1)	2·938 (1)		
Pt–Pu(1)	4·149 (3)		
Pt–Pu(2)	2·934 (2)		
Pt–2Pu(2)	3·048 (2)		
Pt–2Pu(2)	3·512 (2)		
Pt–Pu(2)	4·212 (2)		

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[*] Listings of the final least-squares cycle containing the anisotropic thermal parameters, structure factors, thermal ellipsoid calculations, interatomic distance calculations and polyhedron calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33532 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

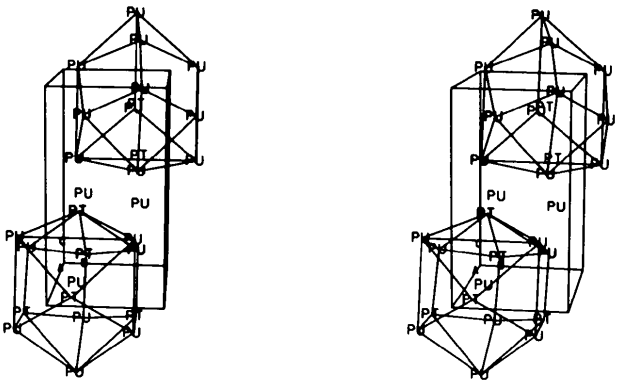

Fig. 1. The Pu(1) and Pt polyhedra in Pu_2Pt. View is approximately along x. The origin is at the lower left rear. Pu(1) is at 0·847, ¼, 0·079 and the Pt is at 0·741, ¾, 0·900.

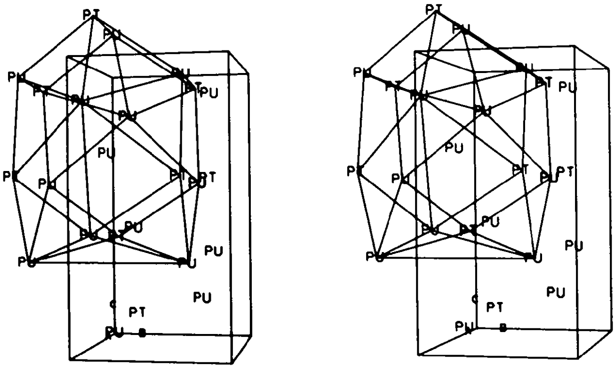

Fig. 2. The Pu(2) polyhedron in Pu_2Pt. Pu(2) is at 0·984, ¼, 0·678.

polyhedra and the number of neighbors for each of the atoms can vary considerably for compounds nominally of the same structure type.

The neighbors and polyhedra were determined as described by Cromer & Larson (1977). The resulting interatomic distances are given in Table 3. These distances are similar to those found in other Pu–Pt compounds. Pu(1) has five Pt and eight Pu neighbors. There are five neighbors in the mirror plane and four on either side of this plane. Pu(2) has six Pt neighbors and ten Pu neighbors with six neighbors in the mirror plane and five on either side. The Pt atom has 11 neighbors, all Pu. There are five neighbors in the mirror plane and three on either side. Stereo drawings of these polyhedra are shown in Figs. 1 and 2.

Thanks are due to R. E. Tate for preparation of the alloy. All calculations were done on a CDC-7600 computer using the *LASL* system of crystallographic programs developed primarily by A. C. Larson.

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Oxysulfure de Gallium et de Lanthane $LaGaOS_2$

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Abstract. Orthorhombic, space group *Pmca*, a = 5·5419 (9), b = 5·767 (1), c = 11·443 (1) Å, Z = 4. μ = 203 cm^{-1}. The structure was solved from single-crystal data. With anisotropic thermal parameters, the