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Compounds of Uranium with the Transition Metals of the Second and Third Long Periods

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In the course of an investigation of the occurrence and structure of compounds UX_2 , where X is Ru, Rh, Pd, Re, Os, Ir or Pt, the existence has been established of the compounds UOs_2 and UIr_2 ($C15$ structure), UPd_3 ($DO24$ structure), URu_3 ($L12$ structure) and UPt_3 ($DO19$ structure).

1. Introduction

In the course of investigations of the occurrence and structure of compounds UX_2 , where X is Ru, Rh, Pd, Re, Os, Ir or Pt, the existence of a number of compounds has been established. They are UOs_2 and UIr_2 with the $C15$ structure (Strukturbericht, 1931c), UPd_3 with the $DO24$ structure (Strukturbericht, 1943), URu_3 with the $L12$ structure (Strukturbericht, 1931b) and UPt_3 with the $DO19$ structure (Strukturbericht, 1940).

2. Preparation of the alloys

All alloys were prepared as 10 g. buttons by arc melting on a water-cooled copper hearth in an atmosphere of purified argon. They were repeatedly remelted to homogenize the ingots. The X elements were of very high purity, approaching that of spectroscopic standards. The uranium was also of high purity; it contained some oxide but was aluminium-free. Heat treatments were carried out on lump specimens in alumina sheaths in evacuated silica tubes. No heat treatments of powdered alloys were necessary, the amount of cold work obtained during powdering being negligible.

3. UX_2 alloys

(i) UOs_2

This alloy crystallizes in a face-centred cubic lattice and is isostructural with $MgCu_2$, the $C15$ structure type. Only Debye-Scherrer powder patterns were necessary to determine the structure. Chemical analysis of the powder used gave 33.5 atomic% uranium. The patterns from the 'as cast' and the heat treated alloy (2 weeks at 900° C.) were identical. The lattice

parameter was determined using Co radiation and the Nelson-Riley (1945) extrapolation as

$$a = 7.4974 \pm 0.0005 \text{ kX.}^* \text{ at } 24^\circ \text{ C.},$$

which gave the X-ray density as 19.42 g.cm.⁻³.

The $C15$ structure has space group $O_h^2-Fd\bar{3}m$ and the atomic sites are as given in *International Tables* (1952, No. 227), i.e. equivalent positions 0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{2}$; $\frac{1}{2}$, 0, $\frac{1}{2}$; $\frac{1}{2}$, $\frac{1}{2}$, 0 with

$$8 \text{ U at } (a) \ 0, 0, 0; \frac{1}{4}, \frac{1}{4}, \frac{1}{4};$$

$$\text{and } 16 \text{ Os at } (d) \ \frac{5}{8}, \frac{5}{8}, \frac{5}{8}; \frac{5}{8}, \frac{7}{8}, \frac{7}{8}; \frac{7}{8}, \frac{5}{8}, \frac{7}{8}; \frac{7}{8}, \frac{7}{8}, \frac{5}{8}.$$

Observed and calculated intensities are given in Table 1.

Since the structure is parameterless, visual intensity estimates have been compared with calculated intensities from which the absorption and temperature factors have been omitted. The observed and calculated values of I are seen to be in good agreement for diffractions occurring at similar θ values. Interatomic distances of near neighbours are given in Table 2.

(ii) UIr_2

The Debye-Scherrer patterns of the UIr_2 alloy were identical with those of UOs_2 , apart from weak additional lines identified as iridium lines. Analysis of the powder used gave a uranium content of 31.2 atomic%. Assuming the uranium to be combined as UIr_2 , 6.4% free iridium would be present; a finding

* Wavelengths of X-radiations used:

Cu $K\alpha_1$ 1.537395 kX.
 Co $K\alpha_1$ 1.78529 kX.
 Cr $K\alpha_1$ 1.28503 kX.

Table 1. *Calculated and observed intensities for UOs₂ and UIr₂*

<i>hkl</i>	UOs ₂		UIr ₂	
	<i>I_c</i>	<i>I_o</i>	<i>I_c</i>	<i>I_o</i>
111	< 1.2	<i>a</i>	< 1.9	<i>a</i>
200	0	<i>a</i>	0	<i>a</i>
220	69.0	<i>m</i>	69.0	<i>wm</i>
311	195.0	<i>s</i>	200.0	<i>s</i>
222	66.6	<i>ms</i>	68.8	<i>ms</i>
400	4.6	<i>w</i>	5.2	<i>w</i>
331	< 0.2	<i>a</i>	< 0.2	<i>a</i>
420	0	<i>a</i>	0	<i>a</i>
422	26.0	<i>m</i>	26.0	<i>m</i>
333	60.0	<i>s</i>	65.6	<i>s</i>
511		<i>s</i>		<i>s</i>
440	58.0	<i>s</i>	59.6	<i>s</i>
531	< 0.2	<i>a</i>	< 0.3	<i>a</i>
600	14.1	<i>a</i>	14.1	<i>a</i>
442		<i>a</i>		<i>a</i>
620	<i>m</i>	<i>m</i>	14.1	<i>m</i>
533	30.4	<i>s</i>	30.7	<i>s</i>
622	34.2	<i>s</i>	35.1	<i>s</i>
444	1.4	<i>vw</i>	1.7	<i>vw</i>
711	< 0.15	<i>a</i>	< 0.19	<i>a</i>
551		<i>a</i>		<i>a</i>
640	0	<i>a</i>	0	<i>a</i>
642	33.1	<i>s</i>	33.1	<i>s</i>
731	119.0	<i>vs</i>	122.0	<i>vs</i>
553		<i>vs</i>		<i>vs</i>
800	40.0	<i>ms</i>	41.0	<i>m</i>

a=absent; *s*=strong; *m*=medium; *w*=weak; *v*=very.

Table 2. *Interatomic distances in UOs₂ and UIr₂*

Atom	Neighbours	Distance (kX.)
U	12 Os	3.1085
	4 U	3.2465
Os	6 Os	2.6508
	6 U	3.1085
U	12 Ir	3.1069
	4 U	3.2449
Ir	6 Ir	2.6495
	6 U	3.1069

in good accord with the relative intensities on the powder photographs. The observed and calculated intensities for UIr₂ on the assumption of a *C15* structure are given in Table 1. The interatomic distances are given in Table 2. The parameter was determined as

$$a = 7.4939 \pm 0.0005 \text{ kX. at } 20^\circ \text{ C.,}$$

which gave an X-ray density of 19.62 g.cm.⁻³.

4. UX₃ alloys

(i) UPd₃

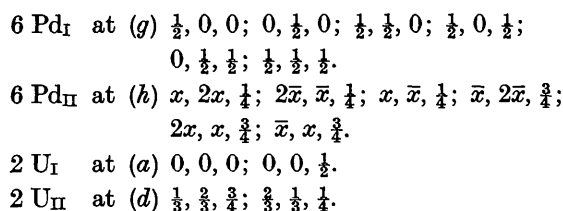
After annealing for 19 days at 1000° C. an 'as cast' alloy of nominal composition UPd₂ showed fairly obvious evidence of two layers of presumably different structures. The powder pattern of the outer layer was simplified compared with the inner layer, a number of lines occurring in the latter having disappeared and the remaining lines being common to both patterns. It was suspected that uranium losses

Table 3. *Calculated and observed intensities for UPd₃*

<i>hkl</i>	$ F ^2_p$	<i>I_o</i>	<i>I'_o</i>
100	1	<i>a</i>	<i>a</i>
002	0	—	—
101	6	<i>a</i>	<i>a</i>
102	17	<i>vw</i>	<i>vw</i>
003	0	—	—
110	15	<i>a</i>	<i>a</i>
111	0	—	—
103	5	<i>a</i>	<i>a</i>
200	24	<i>a</i>	<i>vwv</i>
112	0	—	—
201	126	<i>s</i>	<i>ms</i>
004	110		
202	370	<i>ms</i>	<i>s</i>
104	< 2	<i>a</i>	<i>a</i>
113	0	—	—
203	126	<i>m</i>	<i>wm</i>
005	0	—	—
120	< 2	<i>a</i>	<i>a</i>
121	10	<i>vw</i>	<i>vw</i>
114	29		
105	5	<i>a</i>	<i>a</i>
122	27	<i>vvw</i>	<i>vw</i>
204	32	<i>vw</i>	<i>vw</i>
300	13	<i>a</i>	<i>a</i>
301	0	—	—
123	10	<i>a</i>	<i>a</i>
006	0	—	—
115	0	—	—
302	0	—	—
205	2	<i>ms</i>	<i>wm</i>
106	17		
124	< 4	<i>a</i>	<i>a</i>
303	0		
220	255	<i>ms</i>	<i>m</i>
221	0	—	—
116	0	—	—
130	< 4	<i>a</i>	<i>a</i>
222	0	—	—
007	0	<i>a</i>	<i>a</i>
131	< 10		
304	< 20	<i>vw</i>	<i>a</i>
206	205	<i>s</i>	<i>m</i>
125	< 10		
132	24	<i>vw</i>	<i>a</i>
107	4	<i>a</i>	<i>a</i>
223	0	—	—
133	8	<i>a</i>	<i>a</i>
305	0	—	—
400	12	<i>a</i>	<i>a</i>
401	23	<i>vs</i>	<i>s</i>
117	0		
224	365	<i>vw</i>	<i>a</i>
126	24	<i>s</i>	<i>m</i>
402	205		
207	68	<i>a</i>	<i>a</i>
008	64		
134	3	<i>w</i>	<i>w</i>
108	< 2		
403	68		

would have occurred by distillation from the outer layer, and that UPd₂ did not exist under the conditions of experiment, but that UPd_{*n*}, where *n* > 2, did exist. Grogan (private communication) kindly allowed the authors access to unpublished work which confirmed this view, and suggested that the compound UPd₃ existed. An 'as cast' alloy of composition UPd₃ gave sharp powder spectra, the pattern clearly being

that to which the outer layer of the UPd₂ ingot was tending as heat treatment proceeded. Laue photographs of a single crystal of this alloy showed the structure to be hexagonal with Laue symmetry 6/m. Rotating-crystal photographs established the approximate *c* and *a* values as *c* = 9.59 kX. and *a* = 5.69 kX., and permitted indexing of the powder spectra. Examination of the structure factors of a few chosen lines suggested that the DO24 structure was the only possible hexagonal structure commonly occurring in intermetallic compounds capable of giving calculated intensities in agreement with the observed powder spectra. The DO24 structure, (International Tables, 1952, No. 194), space group *D*_{6h}², has atomic sites:



The ideal value of the parameter *x* is $\frac{1}{3}$. Assuming this ideal value, the structure factors for the first 60 possible lines were calculated and the results are presented in Table 3. After introducing the multiplicity factor *p*, a comparison of $|F_{UPd_2}|^2 p$ with the observed intensities for lines of similar θ values exposed significant discrepancies. Thus the 110 and 200 lines of calculated intensities 15 and 24 were not detected, but the 102 of intensity 17 was observed. Further

- (i) $I(202)_o < I(201)_o + I(004)_o$
 but $I(202)_c > I(201)_c + I(004)_c$;
 (ii) $I(114)_o \gg I(122)_o$ and $I(204)_o \gg I(122)_o$
 but $I(114)_c \sim I(122)_c$ and $I(204)_c \sim I(122)_c$;
 (iii) $I(205)_o + I(106)_o \sim I(220)_o$
 but $I(205)_c + I(106)_c \ll I(220)_c$.

The observed discrepancies were all due to planes of high *l* index having anomalously high intensities relative to adjacent planes of low *l* index. This correlation of the intensity discrepancies with an apparent preferred orientation of the basal planes of the powder fragments parallel to the axis of the specimen made any successful modification of the *x* parameter unlikely. Variation of *x* is equivalent to variation of the co-ordinates of the 6 Pd_{II} atoms in the planes $z = \frac{1}{4}$ and $z = \frac{3}{4}$. The intensities of planes essentially parallel to the plane $z = 0$ cannot be significantly affected by such variations. Experimental verification of the assumption of preferred orientation was therefore sought. Laves & Wallbaum (1939) have reported the solution of a similar problem by mixing their crushed alloy with a molten resin and then crushing the solidified resin in order to obtain random fracture surfaces. A

specimen was prepared in a similar manner, and modified intensities were obtained; these have been recorded in Table 3 as *I*'_o and can be seen to be in better accord with the calculated intensities. They show that preferred orientation has undoubtedly existed in the previous powder specimens, and allow the remaining intensity discrepancies to be ascribed to residual preferred orientation. The structure of the alloy is therefore DO24 with an *x* parameter $\sim \frac{1}{3}$. The accurate lattice constants were obtained from Debye-Scherrer films taken with chromium radiation. Using the value of *c/a* obtained from the single-crystal films, values of *a* were plotted against the Nelson-Riley (1945) extrapolation for 13 lines. A straight line was then drawn through the two lowest *l* index points 220 and 201 and the *c/a* value was adjusted until the scatter of high *l* index points was a minimum; extrapolation to $\theta = 90^\circ$ then gave the best value of *a*. The final values thus obtained were

$$a = 5.757 \pm 0.001, c = 9.621 \pm 0.001 \text{ kX.}, c/a = 1.671.$$

The interatomic distances are given in Table 4. In contrast to the Laves phases UX₂, where there are

Table 4. Interatomic distances in UPd₃

Atom	Neighbours	Distance (kX.)	Remarks
U _I	6 Pd _I	2.878	Same layer
	6 Pd _{II}	2.923	Layers <i>c</i> /4 removed
	6 U _{II}	4.102	Layers <i>c</i> /4 removed
	2 U _I	4.810	Direction <i>c</i> /2 removed
	6 U _I	5.757	Same layer
U _{II}	6 Pd _{II}	2.878	Same layer
	6 Pd _I	2.923	Layers <i>c</i> /4 removed
	6 U _I	4.102	Layers <i>c</i> /4 removed
	6 U _{II}	5.757	Same layer
	6 U _{II}	5.847	Layers <i>c</i> /2 removed
Pd _I	4 Pd _I	2.878	Same layer
	2 U _I	2.878	Same layer
	4 Pd _{II}	2.923	Layers <i>c</i> /4 removed
	2 U _{II}	2.923	Layers <i>c</i> /4 removed
Pd _{II}	4 Pd _{II}	2.878	Same layer
	2 U _{II}	2.878	Same layer
	4 Pd _I	2.923	Layers <i>c</i> /4 removed
	2 U _I	2.923	Layers <i>c</i> /4 removed

U-U and X-X contacts only, in UPd₃ there are U-Pd contacts only. Analysis of the powder used for the Debye-Scherrer films gave 75.05 atomic% palladium.

The calculated density is 13.39 g.cm.⁻³.

(ii) URu₃

An alloy of composition URu₂ showed many analogies with UPd₂. Heat treatment led to sharpening and simplification of the Debye-Scherrer spectra obtained from the 'as cast' alloy, but none of the heat treatments employed produced really sharp spectra. This was particularly noticeable in the outer layers of the ingot and an alloy of composition URu₃ gave a

simplified pattern. The principal lines of this pattern could be indexed on a face-centred cubic lattice of side

$$a = 3.980 \pm 0.002 \text{ kX.}$$

The remaining weak lines suggested a primitive cubic lattice of the same cell size. These findings were in accordance with an ordered face-centred cubic lattice of structure type $L12$, space group $O_h^1-Pm\bar{3}m$, with atomic sites:

$$\begin{aligned} 1 \text{ U at } (a) & 0, 0, 0. \\ 3 \text{ Ru at } (c) & 0, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, 0, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 0. \end{aligned}$$

With this structure the intensities of all face-centred cubic diffractions are functions of $|f_U + 3f_{Ru}|^2$ and those of the remaining lines of $|f_U - f_{Ru}|^2$. In Table 5

Table 5. *Calculated and observed intensity for URu₃*

<i>hkl</i>	$ F ^2 p$	I_o
100	1.2	<i>vwv</i>
110	2.0	<i>vw</i>
111	24.7	<i>s</i>
200	16.5	<i>s</i>
210	3.7	<i>w</i>
211	3.6	<i>w</i>
220	24.1	<i>s</i>
300	3.9	<i>w</i>
221		
310	3.0	<i>w</i>
311	41.3	<i>vs</i>
222	13.3	<i>m</i>
320	2.7	<i>vw</i>
321	4.9	<i>w</i>
400	8.3	<i>m</i>
410	4.2	<i>w-m</i>
322		
411		
330		
331	29.8	<i>vs</i>

the observed visual estimates of the Debye-Scherrer spectra I_o are compared with the product $|F_{URu_3}|^2 p$ and the agreement confirms the assumed structure. The observed intensities recorded in Table 5 refer to a film taken with cobalt radiation of an alloy heat treated at 870° C. for 21 days and water quenched. The U-Ru and Ru-Ru distances are 2.815 kX. the U-U distances 3.980 kX. The calculated density is 14.24 g.cm.⁻³.

(iii) UPt₃

The Debye-Scherrer spectra of this alloy could be indexed on a simple close-packed hexagonal ($A3$) structure (Strukturbericht, 1931a). This structure, space group D_{6h}^4-P6/mmc , has atomic sites

$$(d) \frac{2}{3}, \frac{1}{3}, \frac{1}{4}; \frac{1}{3}, \frac{2}{3}, \frac{3}{4}.$$

Calculation of the structure factors on an assumption of random distribution of the U and Pt atoms revealed major discrepancies between the observed and calculated intensities, as shown in Table 6.

Table 6. *Calculated and observed intensities for UPt₃*

<i>hkl</i>	$ F ^2 p$	I_o	I'_o
100	6	<i>vw</i>	<i>m-w</i>
002	8	<i>s</i>	<i>m-w</i>
101	36	<i>s</i>	<i>s</i>
102	12	<i>m</i>	<i>m-w</i>
110	24	<i>m</i>	<i>m</i>
103	36	<i>s</i>	<i>m</i>
200	54	<i>s</i>	<i>m-s</i>
112			
004	8	<i>m</i>	<i>vwv</i>
201	36	<i>m</i>	<i>m</i>
202	12	<i>w</i>	<i>vw</i>
104	12	<i>m</i>	<i>vw</i>
203	36	<i>m-s</i>	<i>m</i>
210	12	<i>vw</i>	<i>vw</i>
114	48	<i>vs</i>	<i>m-s</i>
211	72	<i>s</i>	<i>s</i>
105	36	<i>vs</i>	<i>m</i>

- (i) $I(100)_c \sim I(002)_c$ but $I(100)_o \ll I(002)_o$;
(ii) $I(201)_c \gg I(004)_c$ but $I(201)_o \sim I(004)_o$.

The discrepancies can all be associated with preferred orientation of the basal planes of the powder specimen. The expedient adopted in the case of UPd₃ confirmed the assumption of preferred orientation. The revised intensities are given as I'_o in Table 6 and are seen to be in good accord with the calculated intensities. It was considered that UPt₃ was very likely to be an ordered structure despite the apparent lack of evidence in support of this view. The only ordered structure consistent with the observed Debye-Scherrer patterns is $DO19$, which is a true superlattice of the $A3$ structure with all superlattice lines having intensities proportional to $|f_U - f_{Pt}|^2$ and all main ($A3$) lines having intensities proportional to $|f_U + 3f_{Pt}|^2$. Taking an average value of $\sin \theta/\lambda$ the ratio

$$|f_U - f_{Pt}|^2 \div |f_U + 3f_{Pt}|^2 \text{ is approximately } 2.5 \times 10^{-3}.$$

With suitable monochromatic techniques, lines of this order of intensity should be detectable, particularly lines of high l index with anomalously high intensities due to preferred orientation. Debye-Scherrer photographs were therefore taken using a LiF curved-crystal focusing monochromator of long focal length and a copper tube operated at 28 kVp. to reduce the $\frac{1}{2}\lambda$ harmonic of the $K\alpha$ radiation. 28 kVp. was chosen as a compromise between unduly long exposures and excessive $\frac{1}{2}\lambda$ interference. These photographs showed the presence of a number of very very faint extra lines in the expected superlattice positions. These positions would also be occupied by $\frac{1}{2}\lambda$ $A3$ diffractions. The relative amounts of λ and $\frac{1}{2}\lambda$ radiation could not readily be determined and were known to be critically dependent on the state and type of X-ray tube; published results of other workers were therefore not applicable. The use of differential filters would have led to a prohibitive increase in the already large (240 mA. hr.) exposure times. The expedient was therefore adopted of taking a Debye-Scherrer pattern of pure platinum under identical conditions. No

evidence of $\frac{1}{2}\lambda$ diffractions could be detected. The *DO19* unit cell is obtained by doubling the *a* parameter of the *A3* unit cell whilst leaving the *c* parameter unchanged. Thus

$$\begin{aligned}(100) A3 &\equiv (200) DO19 \\ (101) A3 &\equiv (201) DO19,\end{aligned}$$

so that, although the $\frac{1}{2}\lambda$ diffraction from the (100) *A3* plane falls on the 100 *DO19* line, the $\frac{1}{2}\lambda$ diffraction of the (101) *A3* plane falls at the position of a non-existent $10\frac{1}{2}$ *DO19* line. A number of such lines with non-integral indices on the *DO19* unit cell should occur if the faint extra diffractions were due to $\frac{1}{2}\lambda$ radiation. No such lines were detected. Table 7 summarizes some

Table 7

<i>hkl</i>	<i>I_c</i>		<i>I_o</i>	Remarks
	<i>DO19</i> in units $ f_U - f_{Pt} ^2$	$\frac{1}{2}\lambda$ in units $(1/K) f_U + 3f_{Pt} ^2$		
100	6	6	—	
001	0	8	—	
10 $\frac{1}{2}$	0	36	—	
101	36	12	†	3rd strongest line
110	24	24	†?	
10 $\frac{3}{2}$	0	36	—	
111	0	48	—	Too near 200, 002 to be seen
20 $\frac{1}{2}$	0	36	—	
102	12	12	—	
20 $\frac{3}{2}$	0	36	—	
210	12	12	—	
112	48	48	†	
10 $\frac{5}{2}$	0	36	—	
211	72	24	—	Too near 202 to be seen
300	24	6	—	Too near 202 to be seen
30 $\frac{1}{2}$	0	36	—	
20 $\frac{5}{2}$	0	36	—	
21 $\frac{3}{2}$	0	72	—	
103	36	12	†	2nd strongest line
20 $\frac{7}{2}$	0	36	—	
212	24	24	†	
311	72	24	†	
104	12	12	†?	
320	12	12	†?	
114	48	48	†	Strongest line

†: present; †?: possibly present.

of the findings; it is complete up to line 212 but subsequently, for brevity, only lines actually observed are listed. The calculated *DO19* intensities are given in units of $|f_U - f_{Pt}|^2$, the $\frac{1}{2}\lambda$ intensities in units of $(1/K)|f_U + 3f_{Pt}|^2$, where *K*, and hence the relationship to $|f_U - f_{Pt}|^2$, is not known. In general it will be seen that the lines most readily detected have relatively strong *DO19* intensities and are favoured by the known preferred orientation.

Subsequently a few of the stronger superlattice lines 114, 103 and 112 were detected on heavily over-

exposed films taken with polychromatic radiation. A number of very faint superlattice spots were also detected on single-crystal photographs, but this evidence was reduced in significance by the presence of many faint extra spots due to fragments of other crystals. Accurate values of the parameters were obtained from the 205, 421, 224, 420, 004 and 220 spectra on the Debye-Scherrer films by the method adopted in the case of UPd₃; the values are

$$a = 5.752 \pm 0.001, \quad c = 4.889 \pm 0.001 \text{ kX.}, \quad c/a = 0.851.$$

The atoms in the *DO19* unit cell, space group $D_{6h}^4 - C6/mmc$, are

$$\begin{aligned}2 \text{ U} &\text{ at } (c) \frac{1}{2}, \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, \frac{1}{2}, \frac{3}{2}. \\ 6 \text{ Pt} &\text{ at } (h) x, 2x, \frac{1}{2}; 2\bar{x}, \bar{x}, \frac{1}{2}; x, \bar{x}, \frac{1}{2}; \bar{x}, 2\bar{x}, \frac{3}{4}; \\ &2x, x, \frac{3}{4}; \bar{x}, x, \frac{3}{4}.\end{aligned}$$

The ideal value of the parameter *x* is $\frac{5}{8}$. Taking this value the interatomic distances are as shown in Table 8.

Table 8. Interatomic distances in UPt₃

Atom	Neighbours	No.	Distance (kX.)	Remarks
U _I	Pt _I	6	2.876	Same layer
	Pt _{II}	6	2.955	Adjacent layers
	U _I	2	4.889	Same vertical line
	U _{II}	2	4.123	Adjacent layers
Pt _I	Pt _I	4	2.876	Same layers
	Pt _{II}	4	2.955	Adjacent layers
	U _I	2	2.876	Same layer
	U _{II}	2	2.955	Adjacent layers

Analysis of the powder used for the Debye-Scherrer films gave 74.9 atomic% platinum. The calculated density is 19.43 g.cm.⁻³.

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