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The unit-cell constants of some PuNi₃-type compounds*. By A. E. DWIGHT, *Metallurgy Division, Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.*

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Crystal structure data, including unit-cell constants and observed intensities obtained from powder patterns, are presented for UCo₃ and other PuNi₃-type compounds.

Earlier work (Elliott, 1965) on the U-Co system indicated that the compound UCo₃ was formed at ~880°C by a peritectoid reaction. The crystal structure of the compound was not identified. Our investigation shows that UCo₃ is isostructural with PuNi₃, which was reported (Cromer & Olsen, 1959) to be rhombohedral, $R\bar{3}m$.

The UCo₃ compound investigated was prepared by arc melting electrolytic uranium and 99.99% Co under an argon-helium atmosphere. The button was homogenized at 800°C for four days, and a powdered specimen was annealed at 800°C for 18 hours. X-ray diffraction patterns were obtained with a Debye-Scherrer camera and chromium $K\alpha$ radiation. Although the structure is rhombohedral, the diffraction pattern was indexed on the basis of the related hexagonal unit cell. The unit-cell constants were cal-

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Table 1. UCo₃ structural data based on a hexagonal unit cell

<i>h k l</i>	<i>d</i> _o	<i>d</i> _c	<i>I</i> _o
	Cr radiation ($K\alpha_1 = 2.28962 \text{ \AA}$)		
1 0 1	4.105 Å	4.138 Å	w
0 0 6		4.052	
1 0 2		3.969	
1 0 4		3.455	
1 0 5		3.179	
0 0 9		2.702	
1 0 7	2.66	2.677	m
1 0 8	2.45	2.462	m
1 1 0	2.412	2.425	m
1 1 3		2.329	
1,0,10		2.104	
2 0 1	2.09	2.092	m
1 1 6	2.075	2.081	s
2 0 2		2.069	
0 0,12	2.022	2.026	vw
2 0 4	1.98	1.985	vw
1,0,11	1.95	1.956	vw
2 0 5	1.925	1.928	w

Table 1 (cont.)

<i>h k l</i>	<i>d</i> _o	<i>d</i> _c	<i>I</i> _o
1 1 9	1.80	1.805	w
2 0 7		1.797	
2 0 8		1.728	
1,0,13		1.709	
0 0,15	1.619	1.621	w
1,0,14	1.604	1.605	w
2 0,10		1.589	
2 1 1	1.581	1.584	w
2 1 2		1.574	
1,1,12		1.555	
2 1 4		1.536	
2,0,11		1.522	
2 1 5		1.509	
2 1 7	1.443	1.444	m
1,0,16	1.429	1.429	vw
2 1 8	1.407	1.407	w
3 0 0	1.400	1.400	m
2,0,13	1.397	1.397	w
3 0 3		1.379	
1,0,17		1.354	
0 0,18		1.351	
1,1,15	1.347	1.348	m
2 0,14	1.338	1.338	m
2,1,10		1.329	
3 0 6	1.322	1.323	s
2,1,11	1.289	1.289	m
3 0 9	1.2425	1.2429	w
2,0,16		1.2312	
1,0,19	1.225	1.2242	w
2 2 0	1.2123	1.2123	s
2,1,13		1.2103	
2 2 3		1.1990	
2,0,17	1.182	1.1822	m
1,1,18		1.1801	
2,1,14	1.1718	1.1717	s
1,0,20		1.1679	
3 1 1	1.1632	1.1634	m
2 2 6		1.1615	
3 1 2		1.1594	
0,0,21	1.158	1.1579	m
3,0,12		1.1518	

Table 2. Unit-cell constants of PuNi₃-type compounds based on the related hexagonal unit cell

Compound	<i>a</i>	<i>c</i>	<i>c/a</i>	Vol/ <i>M</i>	Heat treatment*
UCo ₃	4.8492 (2)	24.317 (1)	5.02	55.03	
GdFe ₃	5.1654 (7)	24.707 (2)	4.78	63.43	(a)
HoFe ₃	5.1097 (3)	24.526 (1)	4.80	61.6	(b)
TbCo ₃	5.0156 (3)	24.424 (1)	4.87	59.13	(c)
LuCo ₃	4.955 (2)	24.101 (9)	4.86	56.94	(d)
HoNi ₃	4.958 (3)	24.33 (1)	4.91	57.4	(a)
ErNi ₃	4.948 (2)	24.27 (1)	4.91	57.18	(a)
TmNi ₃	4.937 (2)	24.213 (9)	4.90	56.79	(a)

* (a) Button homogenized 3 days at 1000°C; powder not annealed.

(b) Button homogenized 19 hr at 900°C; powder not annealed.

(c) Button homogenized 5 days at 500°C; powder annealed 3 hr at 500°C.

(d) Button homogenized 5 days at 900°C; powder annealed 21 hr 900°C.

culated by the computer program of Mueller, Heaton & Miller (1960), and the d spacings were obtained by the program of Mueller, Meyer & Simonsen (1962). The density, measured by the immersion method, is 12.44 g.cm^{-3} , and the X-ray density is 12.52 g.cm^{-3} . The observed and calculated d spacings and observed intensities are listed in Table 1. The observed intensities are in satisfactory agreement with the observed and calculated F^2 values reported by Bertaut, Lemaire & Schweizer (1965) for HoCo_3 . The unit-cell constants of UCo_3 and of several isostructural rare-earth compounds are listed in Table 2. In this Table the Figure in parentheses is the least-squares standard error of the last significant digit. The rare-earth compounds received various heat treatments (see Table 2), but all X-ray patterns were equally well resolved.

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Crystallographic data on disubstituted symmetric ureas. By S. V. DESHAPANDE, *Physics Department, Sardar Patel University, Vallabh Vidyanagar, Gujarat State, India* and C. C. MEREDITH and R. A. PASTERNAK, * *Stanford Research Institute, Menlo Park, California 94025, U.S.A.*

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The unit-cell dimensions and space groups of six disubstituted, symmetric ureas $(\text{RHN})_2\text{C}=\text{O}$ have been established. The substituents R in this series were phenyl, *p*- and *m*-tolyl, *m*- and *o*-chlorophenyl and *p*-anisyl. Similar packing of the molecules in the unit cells is suggested by the data.

We report here the unit cells and space groups of six disubstituted symmetric ureas, $(\text{RHN})_2\text{C}=\text{O}$, with R = phenyl, *p*- and *m*-tolyl, *m* and *o*-chlorophenyl and *p*-anisyl.

Needle crystals were obtained for all the compounds by slow evaporation of their solutions in 96% ethanol. They all showed good cleavage along two directions parallel to the needle axis and no cleavage perpendicular to it. Preliminary unit-cell dimensions were derived by indexing rotation photographs around the needle axis which was

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Table 1. *Crystal data for urea derivatives*

	Molecular weight	Axial lengths			Measured density	Number of molecules	Space group	Crystal system	Remarks
		<i>a</i>	<i>b</i>	<i>c</i>					
Urea*	60.06	5.66 Å	5.66 Å	4.72 Å	1.33 g.cm ⁻³	2.02	$P4_21m$	Tetragonal	
Diphenylurea	212.25	10.51	11.73	9.07	1.23	3.90	$P2_1cn$	Orthorhombic	
Di- <i>p</i> -tolylurea	240.29	9.85	27.77	4.66	1.26	4.02	$Pn2_1a$	Orthorhombic	
Di- <i>m</i> -tolylurea	240.29	9.72	14.56	4.60	1.25	2.04	$P2_12_12$ ($P2_12_12_1$)	Orthorhombic	
Di- <i>m</i> -chlorophenylurea	281.14	9.72	14.36	4.55	1.47	2.00	$P2_12_12$ ($P2_12_12_1$)	Orthorhombic	
Di- <i>o</i> -chlorophenylurea	281.14	23.00	23.20	4.64	1.48	7.85	$Pban$	Orthorhombic	Poor crystals. $h=2n$, very weak for $h00$, $h01$. $k=2n$, very weak for $0k0$, $0k1$.
Di- <i>p</i> -anisylurea	272.29	$(\gamma^* = 81^\circ)$ 21.20 13.38 9.31 ($=d_{100}$) ($=d_{010}$)			1.35	7.95	$P1$ or $P\bar{1}$	Triclinic	Odd layer lines on rotation about c axis very weak. $hk0$ with $h+k$ odd absent; h and k odd very weak.

* Vaughan & Donohue (1952).