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Some AB_3 compounds of the transition metals. By A. E. DWIGHT, J. W. DOWNEY and R. A. CONNER, JR.,
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1. Introduction

An investigation is underway to identify new intermetallic compounds of AB_3 composition. This paper presents crystal structure data for fifteen AB_3 compounds which have been studied since those reported in a paper by Dwight & Beck (1959).

2. Experimental methods

Alloys were made by arc melting 3- or 5-gram charges in a water-cooled copper crucible. All alloys were found to be sufficiently brittle that powder could be made by hammering the cast buttons in a closed carbide die. After screening through silk cloth, specimens of powder were wrapped in Mo foil, sealed in evacuated Vycor capsules and annealed. Diffraction patterns were taken on a Straumanis-type Debye-Scherrer camera of 114.6 mm. diameter. The Nelson-Riley extrapolation was used on patterns of the cubic Cu_3Au -type compounds to obtain

Table 1. AB_3 compounds with the Cu_3Au -structure, Ll_2 , space group $Pm\bar{3}m$

AB_3	a_0	AB_3	a_0	AB_3	a_0
ScRh ₃	3.900 Å	YPt ₃	4.075 Å	ThRh ₃	4.139 Å
ScPd ₃	3.981	LaPd ₃	4.235	URh ₃	3.991
ScPt ₃	3.958	HoPd ₃	4.064	UIr ₃	4.023
YPd ₃	4.074	HoPt ₃	4.064		

Table 2. AB_3 compounds with close packed ordered structures

AB_3	Type	c_0	a_0	c/a
ThPd ₃	TiNi ₃	9.826 Å	5.856 Å	1.678
VPd ₃	TiAl ₃	7.753	3.847	2.015
VPt ₃	TiAl ₃	7.824	3.861	2.027
HfAl ₃	ZrAl ₃	17.155	3.989	4.301

Table 3. Powder diffraction data for ThPd₃, DO_{24} , Cr $K\alpha$ radiation, space group $P6_3/mmc$

hkl	d_o	d_c	I_o	I_c
102	3.506 Å	3.523 Å	<i>w</i>	30.9
110	2.910	2.927	<i>vwv</i>	17
200	2.526	2.535	<i>vw</i>	15.9
004	2.444	2.450	<i>vs</i>	78.5
202	2.247	2.252	<i>vs</i>	200
203	1.997	2.003	<i>s</i>	46.4
114	1.876	1.879	<i>w</i>	10
212	1.782	1.785	<i>vw</i>	9.9
204	1.759	1.762	<i>w</i>	10.7
205	1.5485	1.5506	<i>ms</i>	24.8
220	1.4624	1.4636	<i>s</i>	62.9
304	1.3903	1.3912	<i>vw</i>	6.7
206	1.3722	1.3730	<i>s</i>	72.3
312	1.3509	1.3516	<i>vw</i>	7.8
224	1.2566	1.2565	<i>vs</i>	192
401		1.2571		
402		1.2272		
207	1.2251	1.2255	<i>s</i>	66.6
008		1.2250		
403		1.1819		

Table 4. Powder diffraction data for VPd₃ and VPt₃, DO_{22} , Cr $K\alpha$ radiation, space group $14/mmm$

hkl	VPd ₃			VPt ₃			VNi_3^*
	I_o	d_o (Å)	d_c (Å)	I_o	d_o (Å)	d_c (Å)	
002				<i>vvw</i>	3.86	3.912	<i>vvw</i>
101	<i>w</i>	3.427	3.446	—	—	—	<i>w</i>
110	<i>vvw</i>	2.70	2.720	<i>vw</i>	2.711	2.730	<i>vvw</i>
112	<i>vs</i>	2.219	2.227	<i>vs</i>	2.228	2.239	<i>vs</i>
103	<i>vw</i>	2.142	2.145	—	—	—	<i>vwv</i>
004	<i>m</i>	1.933	1.938	<i>m</i>	1.949	1.956	<i>m</i>
200	<i>ms</i>	1.919	1.923	<i>s</i>	1.923	1.930	<i>ms</i>
202	<i>vw</i>	1.719	1.723	<i>w</i>	1.726	1.731	<i>vvw</i>
211	<i>w</i>	1.678	1.680	<i>w</i>	1.703	1.686	<i>vw</i>
114	<i>vvw</i>	1.576	1.579	<i>w</i>	1.588	1.590	<i>vvw</i>
105	<i>w</i>	1.430	1.438	—	—	—	<i>vvw</i>
213			1.432	—	—	<i>w</i>	
204	<i>s</i>	1.364	1.365	<i>s</i>	1.3724	1.3740	<i>s</i>
220	<i>ms</i>	1.359	1.360	<i>ms</i>	1.3636	1.3649	<i>ms</i>
222	<i>w</i>	1.284	1.283	<i>w</i>	1.2879	1.2888	<i>vvw</i>
301	<i>w</i>	1.265	1.265	<i>vw</i>	—	—	<i>vvw</i>
310	<i>w</i>	1.2163	1.2165	<i>w</i>	1.2205	1.2208	
116	<i>s</i>	1.1672	1.1672	<i>vs</i>	1.1765	1.1767	
312	<i>vs</i>	1.1606	1.1606	<i>vs</i>	1.1653	1.1654	
215	<i>m</i>	1.1518	1.1518				

* VNi_3 data from Pearson & Hume-Rothery (1952).

Table 5. Powder diffraction data for DO_{23} -type compounds

hkl	HfAl ₃ Cr $K\alpha$		ZrAl ₃ * Cu $K\alpha$
	I_o	d_o	I_o
004	<i>m</i>	4.25	<i>s-m</i>
101	<i>ms</i>	3.86	<i>s-m</i>
103	<i>m</i>	3.25	<i>s</i>
110	<i>m</i>	2.81	<i>s</i>
105	<i>ms</i>	2.592	<i>s-m</i>
114	<i>vs</i>	2.351	<i>st</i>
008	<i>m</i>	2.143	<i>m-st</i>
200	<i>ms</i>	1.993	<i>st</i>
204	<i>m</i>	1.810	<i>s</i>
211	<i>m</i>	1.774	<i>s</i>
109;00,10	<i>m</i>	1.722	<i>s</i>
213	<i>m</i>	1.707	<i>s</i>
215	<i>m</i>	1.581	<i>s</i>
208	<i>s</i>	1.460	<i>m-st</i>
217	<i>w</i>	1.442	<i>sss</i>
220	<i>ms</i>	1.410	<i>s-m</i>
224	<i>m</i>	1.339	<i>sss</i>
301	<i>w</i>	1.325	<i>sss</i>
219;20,10	<i>ms</i>	1.302	<i>s</i>
11,12	<i>s</i>	1.275	<i>m</i>
310	<i>m</i>	1.261	<i>ss</i>
10,13	<i>m</i>	1.253	<i>ss</i>
305	<i>m</i>	1.239	<i>sss</i>
314	<i>vs</i>	1.2096	<i>m-st</i>
228	<i>vs</i>	1.1780	<i>m</i>
307	<i>vw</i>	1.1683	—
20,12	<i>ms</i>	1.1619	<i>sss</i>
316	<i>ms</i>	1.1540	—

* $ZrAl_3$ intensities taken from Brauer (1934).

a more accurate lattice parameter. Cohen's least-squares method was applied to the hexagonal and tetragonal patterns.

3. Experimental data

The compounds and lattice parameters found in this investigation are listed in Tables 1 and 2. The observed and calculated intensities and d spacings for ThPd_3 of the hexagonal TiNi_3 -type are given in Table 3. Table 4 lists the observed and calculated d spacings and observed intensities for two compounds, VPd_3 and VPt_3 , of the TiAl_3 -type. No intensity calculations were made for VPd_3 and VPt_3 , but the observed intensities for these compounds are in good agreement with those published by Pearson & Hume-Rothery (1952) for the VNi_3 compound. The intensities observed by Pearson & Hume-Rothery for VNi_3 are reproduced in Table 4.

Table 5 lists similar data for the HfAl_3 compound, which is isostructural with ZrAl_3 . No intensity calculations were made for HfAl_3 , but the observed intensities for HfAl_3 are in good agreement with Brauer's data for ZrAl_3 , considering that the HfAl_3 intensities were obtained with $\text{Cr } K\alpha$ radiation, and the ZrAl_3 intensities with $\text{Cu } K\alpha$.

4. Discussion

With the discovery that ThPd_3 has the TiNi_3 structure, it is noted that the sequence of compounds TiPd_3 , ZrPd_3 , HfPd_3 , ThPd_3 and UPd_3 are isostructural. Likewise, the series TiRh_3 , ZrRh_3 , HfRh_3 , ThRh_3 and URh_3 all have

the Cu_3Au structure. The two compounds VPd_3 and VPt_3 are isostructural with VNi_3 . VPd_3 was previously reported by Koster & Haehl (1958).

The TiAl_3 family of compounds, of which VPd_3 and VPt_3 are members, has been indexed in the older literature with respect to two different unit cells. In this investigation we use the smaller unit cell proposed by Pearson & Hume-Rothery (1952) for VNi_3 . The c_0 parameters are the same for the two unit cells; the a_0 parameters are related by the factor $1/\sqrt{2}$.

The compound HfAl_3 is closely related to the TiAl_3 -type compounds, as was shown by Brauer (1934). The structure of HfAl_3 may be envisioned as containing two TiAl_3 unit cells stacked end to end with one inverted, and with certain layers rippled in the HfAl_3 structure as opposed to flat layers in the TiAl_3 structure.

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Structure cristalline du chloro 9-bromo 10-anthracène par diffraction des rayons X. Par M.

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Le chloro 9-bromo 10-anthracène est isomorphe du dibromo 9-10 anthracène (Trotter, 1958). Les mailles tricliniques sont très semblables.

	Dibromo 9-10 anthracène (Trotter)	Chloro 9-bromo 10-anthracène
a	$8,88 \pm 0,02 \text{ \AA}$	$8,87 \pm 0,02 \text{ \AA}$
b	$16,15 \pm 0,04$	$16,14 \pm 0,03$
c	$4,06 \pm 0,01$	$4,06 \pm 0,01$
α	$97^\circ 05' \pm 10'$	$97^\circ 10' \pm 10'$
β	$100^\circ 21' \pm 10'$	$100^\circ 39' \pm 10'$
γ	$98^\circ 50' \pm 10'$	$98^\circ 27' \pm 10'$
v	$559,3 \text{ \AA}^3$	$558,2 \text{ \AA}^3$

Densité mesurée: 1,75 g.cm.⁻³. Densité calculée: 1,735 g.cm.⁻³.

Les noyaux anthracéniques occupent exactement les mêmes positions dans les 2 structures. Les molécules présentent un centre de symétrie comme dans le dibromo 9-10 anthracène.

La structure du chloro 9-bromo 10-anthracène est une

structure statistique analogue à celle du chloro 1-bromo 4-benzène (Klug, 1947). Les atomes lourds sont des atomes mixtes: $\frac{1}{2}(\text{Br} + \text{Cl})$.

La distance C_9 -atome lourd est de $1,88 \pm 0,01 \text{ \AA}$, intermédiaire entre C_9 -Cl = $1,74 \text{ \AA}$ dans le dichloro 9-10 anthracène (Trotter, 1959) et C_9 -Br = $1,93 \text{ \AA}$ du dibromo 9-10 anthracène (Trotter, 1958). Les atomes de carbone C_9 et C_{10} du noyau anthracénique sont cependant bien localisés et ne sont pas déplacés vers le chlore comme semble l'exiger la différence de $0,2 \text{ \AA}$ entre la liaison C-Br et la liaison C-Cl.

Les déformations du noyau anthracénique que l'on peut constater dans la structure du dibromo 9-10 anthracène (Trotter, 1958) se conservent intégralement dans la structure du chloro 9-bromo 10-anthracène.

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