Short Communications

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The crystal structure of $HoZn_2$.*

By DAVID J. MICHEL and EARLE RYBA, *Department of Metallurgy, The Pennsylvania State University, University Park, Pennsylvania, U.S.A.*

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The crystal structure of $HoZn_2$ has been determined by single-crystal X-ray diffraction techniques, and was found to be isostructural with KHg_2 (Duwell & Baenziger, 1955) and $YbZn_2$ (Michel & Ryba, 1965). The alloy was prepared by melting stoichiometric amounts of 99·5+ % holmium and 99·999 % zinc in a sealed tantalum crucible. The procedure followed in the structure determination was identical with that for $YbZn_2$ (Michel & Ryba, 1965), with the following results.

Space group: *Imma*

$a = 4{\cdot}456 \pm 0{\cdot}001$, $b = 7{\cdot}039 \pm 0{\cdot}003$, $c = 7{\cdot}641 \pm 0{\cdot}005$ Å

Positional parameters:

Ho: 4(*e*) $0\frac{1}{4}z$; $z = 0{\cdot}5281 \pm 0{\cdot}004$
$B = 1{\cdot}37 \pm 0{\cdot}04$ Å^2

Zn: 8(*h*) $0yz$; $y = 0{\cdot}0410 \pm 0{\cdot}0009$,
$z = 0{\cdot}1663 \pm 0{\cdot}0008$
$B = 1{\cdot}45 \pm 0{\cdot}08$ Å^2

$R = 11{\cdot}3$ % (248 reflections)

The Debye–Scherrer data, structure factors for *hkl* (l= 0,1,2) reflections, and interatomic distances are given in Tables 1–3 respectively.

Table 1. *Debye–Scherrer data for* $HoZn_2$

hkl	d_{obs}	d_{calc}	*hkl*	d_{obs}	d_{calc}
002	3·800 Å	3·820 Å	035	1·281 Å	1·281 Å
112	2·660	2·682	152	1·264	1·266
022	2·577	2·588	026	1·200	1·198
013	2·414	2·395	251	1·177	1·176
103	2·219	2·211	314	1·155	1·157
202	1·920	1·925	062	1·121	1·121
004	1·906	1·910	400	1·114	1·114
123	1·870	1·872	402	1·069	1·069
132	1·818	1·824	334	1·048	1·049
040	1·756	1·760	163	1·036	1·036
213	1·633	1·631	055	1·035	1·035
042	1·598	1·598	422	1·024	1·023
231	1·578	1·581	413	1·010	1·010
134	1·403	1·406	262	1·002	1·002
240	1·381	1·381	431	0·998	0·998
143	1·374	1·377	352	0·988	0·987
312	1·359	1·358			
321	1·346	1·347			
125	1·336	1·337			
242	1·298	1·299			

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Table 2. *Observed and calculated structure factors for* $HoZn_2$

hkl	F_o	F_c	*hkl*	F_o	F_c
200	181	182	091	8	−11
400	97	107	202	53	48
600	50	57	402	28	32
800	25	28	602	17	18
020	31	−27	112	63	−57
220	25	−25	312	38	−38
420	15	−18	512	18	−22
620	15	−11	712	11	−11
040	129	125	022	156	−137
240	109	104	222	111	−110
440	67	68	422	62	−69
640	36	38	622	32	−38
060	65	−62	822	14	−19
260	53	−54	132	13	−14
460	39	−38	332	11	−9
660	23	−22	532	3	−4
080	32	28	042	61	60
280	28	25	242	51	51
480	14	18	442	31	35
101	82	−64	642	20	20
301	47	−44	152	58	−69
501	26	−27	352	49	−51
701	11	−14	552	29	−31
121	161	143	752	17	−17
321	105	96	062	53	−57
521	52	56	262	46	−50
721	29	29	462	36	−35
031	75	−68	662	22	−21
231	60	−54	172	5	−15
431	34	−34	572	6	−7
631	18	−18	082	43	47
141	66	−64	282	39	42
341	52	−47	482	29	30
541	29	−29	192	18	−28
741	12	−16	392	19	−22
051	36	−36			
251	29	−30			
451	17	−20			
161	20	60			
181	15	−49			

Table 3. *Interatomic distances in* $HoZn_2$

Ho–2Ho	4·060 ± 0·008 Å	Zn–2Ho	3·207 ± 0·005 Å
Ho–2Ho	3·546 ± 0·003	Zn–1Ho	3·132 ± 0·007
Ho–4Zn	3·207 ± 0·005	Zn–1Ho	3·107 ± 0·007
Ho–2Zn	3·132 ± 0·007	Zn–2Ho	3·057 ± 0·005
Ho–2Zn	3·107 ± 0·007	Zn–1Zn	2·942 ± 0·018
Ho–4Zn	3·057 ± 0·005	Zn–1Zn	2·606 ± 0·018
		Zn–2Zn	2·572 ± 0·009

References

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