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The crystal structure of YCu_2.*

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Four intermetallic compounds have been reported in the yttrium–copper system (Daane & Spedding, 1957; Domagala, Rausch & Levinson, 1961). The crystal structure of one of these compounds, YCu_2, is the subject of this communication. Storm & Benson (1963) have determined from powder X-ray data that the compound YCu_2 is isostructural with $CeCu_2$ (Larson & Cromer, 1961). We also found this and discuss here our independent determination of the structure of YCu_2 by single-crystal techniques.

Several samples of YCu_2, prepared by conventional arc melting techniques, were examined by powder and single-crystal methods. Cu $K\alpha$ radiation was used. Oscillation and Weissenberg photographs for a number of single crystals indicated that the compound was body-centered orthorhombic with $a=4{\cdot}3$, $b=6{\cdot}9$, $c=7{\cdot}3$ Å. A Debye–Scherrer pattern of YCu_2 was subsequently indexed and the lattice constants found were $a = 4{\cdot}308 \pm 0{\cdot}003$, $b = 6{\cdot}891 \pm 0{\cdot}008$, $c = 7{\cdot}303 \pm 0{\cdot}007$ Å. These results substantially agree with those of Storm & Benson, who report $a=4{\cdot}305 \pm 0{\cdot}005$, $b=6{\cdot}800 \pm 0{\cdot}005$, $c=7\ 315 \pm 0{\cdot}005$ Å, except for the b parameter.

Table 1. *Final parameters in* YCu_2 *from the least squares refinement*

Atom	Position	x	y	z	B (Å^2)
Y	4*e*	0	$\frac{1}{4}$	$0{\cdot}546 \pm 0{\cdot}002$	0·46
Cu	8*h*	0	$0{\cdot}052 \pm 0{\cdot}002$	$0{\cdot}162 \pm 0{\cdot}002$	1·50

Table 2. *Observed and calculated structure factors of* YCu_2

hkl	F_o	F_c	*hkl*	F_o	F_c
002	35	26	053	62	53
004	47	−39	055	140	140
006	98	83	060	127	−114
008	64	−61	062	52	−48
011	26	−16	064	18	−11
013	89	83	071	71	−65
015	124	125	073	46	−53
017	38	46	075	24	−19
019	29	25	082	91	72
020	13	17	044	N.O.	19
022	116	−160	035	N.O.	−6
024	81	−100	046	N.O.	8
026	73	82	057	N.O.	11
031	129	−143	028	N.O.	26
033	70	−85	066	N.O.	−13
037	84	−104			
040	154	136			
042	68	67			
048	40	−41			
051	82	−67			

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Table 3. *Interatomic distances in* YCu_2

Y–2 Y	3·679 Å	Cu–1 Y	3·114 Å
Y–2 Y	3·508	Cu–2 Y	3·113
Y–2 Cu	3·114	Cu–1 Y	2·982
Y–4 Cu	3·113	Cu–2 Y	2·963
Y–2 Cu	2·982	Cu–1 Cu	2·722
Y–4 Cu	2·963	Cu–2 Cu	2·506
		Cu–1 Cu	2·474

The orthorhombic unit cell contains four formula units of YCu_2, and the calculated X-ray density is 6·62 g.cm^{-3}. Systematic absences of reflections from single crystals indicated that the space group is either *Im2a* or *Imma*. Visual estimation of intensities from equiinclination Weissenberg photographs was made for two single crystals. For crystal *A*, (*hkl*) data with $l=0$ to 4 were obtained; for crystal *B*, (0*kl*) data were obtained. The resulting intensities were corrected for Lorentz and polarization factors, but only the data for crystal *A* were corrected for absorption since crystal *B* was very irregular in shape.

(*hk*0), (*h*0*l*), and (0*kl*) Patterson projections were found in satisfactory agreement only with a postulated structure in which four yttrium atoms and eight copper atoms are in the 4*e* and 8*h* equipoint positions, respectively, of the space group *Imma*. Since this postulated structure is the same as the structure of $CeCu_2$, the parameters given for $CeCu_2$ were chosen as the trial parameters for YCu_2. The trial structure of YCu_2 was refined for both sets of intensity data by the diagonal least-squares method. The residuals for the data for crystals *A* and *B* were found to be 16·6% and 13·6%, respectively, after 15 cycles of refinement. The positional parameters obtained from two sets of data were almost identical. The results of the refinement of the data for crystal *B* are given in Table 1. The calculated and observed structure factors for this data are given in Table 2, and the interatomic distances are given in Table 3.

All of the crystals of this compound which were examined exhibit some twinning, and it was expected that the intensity measurements would be somewhat in error. The possibility of a phase transformation in this compound which would produce the twinning is being investigated.

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