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The crystal structure of CeCu.*

By ALLEN C. LARSON and DON T. CROMER. *University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, U.S.A.*

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In the Ce–Cu system there are four binary compounds. The structures of $CeCu_6$, $CeCu_4$ and $CeCu_2$ have been determined by Cromer, Larson & Roof (1960), Byström, Kierkegaard & Knop (1952) and Larson & Cromer (1961), respectively. The structure of the remaining compound in this series, CeCu, is the subject of the present communication.

A stoichiometric CeCu alloy was vacuum inductiou melted at 1075 °C. in an MgO crucible. The alloy was then placed under a helium atmosphere in a resistance furnace and held overnight at 500 °C. It was cooled to 400 °C. at a rate of 5°/hr. and then cooled to room temperature at a more rapid rate. Because the alloy oxidizes rather easily, fragments were sealed in thin pyrex capillaries for X-ray examination.

The alloy is rather soft, and it was impossible to obtain single crystal fragments by crushing the ingot at room temperature. Therefore a portion of the ingot was cooled

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Table 1. *Parameters from the least-squares refinement of* CeCu

	x	y	z	B (Å²)
Ce	0·1670 ± 0·0006	¼	0·1469 ± 0·0007	1·7 ± 0·1
Cu	0·0413 ± 0·0015	¼	0·6034 ± 0·0017	2·5 ± 0·3

Table 2. *Observed and calculated structure factors for* CeCu

If F_o is negative the minus sign should be interpreted as 'less than'

h0l

h	F_o	F_c
	$l=0$	
2	26	−12
4	37	−35
6	97	98
8	51	−46
10	39	−31
	$l=1$	
1	26	−19
2	111	−101
3	143	−143
4	118	129
5	31	24
6	31	23
7	35	29
8	39	−33
9	35	−23
10	42	34
	$l=2$	
0	30	−26
1	159	−174
2	45	42
3	47	−47
4	27	25
5	50	46
6	29	−24
7	87	−90
8	−18	6
9	−17	−10
	$l=3$	
1	46	−44
2	17	−13
3	125	134
4	82	75
5	49	−42
6	36	26
7	35	−34
8	−18	−2
9	49	40
	$l=4$	
0	138	−158
1	52	49
2	−15	11
3	16	−17
4	21	23
5	54	−54
6	71	−63
7	26	18
8	35	29
	$l=5$	
1	44	36
2	77	81
3	45	34
4	77	−73
5	−18	3
6	−18	−1
7	−17	−7
8	40	37
	$l=6$	
0	41	38
1	47	54
2	55	−48
3	19	13
4	38	−33
5	27	−22
6	44	38
7	46	36
	$l=7$	
1	33	36
2	23	−20
3	60	−56
4	−18	−7
5	32	25
	$l=8$	
0	37	31
1	39	−36
2	−18	−5

h1l

h	F_o	F_c
	$l=0$	
4	54	62
6	34	−40
8	55	−75
	$l=1$	
2	113	114
3	44	41
4	65	69
5	82	93
6	63	−73
7	−21	−18
8	−22	20
9	−23	10
	$l=2$	
1	188	−157
2	32	26
3	95	88
4	43	−41
5	58	−62
6	−20	−9
7	26	−28
8	−23	9
9	43	57
	$l=3$	
0	15	12
1	112	108
2	87	75
3	19	−15
4	46	41
5	74	−87
6	25	−28
7	38	46
8	−23	2
	$l=4$	
1	−15	4
2	109	103
3	68	−70
4	41	−44
5	24	17
6	21	23
7	−22	18
8	46	48
	$l=5$	
0	91	93
1	−17	−2
2	51	−50
3	23	−24
4	39	−40
5	29	−30
6	62	60
7	−23	−11
	$l=6$	
1	50	46
2	34	−38
3	32	−36
4	45	56
5	22	24
6	−22	11
	$l=7$	
0	36	−33
1	51	−55
2	26	−12
3	−22	−2
4	−22	−4
5	39	38
	$l=8$	
1	−22	−9
2	23	−22
3	43	49

by immersing it in liquid nitrogen. At this low temperature it was crushed without deformation, and a single crystal was found among the fragments. A precession camera and Mo $K\alpha$ X-rays ($\lambda = 0{\cdot}7107$ Å) were used to examine the crystal, which was found to be orthorhombic with $a = 7{\cdot}30$, $b = 4{\cdot}30$ and $c = 6{\cdot}36$ Å, all $\pm 0{\cdot}02$ Å. Systematic absences were $hk0$ with $h = 2n + 1$ and $0kl$ with $k + l = 2n + 1$. Thus the space group, if centric, is *Pnma*. The structural analysis showed that this space group is correct. With four formula units per unit cell the calculated density is 6·78 g.cm.$^{-3}$. A measured density was not obtained.

For intensity measurements a series of timed precession photographs of the $h0l$ and $h1l$ levels was made with Mo $K\alpha$ radiation. The intensities were estimated visually by comparing them with a series of calibration spots of known relative intensities. No absorption corrections were made.

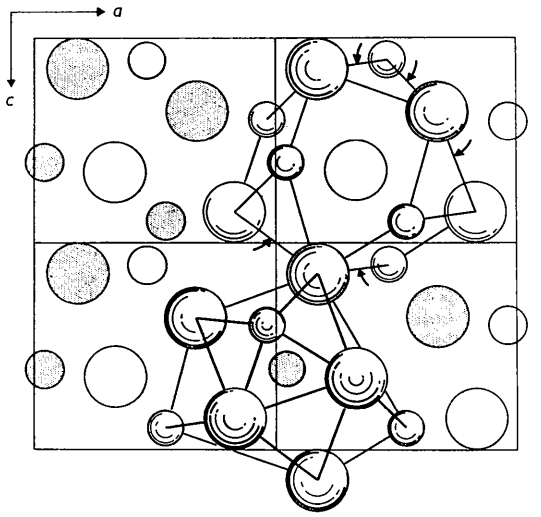

Fig. 1. The structure of CeCu in projection down the b axis. The large circles are Ce atoms and the small circles are Cu atoms. The shaded circles are at $y = \frac{1}{4}$ and the open circles are at $y = \frac{3}{4}$. The shading is omitted for atoms making up the polyhedra.

The axial ratios and space group suggested that CeCu might have the FeB structure. An $h0l$ Patterson projection showed this to be true. A full-matrix, least-squares refinement was then computed on an IBM 704. Separate scale factors for the two layers, and isotropic temperature factors were included as parameters. Form factors were used in functional form by using the parameters given by Forsyth & Wells (1959). The final results are given in Table 1, and the observed and calculated structure factors are given in Table 2. The overall value of R was 11·0%. For the $h0l$ data, $R = 11{\cdot}3\%$ and for the $h1l$ data, $R = 10{\cdot}7\%$, with $F = 0$ terms omitted in all cases. A projection of the structure along the b axis is shown in Fig. 1. The interatomic distances are listed in Table 3. The definition of a neighbor as given by Frank & Kasper (1958) was used to determine which atoms should be included in Table 3. The Ce atoms has 15 neighbors including seven Cu atoms and eight Ce atoms. The *convex* polyhedron formed by these 15 neighbors has two five-sided faces, four four-sided faces and twelve three-sided faces. The arrows in Fig. 1 point to vertical three-sided faces which are bisected by the mirror at $y = \frac{1}{4}$. The Cu atom has 11 neighbors including seven Ce atoms and four Cu atoms. These 11 neighbors form a convex polyhedron having 18 three-sided faces. The lines forming the convex polyhedra do not necessarily join atoms that are themselves neighbors in the Frank & Kasper sense. Furthermore, some lines joining common neighbors are interior to the convex polyhedra.

Table 3. *Interatomic distances in* CeCu

Standard deviations are approximately 0·009, 0·017 and 0·022 Å for Ce–Ce, Ce–Cu and Cu–Cu distances, respectively. The numerals in parentheses indicate the number of crystallographically equivalent distances

Ce–Ce	(2)	3·750 Å	Cu–Cu	(2)	2·591 Å
	(2)	3·878		(2)	4·099
	(4)	4·025	–Ce	(2)	3·039
–Cu	(2)	3·039			3·045
		3·045		(2)	3·075
	(2)	3·075			3·162
		3·162			3·576
		3·576			

In FeB itself, the Fe atom has 17 neighbors. The b axis in this compound is so short that the Fe atoms displaced by one unit cell in this direction also become neighbors. These two extra neighbors lie out from the centers of the five-sided faces. The neighbors of the B atom in FeB are the same crystallographically as those of the Cu atom in CeCu.

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