

## The Crystal Structure of CeCu<sub>6</sub>\*

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The crystal structure of CeCu<sub>6</sub> has been determined by single crystal X-ray diffraction methods. The crystal system is orthorhombic with

$$a = 8.112, b = 5.102, c = 10.162 \text{ \AA}.$$

The unit cell contains four formula units and the probable space group is *Pnma*. Three-dimensional X-ray data were obtained by two different counter techniques and the results are compared. The trial structure was determined by application of the sign relation  $S_H = S_K \cdot S_{H+K}$  to the  $h0l$  zone. The final structure was obtained by a least-squares refinement with anisotropic temperature factors included. The structure contains typical metallic bonds. There are no Ce-Ce contacts and each Ce atom is surrounded by 19 Cu atoms in a manner quite similar to the surroundings of Ca in the CaCu<sub>6</sub> structure. The average Ce-Cu distance is 3.146 Å. The Cu-Cu distances are in reasonable agreement with those found in Cu metal.

### Introduction

CeCu<sub>6</sub> is one of four inter-metallic compounds reported in the binary system Ce-Cu (Hanaman, 1915; Hansen, 1958). The space group and lattice constants of CeCu<sub>6</sub> have been reported by Byström, Kierkegaard & Knop (1952) but these authors did not determine its structure. As part of a program of structural studies of compounds of cerium and of plutonium with other metals we have completed the structure determination of CeCu<sub>6</sub>.

### Preparation, unit cell and space group of CeCu<sub>6</sub>

A Ce-Cu alloy containing about 20 at.% Ce was melted at about 900 °C. and then heat treated for 68 hr. at 765 °C. The alloy was crushed, and single crystals of CeCu<sub>6</sub> were found among the fragments. Weissenberg photographs established the crystal system as orthorhombic, space group *Pnma*, provided that the crystal is centro-symmetric. Lattice constants were determined with the General Electric Co. 'single crystal orienter' (Furnas & Harker, 1955; Furnas, 1957) using Cu  $K\alpha_1$  radiation ( $\lambda = 1.54051 \text{ \AA}$ ) and they are

$$a = 8.112 \pm 0.001, b = 5.102 \pm 0.001, \\ c = 10.162 \pm 0.005 \text{ \AA}.$$

Except for the value of  $a$ , these lattice constants agree well with those reported by Byström *et al.*, which are

$$a = 8.085, b = 5.097, c = 10.172 \text{ \AA}.$$

The calculated density with four formula units per unit cell is 8.23 g.cm.<sup>-3</sup>. Olsen (1959), using a 10 g. sample from an ingot of stoichiometric CeCu<sub>6</sub> which

had been arc melted and then annealed for 72 hr. at 750 °C., found the measured density to be 8.24 g.cm.<sup>-3</sup>.

### Intensity measurements

The first crystal used for intensity measurements had some small satellite crystals adhering to it. This crystal was used only for intensity measurements of the  $h0l$  zone using Ag  $K\alpha$  radiation and the single crystal orienter. Reflections for  $\theta_{Ag} \leq 30^\circ$  were investigated. This limited set of data will be referred to as the 'Ag' data. A better crystal was subsequently found and it was used to collect three-dimensional data using Mo  $K\alpha$  radiation and the single crystal orienter. Out of 1856 possible reflections, 1352 were observed. This set of data will be referred to as the 'SCO' data. This same crystal, mounted on the  $c$  axis, was also used to collect three-dimensional data on the North American Philips Co. counter device which is adapted to a Weissenberg camera (Evans, 1953). Intensities were measured for the levels  $l=0$  through  $l=13$  and 1101 out of a possible 1568 reflections were observed. This set of data will be referred to as the 'W' data. In both of these latter cases, reflections were measured within a sphere defined by  $\theta_{Mo} \leq 45^\circ$ . A proportional counter was used for the Ag and SCO data and a scintillation counter for the W data.

For both counter techniques, angular settings were computed on an IBM 704. In the W technique, the crystal is rocked through the reflecting position and this motion permits the measurement of both the  $\alpha_1$  and  $\alpha_2$  components of the diffracted beam over a considerably larger sphere than is possible in the SCO technique. Geometric considerations were such that the entire  $\alpha_1, \alpha_2$  doublet was recorded in the W method over the entire range investigated, and in the SCO method an increasing portion of the  $\alpha_2$

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component was lost for  $\theta$  greater than approximately  $20^\circ$ . No attempt was made to correct for this intensity loss and the effect of this neglect will be discussed later.

No absorption corrections were made. The fact that two independent sets of intensities, which were recorded with different geometries and hence different absorption errors, lead to essentially the same atomic positions indicates that absorption errors were unimportant.

### Determination of the trial structure

For space group  $Pnma$  the Ce atoms must be in the set  $4c$  because in the other fourfold sets the atoms would be  $b/2 = 2.55 \text{ \AA}$  apart and this distance is much too small for a Ce-Ce contact. The 24 Cu atoms could conceivably be placed in a variety of four and eightfold positions. Those Cu atoms in eightfold sets, however, must have  $y \sim 0$  because of the short  $b$  axis and the mirror at  $y = \frac{1}{4}$ . The problem is such that once the  $xz$  projection is known the structure is essentially solved. This compound appeared to be a particularly favorable one for which to use a direct method, rather than the usual Patterson technique, to determine its approximate structure.

The  $h0l$  Ag data were converted to unitary structure factors by use of the relation given by Lipson & Cochran (1953). The signs of two reflections were arbitrarily chosen and the inequality relation

$$(|U_H| + |U_K|)^2 \leq 1 + S_H S_K (U_{H+K} + U_{H-K}) + U_{H+K} U_{H-K}$$

established with reasonable certainty the signs of two other reflections. Then the sign relation  $S_H = S_K \cdot S_{H+K}$ , which is probably true for reflections with large unitary structure factors, was systematically applied. A self consistent set of signs for 47 out of 155 observed  $F(h0l)$  was thus obtained. A Fourier projection on (010) was calculated using these terms and this projection is shown in Fig. 1. Two large peaks and four smaller peaks of about half the size of the larger ones were observed. One of the large peaks is the Ce atom and the other large peak is an eightfold Cu atom. In the eightfold set two atoms superpose in projection on (010), and because the scattering factor of Cu is about one half that of Ce, two superposed Cu atoms will have a peak approximately the same as that of one Ce atom. The four smaller peaks are fourfold Cu atoms. The  $y$  parameter of  $\frac{1}{4}$  or  $\frac{3}{4}$  for the fourfold Cu atoms, the identification of the large peaks and the assignment of  $y = \frac{1}{4}$  or  $\frac{3}{4}$  to the Ce atom could be

unambiguously decided by consideration of the resulting interatomic distances.

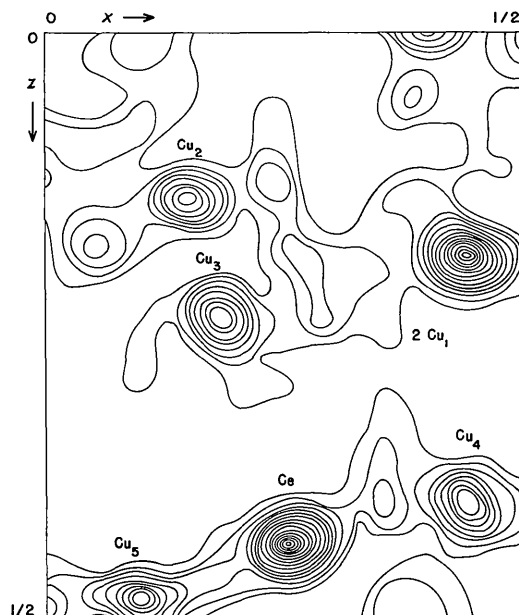


Fig. 1. Fourier projection on (010) using  $47F(h0l)$  terms whose signs had been determined by the direct method. Contours are at equal arbitrary intervals.

This trial structure was physically reasonable in that there were no unduly short interatomic distances and all of the atoms were accounted for. Also, all of the signs used in the Fourier projection had been correctly predicted. Harker syntheses were computed along the lines  $\frac{1}{2}, 0, z$  and  $x, \frac{1}{2}, \frac{1}{2}$ . These line calculations, which, of course, used all of the data, were in complete agreement with the structure deduced from only the  $h0l$  reflections.

### Refinement of the structure with the SCO data

An IBM 704 was used for all least-squares calculations. The Ce form factor was taken from the *Internationale Tabellen* (1935) and the Cu form factor was that of Viervoll & Øgrim (1949). Anomalous dispersion corrections of  $\Delta f' = -1.3$  electrons and  $+0.4$  electrons were applied to the Ce and Cu form factors, respectively (James, 1948). The quantity  $\Delta f''$  was ignored. In all cases the full matrix was used to compute shifts and this matrix was inverted for standard deviation calculations.

Table 1. Parameters from the isotropic refinement of the SCO data

Atom	$x$	$y$	$z$	$B (\text{\AA}^2)$
Cu <sub>1</sub>	$0.4354 \pm 0.0003$	$0.0041 \pm 0.0005$	$0.1908 \pm 0.0004$	$1.03 \pm 0.02$
Cu <sub>2</sub>	$0.1467 \pm 0.0005$	$\frac{1}{4}$	$0.1418 \pm 0.0005$	$1.24 \pm 0.04$
Cu <sub>3</sub>	$0.1821 \pm 0.0004$	$\frac{3}{4}$	$0.2451 \pm 0.0005$	$1.03 \pm 0.04$
Cu <sub>4</sub>	$0.4380 \pm 0.0005$	$\frac{3}{4}$	$0.4023 \pm 0.0004$	$1.30 \pm 0.04$
Cu <sub>5</sub>	$0.0987 \pm 0.0005$	$\frac{3}{4}$	$0.4846 \pm 0.0005$	$1.12 \pm 0.04$
Ce	$0.2602 \pm 0.0005$	$\frac{1}{4}$	$0.4354 \pm 0.0003$	$0.92 \pm 0.02$

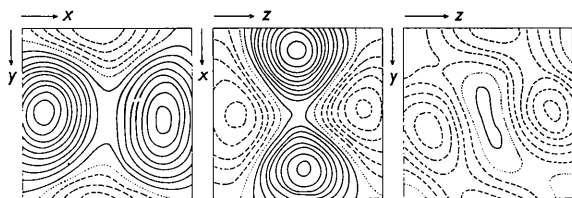


Fig. 2. Sections of the  $(F_o - F_c)$  Fourier through the  $\text{Cu}_1$  atom. Each section is  $1 \text{ \AA} \times 1 \text{ \AA}$  and the atomic position is at the center. The zero contour is dotted, the negative contours are dashed and the positive contours are solid. The contour interval is 1 electron per  $\text{\AA}^3$ .

The initial refinement was made with the SCO data and individual isotropic temperature factors were included as parameters. After a few cycles,  $R$  dropped to 10.8%. The final parameters for this refinement are given in Table 1. An  $(F_o - F_c)$  Fourier was then calculated. The density was flat and near zero at the positions of all of the atoms. However, there were peaks and holes near all of the atoms indicating a very definite anisotropy in thermal motion. The principal axes of the vibration ellipsoid were in all cases parallel, or very nearly parallel, to the crystallographic axes. As an example, sections of the  $(F_o - F_c)$  Fourier, normal to the axes and through the center of  $\text{Cu}_1$  are shown in Fig. 2. It is evident from these sections that  $\text{Cu}_1$  is vibrating with greatest amplitude in a direction parallel to  $a$ .

Refinement was continued with the addition of anisotropic temperature factors. For those atoms lying on the mirror planes the  $B_{12}$  and  $B_{23}$  terms of the temperature factor reduce to zero. Thus  $\text{Cu}_1$ , in the general position, has six thermal parameters and the other atoms each have four thermal parameters. After a few cycles,  $R$  dropped to 7.66%. The final position parameters for this refinement are given in Table 2,

Table 2. Final position parameters from the anisotropic refinement of the SCO data

Atom	$x$	$y$	$z$
$\text{Cu}_1$	$0.4354 \pm 0.0002$	$0.0042 \pm 0.0003$	$0.1908 \pm 0.0001$
$\text{Cu}_2$	$0.1467 \pm 0.0003$	$\frac{1}{2}$	$0.1418 \pm 0.0002$
$\text{Cu}_3$	$0.1821 \pm 0.0003$	$\frac{1}{2}$	$0.2450 \pm 0.0002$
$\text{Cu}_4$	$0.4381 \pm 0.0003$	$\frac{1}{2}$	$0.4024 \pm 0.0002$
$\text{Cu}_5$	$0.0986 \pm 0.0003$	$\frac{1}{2}$	$0.4846 \pm 0.0002$
Ce	$0.2602 \pm 0.0001$	$\frac{1}{2}$	$0.4354 \pm 0.0001$

the final thermal parameters are given in Table 3 and the observed and calculated structure factors are given in Table 4. The atomic coordinates have changed from the isotropic refinement by 0.0001 at most but the

Table 3. Thermal parameters in  $\text{\AA}^2$  obtained from the anisotropic refinement of the SCO data

Atom	$B_{11}$	$B_{22}$	$B_{33}$	$B_{13}$	$B_{12}$	$B_{23}$
$\text{Cu}_1$	$1.43 \pm 0.04$	$0.92 \pm 0.04$	$0.84 \pm 0.02$	$0.05 \pm 0.04$	$0.05 \pm 0.04$	$0.07 \pm 0.03$
$\text{Cu}_2$	$1.60 \pm 0.07$	$1.53 \pm 0.08$	$0.75 \pm 0.02$	$-0.01 \pm 0.04$		
$\text{Cu}_3$	$1.27 \pm 0.06$	$1.20 \pm 0.07$	$0.75 \pm 0.01$	$0.02 \pm 0.03$		
$\text{Cu}_4$	$1.70 \pm 0.07$	$1.83 \pm 0.09$	$0.63 \pm 0.03$	$0.04 \pm 0.04$		
$\text{Cu}_5$	$1.85 \pm 0.07$	$1.13 \pm 0.07$	$0.58 \pm 0.01$	$-0.02 \pm 0.03$		
Ce	$1.23 \pm 0.03$	$0.96 \pm 0.03$	$0.64 \pm 0.03$	$0.01 \pm 0.01$		

standard deviations have been approximately halved. In Table 3 the parameters used in the least-squares calculations have been reduced to the same form as the isotropic temperature factor (Jeffrey & Shiono, 1959) so that they can be directly compared with those given in Table 1.

The cross terms of the thermal parameters are not significantly different from zero, in agreement with the observations made on the  $(F_o - F_c)$  Fourier.

### Refinement of the structure with the W data

A least-squares refinement with isotropic temperature factors was next made using the W data. Separate scale factors were included for each of the 14 values of  $l$ . Because intensities had been measured for only one mounting of the crystal, no internal layer to layer correlation was possible. In principle, all layers should be on the same scale and indeed, the average deviation of the various scale factors from their mean was only 2.1% even though the measurements had been made over a period of three weeks.

After a few cycles,  $R$  dropped to 7.2%. The final parameters for this set of data are given in Table 5. Except for the temperature factors, in no case is there a significant difference between the parameters listed in Tables 1 and 5. The higher temperature factors given by the SCO data, as well as the higher  $R$ , are undoubtedly caused by partial intensity loss in the high order reflections due to the dispersion of the  $\alpha_1$  and  $\alpha_2$  components of the diffracted beam. However, this intensity loss has not significantly affected the position parameters and these parameters are the important ones. Another reason for the lower  $R$  for the W data is that several scale factors were used and, of course, as the number of parameters increases the agreement between observed and calculated quantities will improve. In addition, separate scale factors for each value of  $l$  will tend to partially correct for anisotropy of thermal motion in the  $c$  direction.

Without first placing all reflections on the same scale in some way, an anisotropic refinement with the W data is impossible because of the high correlation between the scale factors and the  $B_{33}$ 's. Nevertheless, out of curiosity to see exactly what would happen, an anisotropic least-squares calculation with separate scale factors was tried. Somewhat to our surprise the problem quickly converged and there was no significant change in the position parameters. The scale and temperature parameters changed but not by particularly large amounts. As expected, the standard devia-



Table 4 (cont.)

6	7	10	34	35	10	3	11	37	-17	2	7	13	26	-19	9	2	14	-16	13	3	5	17	-15	-14
7	0	10	19	22	10	3	11	37	-17	2	7	13	26	-19	9	2	14	-16	13	3	5	17	-15	-14
7	1	10	22	-25	10	3	11	37	-17	2	7	13	26	-19	9	2	14	-16	13	3	5	17	-15	-14
7	3	10	20	23	10	5	11	24	-23	3	5	15	40	-8	10	2	14	35	36	1	2	17	-13	-10
7	4	10	29	18	11	0	11	-13	5	3	4	13	-12	-8	10	3	14	14	-17	1	4	17	-14	-10
7	5	10	15	-18	12	2	11	24	-28	4	7	0	11	-12	10	2	14	-14	-17	2	5	17	-14	-6
7	6	10	-13	-6	11	2	11	-13	4	3	6	17	27	11	2	14	-16	-18	2	0	17	25	-76	-76
7	7	10	-14	13	11	3	11	-14	-4	3	7	13	28	29	11	2	14	24	-17	2	0	17	-13	-14
7	8	10	-12	-11	4	11	11	-14	-15	4	7	0	11	-12	10	2	14	-14	-17	2	5	17	-14	-6
8	1	10	13	16	17	0	11	-14	7	4	1	13	16	11	0	3	15	-13	-3	2	3	17	-17	-15
8	2	10	-12	-12	17	0	11	10	21	4	2	13	31	-31	0	5	15	-13	-3	2	4	17	-14	-16
8	3	10	-14	-12	18	1	11	15	18	5	4	13	35	-35	0	5	15	-13	-3	2	4	17	-14	-16
8	4	10	59	-57	12	0	11	18	-19	4	4	13	35	33	1	1	15	40	44	3	0	17	-13	-8
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8	6	10	-14	-8	13	1	11	-14	-21	5	6	13	17	-15	1	3	15	38	-41	3	2	17	-13	-7
8	7	10	-14	-8	13	2	11	-14	-2	4	7	11	-14	-8	1	4	15	33	-34	3	3	17	21	21
8	8	10	-12	-60	0	0	12	48	52	5	0	13	-12	6	1	5	15	30	-29	3	4	17	-14	-6
9	1	10	-12	13	0	2	12	83	-79	5	1	13	41	43	1	6	15	-14	-10	3	5	17	14	-17
9	2	10	32	35	0	4	12	33	36	5	2	13	47	-46	2	0	15	47	-50	4	0	17	13	-19
9	3	10	-13	-10	0	6	12	36	-47	5	3	13	35	-33	2	1	15	27	20	4	1	17	34	-35
9	4	10	48	-46	0	8	12	-18	-15	6	2	13	42	-17	3	0	15	-12	-9	4	2	17	-14	-45
9	5	10	-13	10	1	0	12	37	-37	5	5	13	34	31	2	3	15	16	-16	4	1	17	29	11
9	6	10	-12	8	2	1	12	26	-23	5	6	13	26	-27	2	4	15	38	-38	4	4	17	16	17
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10	8	10	21	20	3	0	12	17	-15	6	7	13	12	-12	4	6	15	-14	-6	6	3	17	-14	-18
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13	8	10	14	17	3	3	12	15	11	8	11	13	34	33	5	10	15	77	-77	1	7	18	31	36
13	9	10	14	17	3	3	12	15	11	8	12	13	34	33	5	11	15	77	-77	1	8	18	31	36
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14	2	10	30	25	3	6	12	-99	-104	9	3	13	-13	-8	5	8	15	-14	-3	1	5	18	21	25
14	3	10	30	25	3	6	12	-99	-104	9	4	13	-13	-8	5	9	15	-14	-3	1	6	18	21	25
14	4	10	30	25	3	6	12	-99	-104	9	5	13	-13	-8	5	10	15	-14	-3	1	7	18	21	25
14	5	10	30	25	3	6	12	-99	-104	9	6	13	-13	-8	5	11	15	-14	-3	1	8	18	21	25
14	6	10	30	25	3	6	12	-99	-104	9	7	13	-13	-8	5	12	15	-14	-3	1	9	18	21	25
14	7	10	30	25	3	6	12	-99	-104	9	8	13	-13	-8	5	13	15	-14	-3	1	10	18	21	25
14	8	10	30	25	3	6	12	-99	-104	9	9	13	-13	-8	5	14	15	-14	-3	1	11	18	21	25
14	9	10	30	25	3	6	12	-99	-104	9	10	13	-13	-8	5	15	15	-14						

Table 6. *Interatomic distances in CeCu<sub>6</sub>*

The standard deviation of Ce-Cu distances is 0.004 Å and of Cu-Cu distances 0.005 Å. The number of crystallographically equivalent distances is given in parentheses

Ce-Cu <sub>1</sub> (2)	3.127 Å	Cu <sub>1</sub> -Ce (1)	3.127 Å
-Cu <sub>1</sub> (2)	3.188	-Ce (1)	3.188
-Cu <sub>1</sub> (2)	3.306	-Ce (1)	3.306
-Cu <sub>2</sub> (1)	3.122	-Cu <sub>1</sub> (1)	2.509
-Cu <sub>2</sub> (1)	3.233	-Cu <sub>1</sub> (1)	2.593
-Cu <sub>2</sub> (2)	3.388	-Cu <sub>2</sub> (1)	2.703
-Cu <sub>3</sub> (1)	3.182	-Cu <sub>2</sub> (1)	2.721
-Cu <sub>3</sub> (2)	3.263	-Cu <sub>3</sub> (1)	2.472
-Cu <sub>4</sub> (1)	2.952	-Cu <sub>3</sub> (1)	2.492
-Cu <sub>4</sub> (2)	2.950	-Cu <sub>4</sub> (1)	2.510
-Cu <sub>5</sub> (1)	3.023	-Cu <sub>5</sub> (1)	2.459
-Cu <sub>5</sub> (2)	2.910	-Cu <sub>5</sub> (1)	2.571
Cu <sub>2</sub> -Ce (1)	3.122	Cu <sub>3</sub> -Ce (1)	3.182
-Ce (1)	3.233	-Ce (2)	3.263
-Ce (2)	3.388	-Cu <sub>1</sub> (2)	2.472
-Cu <sub>1</sub> (2)	2.703	-Cu <sub>1</sub> (2)	2.492
-Cu <sub>1</sub> (2)	2.721	-Cu <sub>2</sub> (2)	2.773
-Cu <sub>3</sub> (2)	2.773	-Cu <sub>4</sub> (1)	2.483
-Cu <sub>4</sub> (1)	2.529	-Cu <sub>4</sub> (1)	2.620
-Cu <sub>4</sub> (2)	3.095	-Cu <sub>5</sub> (1)	2.526
-Cu <sub>5</sub> (1)	2.611		
Cu <sub>4</sub> -Ce (1)	2.952	Cu <sub>5</sub> -Ce (1)	3.023
-Ce (2)	2.950	-Ce (2)	2.910
-Cu <sub>1</sub> (2)	2.510	-Cu <sub>1</sub> (2)	2.459
-Cu <sub>2</sub> (1)	2.529	-Cu <sub>1</sub> (2)	2.571
-Cu <sub>2</sub> (2)	3.095	-Cu <sub>2</sub> (1)	2.611
-Cu <sub>3</sub> (1)	2.483	-Cu <sub>3</sub> (1)	2.526
-Cu <sub>3</sub> (1)	2.620	-Cu <sub>4</sub> (1)	2.876
-Cu <sub>1</sub> (2)	3.385	-Cu <sub>5</sub> (2)	3.028
-Cu <sub>5</sub> (1)	2.876		

Cu<sub>2</sub> has four Ce and ten Cu neighbors. The four Ce atoms form a tetrahedron and there is a triangle of three Cu atoms in three of the faces of this tetrahedron. There is a single Cu atom in the center of the fourth face of the tetrahedron. If the single Cu atom were a triangle of three Cu atoms, the coordination about Cu<sub>2</sub> would be like that around the *A* atom in the *AB*<sub>2</sub> Laves or Friauf structures. Cu<sub>4</sub> has three approximately coplanar Ce neighbors and ten Cu neighbors. The coordination polyhedron can best be described as having been derived from a hexagonal close packed arrangement wherein one of the six atoms coplanar with the central atom has been changed to

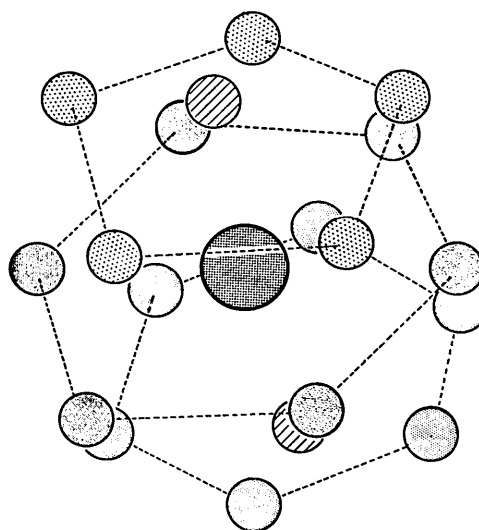


Fig. 4. Drawing of the Ce atom (larger circle) and its 19 neighbors.

two atoms (in this case two Cu<sub>1</sub> atoms) and these two atoms placed in between the close packed layers.

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