

Fig. 1. The resonance scattering amplitudes and the total cross section of ^{239}Pu as a function of neutron energy.

1.391 \AA , from which we obtain a more accurate value, $R' = 0.73 \pm 0.03$.

In spite of the proximate resonance levels, b' and b'' of ^{233}U and ^{235}U are very small and practically constant. The amplitude variation and the imaginary amplitude of ^{239}Pu are also small but by no means negligible in the high-precision structure analysis. In Fig. 1, the resonance amplitudes of ^{239}Pu are plotted in the wider range of the neutron energy. The total cross-section curve is also shown in Fig. 1 so as to demonstrate the effect of the 0.296 eV resonance on the scattering amplitudes. The functional correlation here represents a typical, common feature of the resonance scattering. A resemblance between the b'' and total cross-section curves implies that the neutron structure analysis analogous to the X-ray dispersion technique has to overcome a rapidly increasing absorption effect for the larger b'' value.

The multilevel analysis has suffered from many adjustable parameters and the refined experiment and interpretation have recently revealed a number of smaller probable levels in these nuclei (for example, Lynn, 1964). Moreover,

the bound levels will not be determined unambiguously without the direct method that has yet to be established. Regardless of this apparently provisional status, the following conclusions can be drawn. (1) It is very unlikely that further resonance analysis would alter our b'' values significantly since b'' is strongly related to the capture and fission cross-sections. (2) The $(R' + b')$ values are reliable, although the uranium cases possess large statistical errors. (3) The individual real components, R' and b' are sensitive to the refinement in the resonance analysis, although our conclusion regarding the wavelength dependence of b' will not be affected. (4) The coherent amplitude of naturally occurring uranium, 0.845 ± 0.015 , a statistical average of the reported values (Atoji, 1961; Roof *et al.* 1962), can also be assigned to depleted uranium. Finally, the determination of these small b' and b'' by means of the coherent-intensity analysis using non-centrosymmetric single crystals would require exceedingly high-accuracy measurement.

Note added in proof: - For ^{235}U , it was gratifying to find a reasonable agreement between our result, $|b| = 1.07 \pm 0.09$, and an experimental value, $|b| = 0.98 \pm 0.06$, reported by Willis (1963).

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The crystal structure of the copper complex of L-alanine. By A. DIJKSTRA*, *Central Laboratory, Dutch State Mines, Geleen, The Netherlands*

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Knowledge of the crystal structure of the copper complex of L-alanine was required in order to elucidate the optical properties (in the visible region) of single crystals of this copper complex (Dijkgraaf, 1964*a, b*). The structure was determined by two-dimensional Fourier methods.

Rotation and Weissenberg photographs gave the following unit-cell dimensions:

$$a = 9.24 \pm 0.04, \quad b = 5.05 \pm 0.02, \quad c = 9.59 \pm 0.04 \text{ \AA};$$

$$\beta = 95.2^\circ \pm 0.3^\circ.$$

The density as calculated with two formula units $\text{Cu}(\text{C}_3\text{H}_6\text{O}_2\text{N})_2$ per unit cell is 1.785 g.cm^{-3} , whereas the observed density is approximately 1.81 g.cm^{-3} . Reflexions $0k0$ with k odd are systematically absent. Since the copper complex of L-alanine has no centre of symmetry, the monoclinic space group must be $P2_1$.

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Weissenberg photographs were made of prisms of approximately 0.2 x 0.2 mm cross section elongated along the *b* axis and of prisms of approximately the same dimensions elongated along the *c* axis. These prisms were cut from flat crystals in which the (100) plane predominates. The intensities of the reflexions *h0l* and *hk0* were estimated visually from zero-layer Weissenberg photographs by using a calibrated scale. The intensities of the unobserved, but not systematically absent reflexions were taken as half the threshold value. For all photographs Cu $K\alpha$ radiation was used. Only a small absorption correction like that for cylindrical rods had to be applied to the intensities.

Preliminary *x* and *z* coordinates of the atoms were obtained from the well resolved Patterson projection along the *b* axis. Preliminary *y* values were calculated from the *x* and *z* coordinates and approximate bond lengths. Direct determination of the coordinates from the [001] projection was impossible, because of overlap.

The crystal structure was refined by difference Fourier synthesis (five cycles) of both projections down to an *R* value of 14.2% for the centrosymmetric [010] projection and of 9.6% for the non-centrosymmetric projection along the [010] axis. The positions of the hydrogen atoms were not taken into account. The scattering factors of Cu²⁺, O, N and C were taken from *International Tables for X-ray Crystallography*, Vol. III. All calculations were performed on a Univac III computer for which the programs were written in FORTRAN IV.

The final values of the calculated structure factors (and temperature factors) together with the observed values, are shown in Table 1. The atomic coordinates at the final stage

of refinement are summarized in Table 2. The standard deviations (*International Tables for X-ray Crystallography*, Vol. II) of the *x* and *z* coordinates for the copper atom are 0.004 Å; for the oxygen, nitrogen, and carbon atoms an average value of 0.025 Å was calculated. The standard deviations of the *y* coordinates as derived from the [001] projection are larger, 0.01 Å for the copper atom and 0.05 Å for the resolved carbon atoms. For the unresolved atoms the standard deviations will, most likely, be even larger.

A [010] projection (of one independent complex) is shown in Fig. 1. The coordination of the oxygen and nitrogen atoms around the copper atom is coplanar within experimental error. (The equation of the best plane through

Table 2. Atomic coordinates in fractions of unit cell dimensions [one independent complex of Cu(C₃H₆O₂N)₂]

| Atom | <i>x</i> | <i>y</i> | <i>z</i> |
|------|----------|----------|----------|
| Cu | 0.514 | 0.250 | 0.250 |
| O(1) | 0.457 | 0.043 | 0.411 |
| O(2) | 0.303 | 0.055 | 0.584 |
| O(3) | 0.567 | 0.460 | 0.091 |
| O(4) | 0.704 | 0.424 | 0.905 |
| N(1) | 0.362 | 0.505 | 0.305 |
| N(2) | 0.657 | 0.982 | 0.186 |
| C(1) | 0.314 | 0.125 | 0.464 |
| C(2) | 0.254 | 0.345 | 0.377 |
| C(3) | 0.144 | 0.484 | 0.450 |
| C(4) | 0.667 | 0.333 | 0.018 |
| C(5) | 0.745 | 0.085 | 0.084 |
| C(6) | 0.895 | 0.198 | 0.157 |

Table 1. Comparison of observed and calculated structure factors
Common isotropic temperature factors are 2.9 and 2.7 Å² for [010] and [001] projections.

| h | 1 | 10 | F ₀ | 10 | P _C | h | 1 | 10 | F ₀ | 10 | P _C | h | 1 | 10 | F ₀ | 10 | P _C | h | 1 | 10 | F ₀ | 10 | P _C | h | 1 | 10 | F ₀ | 10 | P _C | α (°) |
|----|-----|-----|----------------|------|----------------|----|-----|-----|----------------|------|----------------|----|-----|-----|----------------|------|----------------|----|-----|-----|----------------|------|----------------|----|-----|-----|----------------|------|----------------|-------|
| 1 | 100 | 100 | 987 | 104 | 180 | 1 | 100 | 100 | 987 | 104 | 180 | 1 | 100 | 100 | 987 | 104 | 180 | 1 | 100 | 100 | 987 | 104 | 180 | 1 | 100 | 100 | 987 | 104 | 180 | 0 |
| 2 | 100 | 100 | 104 | 104 | 180 | 2 | 100 | 100 | 104 | 104 | 180 | 2 | 100 | 100 | 104 | 104 | 180 | 2 | 100 | 100 | 104 | 104 | 180 | 2 | 100 | 100 | 104 | 104 | 180 | 0 |
| 3 | 100 | 100 | 116 | 116 | 180 | 3 | 100 | 100 | 116 | 116 | 180 | 3 | 100 | 100 | 116 | 116 | 180 | 3 | 100 | 100 | 116 | 116 | 180 | 3 | 100 | 100 | 116 | 116 | 180 | 0 |
| 4 | 100 | 100 | 122 | 122 | 180 | 4 | 100 | 100 | 122 | 122 | 180 | 4 | 100 | 100 | 122 | 122 | 180 | 4 | 100 | 100 | 122 | 122 | 180 | 4 | 100 | 100 | 122 | 122 | 180 | 0 |
| 5 | 100 | 100 | 130 | 130 | 180 | 5 | 100 | 100 | 130 | 130 | 180 | 5 | 100 | 100 | 130 | 130 | 180 | 5 | 100 | 100 | 130 | 130 | 180 | 5 | 100 | 100 | 130 | 130 | 180 | 0 |
| 6 | 100 | 100 | 141 | 141 | 180 | 6 | 100 | 100 | 141 | 141 | 180 | 6 | 100 | 100 | 141 | 141 | 180 | 6 | 100 | 100 | 141 | 141 | 180 | 6 | 100 | 100 | 141 | 141 | 180 | 0 |
| 7 | 100 | 100 | 154 | 154 | 180 | 7 | 100 | 100 | 154 | 154 | 180 | 7 | 100 | 100 | 154 | 154 | 180 | 7 | 100 | 100 | 154 | 154 | 180 | 7 | 100 | 100 | 154 | 154 | 180 | 0 |
| 8 | 100 | 100 | 171 | 171 | 180 | 8 | 100 | 100 | 171 | 171 | 180 | 8 | 100 | 100 | 171 | 171 | 180 | 8 | 100 | 100 | 171 | 171 | 180 | 8 | 100 | 100 | 171 | 171 | 180 | 0 |
| 9 | 100 | 100 | 193 | 193 | 180 | 9 | 100 | 100 | 193 | 193 | 180 | 9 | 100 | 100 | 193 | 193 | 180 | 9 | 100 | 100 | 193 | 193 | 180 | 9 | 100 | 100 | 193 | 193 | 180 | 0 |
| 10 | 100 | 100 | 227 | 227 | 180 | 10 | 100 | 100 | 227 | 227 | 180 | 10 | 100 | 100 | 227 | 227 | 180 | 10 | 100 | 100 | 227 | 227 | 180 | 10 | 100 | 100 | 227 | 227 | 180 | 0 |
| 11 | 100 | 100 | 273 | 273 | 180 | 11 | 100 | 100 | 273 | 273 | 180 | 11 | 100 | 100 | 273 | 273 | 180 | 11 | 100 | 100 | 273 | 273 | 180 | 11 | 100 | 100 | 273 | 273 | 180 | 0 |
| 12 | 100 | 100 | 339 | 339 | 180 | 12 | 100 | 100 | 339 | 339 | 180 | 12 | 100 | 100 | 339 | 339 | 180 | 12 | 100 | 100 | 339 | 339 | 180 | 12 | 100 | 100 | 339 | 339 | 180 | 0 |
| 13 | 100 | 100 | 416 | 416 | 180 | 13 | 100 | 100 | 416 | 416 | 180 | 13 | 100 | 100 | 416 | 416 | 180 | 13 | 100 | 100 | 416 | 416 | 180 | 13 | 100 | 100 | 416 | 416 | 180 | 0 |
| 14 | 100 | 100 | 504 | 504 | 180 | 14 | 100 | 100 | 504 | 504 | 180 | 14 | 100 | 100 | 504 | 504 | 180 | 14 | 100 | 100 | 504 | 504 | 180 | 14 | 100 | 100 | 504 | 504 | 180 | 0 |
| 15 | 100 | 100 | 604 | 604 | 180 | 15 | 100 | 100 | 604 | 604 | 180 | 15 | 100 | 100 | 604 | 604 | 180 | 15 | 100 | 100 | 604 | 604 | 180 | 15 | 100 | 100 | 604 | 604 | 180 | 0 |
| 16 | 100 | 100 | 716 | 716 | 180 | 16 | 100 | 100 | 716 | 716 | 180 | 16 | 100 | 100 | 716 | 716 | 180 | 16 | 100 | 100 | 716 | 716 | 180 | 16 | 100 | 100 | 716 | 716 | 180 | 0 |
| 17 | 100 | 100 | 833 | 833 | 180 | 17 | 100 | 100 | 833 | 833 | 180 | 17 | 100 | 100 | 833 | 833 | 180 | 17 | 100 | 100 | 833 | 833 | 180 | 17 | 100 | 100 | 833 | 833 | 180 | 0 |
| 18 | 100 | 100 | 956 | 956 | 180 | 18 | 100 | 100 | 956 | 956 | 180 | 18 | 100 | 100 | 956 | 956 | 180 | 18 | 100 | 100 | 956 | 956 | 180 | 18 | 100 | 100 | 956 | 956 | 180 | 0 |
| 19 | 100 | 100 | 1084 | 1084 | 180 | 19 | 100 | 100 | 1084 | 1084 | 180 | 19 | 100 | 100 | 1084 | 1084 | 180 | 19 | 100 | 100 | 1084 | 1084 | 180 | 19 | 100 | 100 | 1084 | 1084 | 180 | 0 |
| 20 | 100 | 100 | 1217 | 1217 | 180 | 20 | 100 | 100 | 1217 | 1217 | 180 | 20 | 100 | 100 | 1217 | 1217 | 180 | 20 | 100 | 100 | 1217 | 1217 | 180 | 20 | 100 | 100 | 1217 | 1217 | 180 | 0 |
| 21 | 100 | 100 | 1354 | 1354 | 180 | 21 | 100 | 100 | 1354 | 1354 | 180 | 21 | 100 | 100 | 1354 | 1354 | 180 | 21 | 100 | 100 | 1354 | 1354 | 180 | 21 | 100 | 100 | 1354 | 1354 | 180 | 0 |
| 22 | 100 | 100 | 1494 | 1494 | 180 | 22 | 100 | 100 | 1494 | 1494 | 180 | 22 | 100 | 100 | 1494 | 1494 | 180 | 22 | 100 | 100 | 1494 | 1494 | 180 | 22 | 100 | 100 | 1494 | 1494 | 180 | 0 |
| 23 | 100 | 100 | 1635 | 1635 | 180 | 23 | 100 | 100 | 1635 | 1635 | 180 | 23 | 100 | 100 | 1635 | 1635 | 180 | 23 | 100 | 100 | 1635 | 1635 | 180 | 23 | 100 | 100 | 1635 | 1635 | 180 | 0 |
| 24 | 100 | 100 | 1776 | 1776 | 180 | 24 | 100 | 100 | 1776 | 1776 | 180 | 24 | 100 | 100 | 1776 | 1776 | 180 | 24 | 100 | 100 | 1776 | 1776 | 180 | 24 | 100 | 100 | 1776 | 1776 | 180 | 0 |
| 25 | 100 | 100 | 1916 | 1916 | 180 | 25 | 100 | 100 | 1916 | 1916 | 180 | 25 | 100 | 100 | 1916 | 1916 | 180 | 25 | 100 | 100 | 1916 | 1916 | 180 | 25 | 100 | 100 | 1916 | 1916 | 180 | 0 |
| 26 | 100 | 100 | 2054 | 2054 | 180 | 26 | 100 | 100 | 2054 | 2054 | 180 | 26 | 100 | 100 | 2054 | 2054 | 180 | 26 | 100 | 100 | 2054 | 2054 | 180 | 26 | 100 | 100 | 2054 | 2054 | 180 | 0 |
| 27 | 100 | 100 | 2191 | 2191 | 180 | 27 | 100 | 100 | 2191 | 2191 | 180 | 27 | 100 | 100 | 2191 | 2191 | 180 | 27 | 100 | 100 | 2191 | 2191 | 180 | 27 | 100 | 100 | 2191 | 2191 | 180 | 0 |
| 28 | 100 | 100 | 2326 | 2326 | 180 | 28 | 100 | 100 | 2326 | 2326 | 180 | 28 | 100 | 100 | 2326 | 2326 | 180 | 28 | 100 | 100 | 2326 | 2326 | 180 | 28 | 100 | 100 | 2326 | 2326 | 180 | 0 |

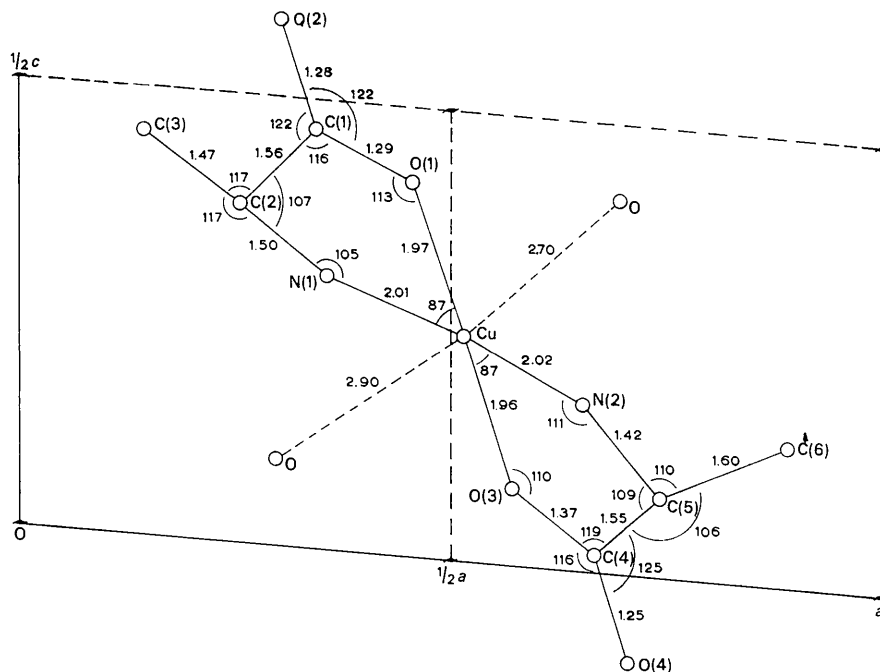


Fig. 1. Bond lengths (Å) and valency angles ($^{\circ}$) shown on a [010] projection of the copper complex.

the copper, oxygen and nitrogen atoms with respect to the a and b axes and an axis (c) perpendicular to these is $0.685x + 0.468y + 0.558z = 5.14$, all distances in Å). The deviations of the copper, oxygen and nitrogen atoms from the best plane are 0.02, 0.01, and 0.05 Å respectively.

The copper ion is surrounded by two nitrogen and two oxygen atoms at distances of approximately 2 Å and two double-bonded oxygen atoms of neighbouring complexes at an average distance of approximately 2.8 Å. These six atoms are at the corners of a distorted octahedron.

The differences in bond lengths and bond angles between the two halves of the copper complex are probably not significant.

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Contribution à l'étude de la structure cristalline de LaAlO_3 . Par C. DE RANGO, G. TSOUCARIS et C. ZELWER, *Laboratoire de Cristallographie, Centre National de la Recherche Scientifique, Bellevue (Seine et Oise), France*

(Reçu le 21 septembre 1965)

La structure cristalline de LaAlO_3 a récemment fait l'objet de plusieurs études au moyen de techniques différentes:

Spectroscopie optique (Couture, Brunetière, Forrat & Trévoux, 1963; Poole, 1964).

Résonance magnétique nucléaire et résonance paramagnétique électronique (Derighetti, Drumheller, Laves, Müller & Waldner, 1964).

Tous ces auteurs s'accordent pour conclure à la nécessité d'une connaissance précise de la structure afin d'expliquer de manière satisfaisante les propriétés optiques et magnétiques du cristal.

Geller & Bala (1956) ont déjà établi que ce cristal est rhomboédrique et ils ont constaté que le groupe le plus symétrique $R\bar{3}m$ était compatible avec leurs diagrammes de rayons X .

Dans une publication antérieure (de Rango, Tsoucaris & Zelwer, 1964) nous avons montré que l'ensemble de nos diagrammes de diffraction de rayons X et de diffraction des neutrons était compatible avec les groupes $R3c$ et $R\bar{3}c$. Dans cette première étude, nous avons supposé que le groupe était $R\bar{3}c$ et cherché la valeur du seul paramètre variable dans ce cas: la coordonnée de l'oxygène x_0 . Nous avons trouvé $x_0 = 0,475$, valeur en bon accord avec les résultats publiés indépendamment par Derighetti *et al.* Les coordonnées relatives à cette hypothèse sont:

| | x | y | z |
|----|-------|-----|---------------|
| Al | 0 | 0 | 0 |
| La | 0 | 0 | $\frac{1}{4}$ |
| O | 0,475 | 0 | $\frac{1}{4}$ |