units, and, assuming three water molecules in each formula unit, the calculated density is 2·15 g.cm.$^{-3}$.

Systematic extinctions occur only for $h0l$ with l odd and $0k0$ with k odd, hence the space group is $P2_1/c$–C_{2h}. A close inspection of the hkl reflexions shows, however, that the crystal very nearly belongs to the space group $C2/c$–C_{2h}^6. The reason for this is that out of 215 spectra recorded for a Patterson–Harker section, only 28 weak spectra did not conform to the extinction conditions implied by this space group.

(2) $(NH_4)_3[Cr(C_2O_4)_3].xH_2O$

The ammonium salt generally crystallizes in the form of flat plates. The crystals are triclinic, class $\bar{1}$–C_i, and not monoclinic as reported by Wyrouboff (1900). Referring the crystals to a set of axes approximately similar to those used in the potassium salt, the following unit-cell dimensions were obtained:

$$a'=7{\cdot}79,\quad b'=20{\cdot}13,\quad c'=10{\cdot}73\ \text{A.};$$
$$\alpha'=91^\circ\,55',\quad \beta'=112^\circ\,36',\quad \gamma'=89^\circ\,18'.$$

This triclinic unit cell and the general appearance of the photographs resemble very closely the corresponding data of the potassium salt. The unit cell as given above is, however, centred on the C face, and the following set of transformations

$$a=a',\quad b=\tfrac{1}{2}a'+\tfrac{1}{2}b',\quad c=c'$$

gives the primitive triclinic cell with dimensions

$$a=7{\cdot}79,\quad b=10{\cdot}90,\quad c=10{\cdot}73\ \text{A.};$$
$$\alpha=98^\circ\,10',\quad \beta=112^\circ\,36',\quad \gamma=67^\circ\,22'.$$

An independent set of measurements confirmed these values.

The density, determined by the method of flotation, is 1·79 g.cm.$^{-3}$. Assuming two formula units, each with three water molecules, in the unit cell, the calculated density is 1·81 g.cm.$^{-3}$.

There are no systematic extinctions, hence the space group is either $P1$–C_1^1 or $P\bar{1}$–C_i^1. An examination of the external crystal form and the close similarity between the two structures, as obtained from detailed structural work now in progress, suggest that the space group is $P\bar{1}$–C_i^1.

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An experimentally determined atomic scattering-factor curve for chromium.

By J. N. van Niekerk and F. R. L. Schoening, *National Physical Laboratory, Council for Scientific and Industrial Research, Pretoria, South Africa*

(*Received* 14 *April* 1951)

While investigating the structure of

$$(NH_4)_3[Cr(C_2O_4)_3].2H_2O$$

by the method of double Fourier synthesis, a projection was obtained in which very nearly all the atoms in the structure were resolved. Using atomic scattering-factor values for carbon as given by Robertson (1935), and reducing the corresponding oxygen and nitrogen values given by James & Brindley (1931) by the same ratio as that by which Robertson's values for carbon differ from those of James & Brindley, the possibility then arises of determining a set of atomic scattering-factor values for chromium in the trioxalato complex.

The intensities of the 124 spectra used for obtaining this projection were carefully estimated by eye by comparing them with a set of previously calibrated intensity spots of approximately the same size. The intensities of a number of these spectra were measured on a Geiger-counter spectrometer in order to find their approximate absolute values. A conversion factor was then calculated by which all the eye-estimated intensities were multiplied, to express the intensities of all the spectra on an approximately absolute scale.

By using atomic scattering-factor values for oxygen, nitrogen and carbon as described above, and values for chromium as previously described by us (van Niekerk & Schoening, 1951), structure factors were calculated for all spectra with $\sin\theta/\lambda \leqslant 0{\cdot}25$. It was estimated that for these low-order spectra the true f values for chromium would not differ appreciably from the theoretical values. These calculated structure factors were then compared with the observed ones, and it was found that on multiplying the observed intensities of the low-order spectra by a further factor of 1·2, excellent agreement was obtained. All spectra were now multiplied by this factor, thus expressing them all on an absolute scale.

Considering spectra with $\sin\theta/\lambda > 0{\cdot}25$, structure factors were calculated using that f factor for chromium which gave the best fit between observed and calculated values in each individual case. These f values for chromium were plotted against $\sin\theta/\lambda$, and the points were found to fall approximately on a smooth curve. The best average curve was then drawn through these points. Using the f values obtained from this curve, the structure factors for all 200 spectra, including absent spectra, were recalculated. The agreement between observed and calculated structure factors was excellent, and seemed to confirm the procedures adopted in deriving a set of f values for chromium in this particular complex. The following table gives the atomic scattering-factor values for chromium finally obtained by the methods outlined above:

$\sin\theta/\lambda$ (A.$^{-1}$)	0	0·1	0·2	0·3	0·4	0·5
f	24·0	21·0	17·1	13·2	9·3	6·5
$\sin\theta/\lambda$ (A.$^{-1}$)	0·6	0·7	0·8	0·9	1·0	1·1
f	4·7	3·5	2·6	2·1	1·8	1·6

During the investigation Mo $K\alpha$ radiation was used throughout.

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Multiplicity of solutions of crystal-structure equations.

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(*Received* 3 *March* 1951)

In a previous note (Hauptman & Karle, 1950), it was stated that $3(N-1)$ independent magnitudes were sufficient to determine the solution of the crystal-structure problem, and that for the case of three atoms in one dimension the solution is unique. The former statement is ambiguous and the latter incorrect. In general, $3(N-1)$ independent magnitudes are sufficient to determine a finite number of solutions of the crystal-structure problem (Karle & Hauptman, 1951). Since, as a general rule, many more than $3(N-1)$ magnitudes are available from experiment, a unique solution (except, of course, for ambiguities of the Patterson (1944) type) is determined by the data. The following example exhibits four solutions determined by the method described by Karle & Hauptman (1951) for the case of three atoms in one dimension when the minimum amount of algebraic data is used (two magnitudes).

Co-ordinates of the atoms

	Solution I	Solution II	Solution III	Solution IV
$x_1=$	0·000 000	0·000 000	0·000 000	0·000 000
$x_2=$	0·159 155	0·386 169	0·320 276	0·159 931
$x_3=$	0·477 465	0·100 825	0·899 699	0·658 078
or, if $\phi_j=2\pi x_j$				
$\phi_1=$	0·000°	0·000°	0·000°	0·000°
$\phi_2=$	57·296°	139·021°	115·299°	57·575°
$\phi_3=$	171·887°	36·297°	323·892°	236·908°

The atomic scattering factors are given by:

	Plane (100)	Plane (200)	Plane (300)
Atom 1	$f_{11}=0{\cdot}40$	$f_{21}=0{\cdot}30$	$f_{31}=0{\cdot}25$
Atom 2	$f_{12}=0{\cdot}30$	$f_{22}=0{\cdot}25$	$f_{32}=0{\cdot}23$
Atom 3	$f_{13}=0{\cdot}20$	$f_{23}=0{\cdot}16$	$f_{33}=0{\cdot}14$

If

$$F_h=\sum_{j=1}^{3} f_{hj}\,e^{-2\pi i h x_j} \quad (h=1,2,3)$$

it is readily verified that

$$|F_1|^2=0{\cdot}211\,336 \quad |F_2|^2=0{\cdot}155\,563$$

for each of the four solutions. However,

$$|F_3|^2=0{\cdot}01921,\quad 0{\cdot}21466,\quad 0{\cdot}21978,\quad 0{\cdot}02565$$

for the respective solutions, so that the specification of $|F_3|^2$ (in addition to $|F_1|^2$ and $|F_2|^2$) would be sufficient to determine a unique solution.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

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Tables for Conversion of X-ray Diffraction Angles to Interplanar Spacing

The National Bureau of Standards announces the publication of *Tables for Conversion of X-ray Diffraction Angles to Interplanar Spacing.* The first six tables give the spacing values for the angles θ from 0 to 90° at intervals of 0·01°. These tables were calculated by using the $K\alpha_1$ wave-