examined to determine the relationship of his result to that given here. Roess's result is given for the mass distribution function, which is simply related to the number distribution. Also using Mellin transforms, he obtained a form involving the differentiation of an integral, namely,

$$M(R)=\frac{-8R}{27\pi B}\frac{d}{dR}\int_0^\infty Rk^4I(k)\,{}_1F_2(\tfrac{1}{2};\ -\tfrac{1}{2},\tfrac{5}{2};\ -k^2R^2)dR \qquad (16)$$

$${}_1F_2(\tfrac{1}{2};\ -\tfrac{1}{2},\tfrac{5}{2};\ -x^2)=-\tfrac{3}{2}J_{\frac{3}{2}}(x)J_{-\frac{3}{2}}(x)\,.$$

Formally differentiating under the integral sign, we obtain, except for differences between the two types of distribution, the result shown in equation (10).

Although X-ray scattering has been discussed here, it is well known that an equation similar to equation (1) has been applied to the determination of size of spherical particles by visible light-scattering (Debye, 1944). It follows that the results obtained here should be applicable to dilute polydisperse solutions of spherical macro-molecules, in which particle–particle interference effects may be neglected.

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The Crystal Structure of Potassium Trioxalatochromate (III), $K_3[Cr(C_2O_4)_3]\,.\,3\,H_2O$

By J. N. van Niekerk and F. R. L. Schoening

National Physical Laboratory, Council for Scientific and Industrial Research, Pretoria, South Africa

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The crystal structure of $K_3[Cr(C_2O_4)_3].3H_2O$ is monoclinic $P2_1/c$–C^5_{2h} with four formula units in a cell of dimensions $a = 7{\cdot}71$, $b = 19{\cdot}74$, $c = 10{\cdot}40$ Å, $\beta = 108°\ 0'$. The structure has the pseudo space group $C2/c$–C^6_{2h}, which was used throughout this investigation. By evaluating the functions $\sigma(x, y)$ and $\sigma(y, z)$, projections of the structure on two crystallographic planes were obtained.

The configuration of the two stereo isomeric complex ions $[Cr(C_2O_4)_3]$ is described. The three oxalato groups in a complex ion are planar, their inner oxygen atoms form a slightly distorted octahedron round the central chromium atom. It is shown that both ionic and hydrogen bonds link the complex ions in the structure. The errors introduced by treating the structure in the wrong space group are estimated not to be very serious, so that the investigation gives a clear picture of the general features of the structure.

1. Preparation and crystal data

The material used in this investigation was prepared by Mr R. W. Burley (1950) of the Leather Industries Research Institute, Grahamstown, South Africa. The crystallographic data of this compound were investigated by Jaeger (1919). We found his data to be substantially correct, except that his unit cell has very nearly three times the volume of our cell. The crystals are monoclinic holohedral and dark blue in colour. They usually crystallise as thick prismatic needles with large, well developed {031} faces. Jaeger calls these the {110} faces. In the literature this compound is usually described as $K_3[Cr(C_2O_4)_3].3H_2O$ (Jaeger, 1919; Wyrouboff, 1900; Rammelsberg, 1854; Schabus, 1854). The crystals are, however, unstable. They lose water in a dry atmosphere, decomposing into a crystalline powder, whereas in a humid atmosphere they absorb water and become liquid. The exact number of water molecules associated with a formula unit is therefore undetermined. Although the crystals were coated with perspex films during photographic exposures, the uncertainty of their exact water content when an exposure was started still remained. The optical data obtained for the crystals are summarised in Fig. 1.

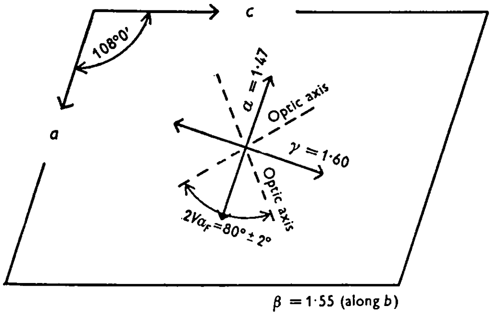

Fig. 1. Directions of refractive indices and optic axes.

2. The unit cell and space group

Oscillation and Weissenberg photographs were taken using filtered Cu $K\alpha$ and Mo $K\alpha$ radiation, and from these the following unit cell dimensions were determined:

$$a = 7{\cdot}71,\ b = 19{\cdot}74,\ c = 10{\cdot}40\ \text{Å},\ \beta = 108°0'\ .$$

The density, determined by the method of flotation, is 2·16 g.cm.$^{-3}$. Taking $K_3[Cr(C_2O_4)_3].3H_2O$ as formula unit, the unit cell contains four of these formula units, corresponding to a calculated density of 2·15 g.cm.$^{-3}$.

Systematic extinctions occur only for $h0l$ with l odd and for $0k0$ with k odd. The space group is therefore $P2_1/c$–C_{2h}^5.

3. Intensity measurements

All the intensity photographs were taken with a single small crystal of approximately cubic dimensions, using filtered Mo $K\alpha$ radiation. In view of the small size of the crystal no absorption corrections were made. The relevant intensities were estimated visually. The intensities of a number of suitable spectra were also measured on a Geiger-counter X-ray spectrometer, using methods similar to those described by Cochran (1950) and Lonsdale (1948). By comparing these intensities with the calculated integrated intensity and the measured intensity of the 200 reflection from a suitable NaCl crystal, the latter intensity also being measured on the spectrometer, it was possible to express all the visually estimated intensities on an approximately absolute scale.

4. Preliminary estimate of the structure

The following survey of the spectra used for the various projections indicates that the crystal very nearly belongs to the space group $C2/c$–C_{2h}^6. For the $b\,c$ projection 94 spectra were recorded. Of these only 16, contributing 8% of the total intensity, do not conform to the condition hkl present only with $h+k$ even. Similarly, out of 55 spectra used in the $a\,b$ projection only 14, with a total intensity contribution of 16%, do not fulfil the above condition. Finally, out of 215 spectra used for a Patterson–Harker section only 28 weak spectra do not fulfil the condition stated above.

Since there are four formula units in the unit cell, it follows that in the $P2_1/c$ space group a formula unit $K_3[Cr(C_2O_4)_3].3H_2O$ must occupy a general position, leading to 75 independent parameters. If, however, the structure is referred to the space group $C2/c$, the formula units must then occupy special positions, reducing the number of independent parameters to 42. For the above reasons it was decided to adopt the space group $C2/c$ during the preliminary treatment of the structure.

For $C2/c$ the special positions are symmetry centres and twofold axes. Stereochemical considerations of the complex ion $[Cr(C_2O_4)_3]$, (Werner, 1912 *a*; Pauling, 1945), rule out symmetry centres but allow twofold axes. During subsequent calculations a twofold axis of the complex ion was taken to coincide with that of the space group $C2/c$.

In an attempt to fix the positions of the potassium and chromium atoms in the $b\,c$ projection, the Patterson–Harker sections $P(0, v, \frac{1}{2}c)$ and $P(u, \frac{1}{2}b, w)$, giving the distances of the atoms from a glide plane and a screw axis respectively, were evaluated. The latter section confirmed with certainty only the position of the chromium atom on the twofold axis. The $P(0, v, \frac{1}{2}c)$ section indicated three big peaks together with some smaller ones, but, because there are three potassium atoms and one chromium atom in a formula unit, this section could not be interpreted with certainty. A Patterson projection $P(0, v, w)$ indicated a heavy atom on the twofold axis in a position corresponding to that of the biggest peak on the $P(0, v, \frac{1}{2}c)$ section. It was provisionally assumed that the chromium atom occupied this position. Later work confirmed this assumption.

5. Evaluation of the Fourier series for the *b c* projection

At the outset only the chromium atom was used for calculating the signs of the observed structure factors, and the series $\sigma(y, z)$ was evaluated. Successive refinements were tried, but it soon became clear that the uncertainty of the positions of the other atoms, particularly the potassium atoms, prevented the expected convergence to the true structure.

Wyrouboff (1900) and Rammelsberg (1854) have reported that this potassium salt and the corresponding ammonium compound are isomorphous. The corresponding ammonium formula unit has the advantage of possessing only one heavy atom, and for this reason it seemed likely that a direct comparison between the two structures would be useful. Although we found the ammonium salt to be triclinic, its deviation from a monoclinic structure was so small, that it could to a first approximation be treated as a monoclinic crystal. Fourier and Patterson projections were made on the *b c* plane, treating the ammonium salt as an average monoclinic crystal. By comparing these projections with the corresponding ones for the potassium salt, it was possible to fix approximately the positions of the potassium atoms as well as the positions of a number of other atoms in the *bc* projection of the potassium salt.

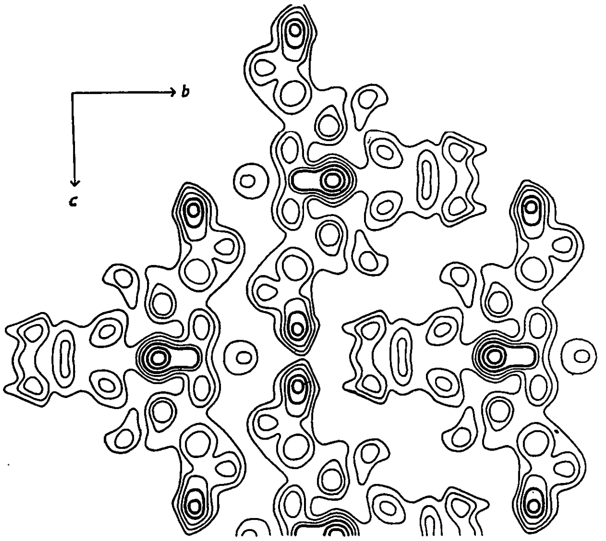

Fig. 2. Electron-density projected along the *a* axis on to the *b c* plane. The electron-density contours are drawn at arbitrary intervals. The heavy contours, drawn at higher intervals, indicate the positions of the potassium and chromium atoms.

The values for $F(0kl)$ were recalculated, using atomic scattering factor values as previously described by us (van Niekerk & Schoening, 1951). Successive refinements led to the final projection shown in Fig. 2, which can be interpreted with the aid of Fig. 3. Because the crystal was treated as belonging to the wrong space group $C2/c$ false detail can be expected on this projection and this probably accounts for the distortion of the lower contour levels in Fig. 2. Even so, the projection shows quite clearly the general configuration of the formula units.

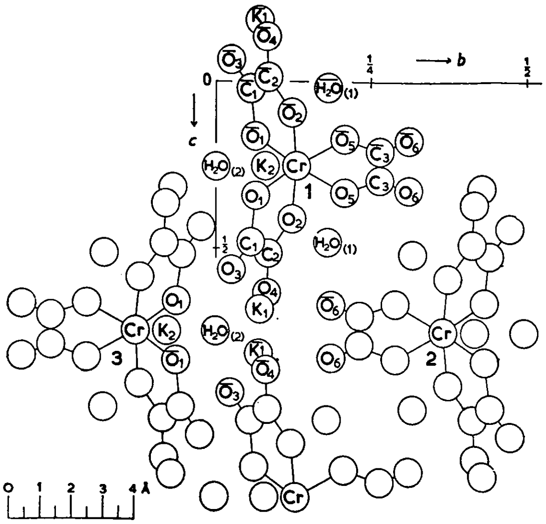

Fig. 3. Projection of the structure along the *a* axis on to the *b c* plane. Unit 2 is derived from unit 1 by the operation of a glide plane parallel to (010). Unit 3 is derived from unit 2 by the operation of a screw axis parallel to *b*.

6. Evaluation of the Fourier series for the *a b* projection

Inspection of the *b c* projection shows that very poor resolution can be expected on the *a b* projection.

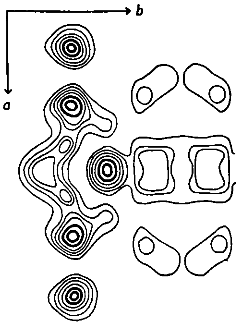

Fig. 4. Electron-density projected against the *c* axis on to the *a b* plane. The electron-density contours are drawn at arbitrary intervals. The heavy contours, drawn at higher intervals, indicate the positions of the potassium and chromium atoms.

The Fourier series $\sigma(x, y)$ was evaluated following the method described by Lipson & Beevers (1936). The projection finally obtained is shown in Fig. 4, and it can be interpreted with the aid of Fig. 5.

7. Estimation of parameters

The *y* and *z* co-ordinates could be estimated with reasonable accuracy from the *b c* projection. The *x* co-ordinates were, however, very uncertain. The *x* co-ordinates finally chosen were those which gave the

Table 1. *Final parameters*

Atom	x/a	y/b	z/c
O_1	0·153	0·065	0·340
O_2	0·447	0·123	0·410
O_3	0·217	0·025	0·567
O_4	0·500	0·083	0·633
O_5	0·167	0·208	0·327
O_6	0·167	0·314	0·327
C_1	0·267	0·057	0·483
C_2	0·417	0·085	0·517
C_3	0·207	0·267	0·293
Cr	0·250	0·130	0·250
K_1	−0·010	0·073	0·683
K_2	0·750	0·079	0·250
$H_2O_{(1)}$	−0·050	0·183	0·483
$H_2O_{(2)}$	0·250	0·000	0·250

Table 2. *Observed and calculated struture factors*

hkl	F_o	F_c
020	99	+156
040	139	−125
060	206	−187
080	141	−165
0,10,0	—	+29
0,12,0	—	+49
0,14,0	115	+126
0,16,0	75	+101
0,18,0	70	−90
0,20,0	92	−134
002	169	−203
004	56	+92
006	12	+34
008	37	+10
00,10	22	−38
00,12	71	+90
011	—	0
021	68	−58
031	21	0
041	48	+43
151	—	0
061	134	+106
071	43	0
081	9	−24
091	—	0
0,10,1	106	−122
0,11,1	—	0
0,12,1	—	+8
0,13,1	—	0
0,14,1	86	+74
0,15,1	13	0
0,16,1	14	−11
0,17,1	—	0
0,18,1	—	+15
0,19,1	—	0
0,20,1	—	+23
0,21,1	—	0
0,22,1	—	+32
0,23,1	—	0
0,24,1	31	−51
012	12	0
022	94	−14
032	—	0
042	69	+68
052	—	0
062	52	+123
072	52	0
082	24	+18
092	—	0
0,10,2	11	+10
0,11,2	—	0
0,12,2	12	−21
0,13,2	25	0
0,14,2	45	−117
0,15,2	—	0
0,16,2	20	−54
0,17,2	—	0
0,18,2	30	+54
0,19,2	16	0
0,20,2	22	+80
0,21,2	—	0
0,22,2	17	+9
013	—	0
023	69	+73
033	8	0
043	95	+71
053	—	0
063	18	−20
073	14	0
083	—	+14
093	34	0
0,10,3	32	+33
0,11,3	—	0
0,12,3	—	+10
0,13,3	—	0
0,14,3	—	+15
0,15,3	—	0
0,16,3	45	+62
0,17,3	—	0
0,18,3	—	+11
0,19,3	—	0
0,20,3	23	−44
0,21,3	—	0
0,22,3	24	−50
014	—	0
024	18	+7
034	18	0
044	53	−40
054	—	0
064	52	+12
074	—	0
084	77	+31
094	11	0
0,10,4	—	−14
0,11,4	25	0
0,12,4	13	−6
0,13,4	13	0
0,14,4	—	+18
0,15,4	—	0
0,16,4	—	+27
0,17,4	—	0
0,18,4	—	−37
0,19,4	—	0
0,20,4	—	−39
0,21,4	—	0
0,22,4	35	+40
015	—	0
025	155	−153
035	—	0
045	22	−50
055	—	0
065	61	+59
075	—	0
085	12	+35
095	12	0
0,10,5	36	+55
0,11,5	13	0
0,12,5	33	+32
0,13,5	—	0
0,14,5	—	+26
0,15,5	—	0
0,16,5	30	−60
0,17,5	—	0
0,18,5	28	−77
0,19,5	—	0
0,20,5	24	+42
0,21,5	—	0
0,22,5	18	+63
016	—	0
026	—	−23
036	—	0
046	51	+50
056	—	0
066	55	−52
076	—	0
086	148	−170
096	—	0
0,10,6	13	+13
0,11,6	—	0
0,12,6	53	+62
0,13,6	—	0
0,14,6	21	+22
0,15,6	—	0
0,16,6	—	+9
0,17,6	—	0
0,18,6	16	+27
0,19,6	—	0
0,20,6	—	+18
0,21,6	—	0
0,22,6	19	−43
017	—	0
027	108	−133
037	—	0
047	26	+88
057	—	0
067	64	−43
077	—	0
087	—	−32
097	—	0
0,10,7	—	−33
0,11,7	—	0
0,12,7	15	−50
0,13,7	—	0
0,14,7	—	−5
0,15,7	—	0
0,16,7	23	+82
0,17,7	—	0
0,18,7	30	+94
018	—	0
028	—	−4
038	—	0
048	68	−62
058	—	0
068	20	+15
078	—	0
088	25	+61
019	—	0
029	62	−99
039	—	0
049	15	−57
0,4,10	22	+35
0,4,11	24	+31
0,4,12	25	−48
100	—	0
200	90	−67
300	78	0
400	168	+228
500	—	0
600	—	−1
110	150	−206
120	—	0
130	29	−22
140	—	0
150	—	−10
160	—	0
170	80	−26
180	47	0
190	119	−85
1,10,0	—	0
1,11,0	39	−75
1,12,0	—	0
1,13,0	77	+74
1,14,0	—	0
1,15,0	36	+44
1,16,0	39	0
1,17,0	39	−29
210	71	0
220	41	+16
230	33	0
240	75	−96

Table 2 (*cont.*).

hkl	F_o	F_c
250	24	0
260	90	−99
270	54	0
280	92	−114
290	—	0
2,10,0	44	+13
2,11,0	—	0
2,12,0	95	+87
2,13,0	—	0
310	102	+49
320	—	0
330	114	−36
340	27	0
350	35	−38
360	29	0
370	36	+41
380	39	0
390	57	+81
3,10,0	41	0
3,11,0	35	+34
3,12,0	—	0
3,13,0	53	−40
410	—	0
420	96	+117
430	—	0
440	110	−80
450	—	0
460	47	−99
470	41	0
480	35	−11
490	50	0
4,10,0	—	−15
4,11,0	—	0
510	—	+24
520	—	0
530	—	−10
540	44	0
550	96	+78
560	—	0
570	—	+54
580	—	0
590	123	−133
5,10,0	—	0
5,11,0	69	−62
610	—	0
620	—	−3
630	—	0
640	39	+42
650	—	0
660	39	−41
670	—	0
680	41	−96

best fit between the observed and calculated values of $F(hk0)$. The final parameters are shown in Table 1.

The parameters given above were obtained on the assumption that the crystal belongs to the space group $C2/c$, and using these parameters the structure factors shown in Table 2 were calculated. Taken on the average there is fair agreement between the observed and calculated structure factors. The discrepancies that occur in spectra ***hkl*** with $h+k$ odd, are due to the fact that the wrong space group $C2/c$ was used, since for this space group the calculated $F(hkl)$ values for the spectra under discussion are necessarily zero.

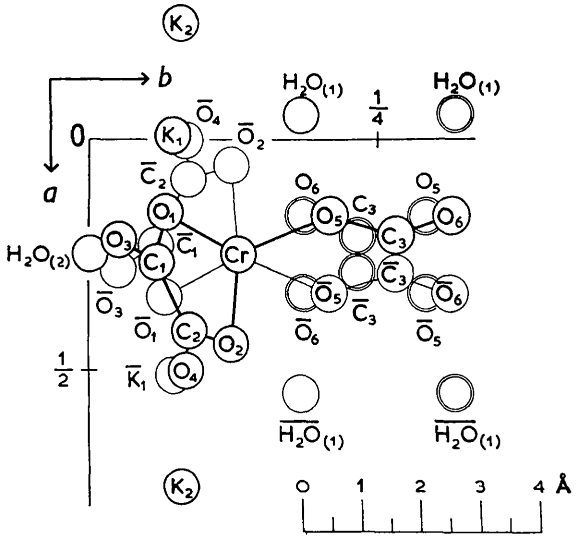

Fig. 5. Projection of the structure against the c axis on to the $a\,b$ plane. Atoms marked with double circles lie at distances $\frac{1}{2}c$ above or below correspondingly marked single circle atoms. Atoms joined by heavy lines lie above whereas atoms joined by thin lines lie below a plane parallel to the paper, this plane containing the chromium atom.

It is doubtful, particularly in the case of the $a\,b$ projection, whether much would be gained in resolution if the crystal were treated in the correct space group $P2_1/c$, so that the x co-ordinates in particular would remain uncertain. Furthermore, the presence of four comparatively heavy atoms in the formula unit causes large errors in the positions of the lighter atoms. No further attempt was therefore made to refine the structure, as it seemed very unlikely at this stage that further refinement by the double-Fourier-series method would lead to a more reliable set of interatomic distances. The difficulties briefly outlined above appear to be less pronounced in the corresponding ammonium compound, and in our opinion a structural investigation of this compound will lead to more definite results.

8. Description of the complex ion $[Cr(C_2O_4)_3]$

With the parameters given in Table 1, the distances tabulated in Table 3 were calculated for the complex ion $[Cr(C_2O_4)_3]$ (see also Fig. 3). These distances can be compared with those previously described by us (van Niekerk & Schoening, 1951) for the complex ion

Table 3. *Interatomic distances and angles*

	$[Cr(C_2O_4)_3]$		$[Cr(C_2O_4)_2(H_2O)_2]$
$Cr–O_1$	1·88 Å	1·90 Å (mean)	1·92 Å
$Cr–O_2$	1·88		
$Cr–O_5$	1·93		
$O_1–O_2$	2·44	2·38 Å (mean)	2·56 Å
$O_5–\bar{O}_5$	2·33		
$O_1–C_1$	1·47	1·39 Å (mean)	1·31 Å
$O_2–C_2$	1·42		
$O_5–C_3$	1·28		
$C_1–C_2$	1·23	1·25 Å (mean)	1·39 Å
$C_3–\bar{C}_3$	1·27		
$C_1\ O_3$	1·25	1·17 Å (mean)	1·23 Å
$C_2–O_4$	1·17		
$C_3–O_6$	1·07		
$O_3–O_4$	2·38	2·35 Å (mean)	2·55 Å
$O_6–\bar{O}_6$	2·33		
$\angle\ O_1CrO_2$	81°	77·5° Å (mean)	83°
$\angle\ O_5Cr\bar{O}_5$	74°		

$[Cr(C_2O_4)_2(H_2O)_2]$, which are shown in the last column of Table 3.

Calculations show that the three oxalato groups in a complex ion are approximately planar, the inner oxygen atoms of these groups forming a slightly distorted octahedral configuration around the central chromium atom (Fig. 6).

9. Discussion of the structure and the bonding

Fig. 7 illustrates diagrammatically the idealized packing of the formula units in the structure. The plan of this diagram shows a layer of complex ions parallel to the *b c* plane. Starting with any complex ion in section *A* of this plan, the other complex ions in section *A* follow by the operation of the glide plane. The same applies to all the complex ions in section *B*. By the operation of the screw axes all the complex ions in section *B* follow from those in section *A* and vice versa. Because of the glide parallel to *c*, all the complex ions in section *A* can be regarded as lying approximately in a layer. The complex ions in section *B* also lie approximately in a layer, but, owing to the operation of the screw axes, this layer is elevated by half a unit in the *a* direction. Cross-sections of these layers of complex ions are shown as unshaded blocks in the *A* and *B* sections of the elevation. The shaded blocks represent cross-sections of sheets of potassium ions and water molecules running through the structure in the *c* direction. These sheets are mainly responsible for holding together the complex ion layers marked I, II and III. In addition complex ions in the same layer are also linked together by the potassium ions and the water molecules.

The way in which the potassium ions form bonds in the structure is best described by referring to Fig. 3. K_1 is linked to O_3 and O_4 in unit 1 and to $\overline{O}_3$ and $\overline{O}_4$ in the repeat of unit 1 along the *c* axis. It is also linked to O_6 in unit 2 and to O_1 in unit 3. K_1 is further linked to $H_2O_{(1)}$ and to $H_2O_{(2)}$. The mean length of these eight ionic bonds is 2·8 Å. Because of the twofold axis, the bonds associated with the second potassium ion, $\overline{K}_1$, are similar to those described for K_1. The third potassium ion, K_2, is linked to $\overline{O}_1$ and O_2 of unit 1, and to O_1 and $\overline{O}_2$ of the repeat of unit 1 in the *a* direction. K_2 is also linked to $\overline{H_2O}_{(1)}$ and to $H_2O_{(1)}$. These six ionic bonds all approach the mean value 3·1 Å.

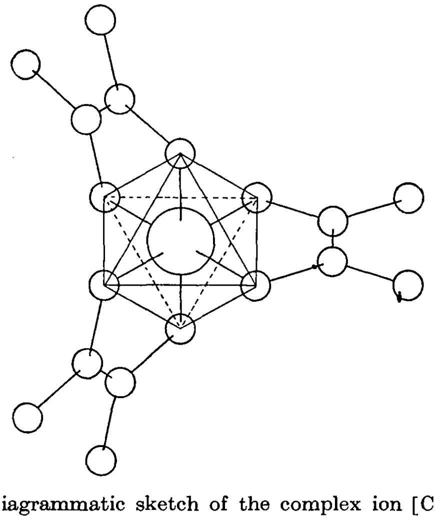

Fig. 6. Diagrammatic sketch of the complex ion $[Cr(C_2O_4)_3]$.

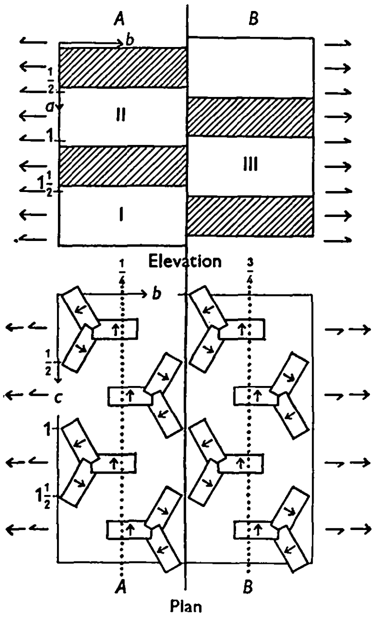

Fig. 7. Diagrammatic illustration of the packing of complex ions in the structure. International symbols are used to illustrate the symmetry elements.

The three water molecules, $H_2O_{(1)}$, $\overline{H_2O}_{(1)}$ and $H_2O_{(2)}$, form hydrogen bonds to oxygen atoms and they are also bonded to the potassium ions. It must be pointed out, however, that the peak obtained for $H_2O_{(2)}$ was considerably smaller than those obtained for the other oxygen atoms in the structure, so that it is doubtful whether or not a water molecule exists in this position. Because of this uncertainty the bond lengths calculated for $H_2O_{(2)}$ must be regarded as unreliable. $H_2O_{(2)}$ is linked to O_1 and $\overline{O}_1$ and also to K_1 and $\overline{K}_1$, the bonds to the potassium ions having a mean value of 2·6 Å. The water molecule, marked $H_2O_{(1)}$, is linked to O_5 in unit 1 and to $\overline{O}_6$ in unit 2, the mean bond length being 2·8 Å. $H_2O_{(1)}$ is further linked to K_1 and to K_2, the average bond length in this case is 3·0 Å. Because of the twofold axis the bonds associated with $\overline{H_2O}_{(1)}$ are similar to those described for $H_2O_{(1)}$.

The economical way in which the complex ions are arranged in the structure can be seen by referring to the plan of Fig. 7, where the arrows on the planes of the oxalato groups indicate their slopes. Inspection shows that neighbouring oxalato groups belonging to different complex ions always slope in the same direction, resulting in the tightest possible fit. The structure considered as a whole is therefore mainly determined by the shape of the complex ions. The figure also illustrates that the two stereo isomeric ions predicted by Werner (1912 *b*) are present in equal numbers in the structure.

Finally, even though the wrong space group was used throughout this investigation, we feel that, for reasons pointed out earlier, the errors introduced will not be very large, and that, although the actual values of the bond lengths discussed may not be very reliable, these bonds do give a clear picture of the main forces holding the structure together.

In conclusion we wish to thank Mr R. W. Burley for preparing the crystals and Dr H. J. Nel, of the Pretoria University Geology Department, for help with the measurements of the optical properties of the crystals.

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The Crystal Structure of Axinite

By T. Ito and Y. Takéuchi

Mineralogical Institute, University of Tokyo, Japan

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The structure of axinite has been studied using Weissenberg photographs (Cu $K\alpha$, $\lambda = 1{\cdot}54$ Å). The unit cell has the dimensions $a = 7{\cdot}14_8$, $b = 9{\cdot}15_6$, $c = 8{\cdot}96_0$ Å, $\alpha = 88°\ 04'$, $\beta = 81°\ 36'$, $\gamma = 77°\ 42'$, and contains two molecules of $H(Fe, Mn)Ca_2Al_2BSi_4O_{16}$. The space group is $P\bar{1}$. Analysis was carried out and the result described with another set of axes: $a' = 7{\cdot}15$, $b' = 12{\cdot}57$, $c' = 13{\cdot}05$ Å, $\alpha' = 91°\ 23'$, $\beta' = 75°\ 30'$, $\gamma' = 93°\ 23'$, the transformation matrix from the proper to the working setting being $100/0\bar{1}1/011$. The structure is composed of separate Si_4O_{12} and BO_3 groups bound together by Fe, Al and Ca atoms. Fe atoms are in the middle of O–OH double-octahedra and one-half of the Al atoms are in the middle of similar oxygen double-octahedra, the remaining half occupying the centres of tetrahedra formed of three oxygen atoms and one OH group. Each Ca atom is surrounded irregularly by ten oxygen atoms of which five exert no bond toward it. The electrostatic balance of bonds determines unequivocally the position of the OH group.

Axinite is one of those common silicate minerals whose crystal structure has been hitherto unknown. As part of our program for boron-containing substances axinite has been studied by the X-ray method with the results described below.

1. Experimental

The specimens used are from Obira, the well-known locality in Japan for axinite and other boron-bearing minerals. Almost colourless to pale violet, transparent crystals of sphenoidal habit, several mm. in size, were available for X-ray examination. Chemical analysis showed that its composition is well expressed by the formula, $H(Fe_{0\cdot7}Mn_{0\cdot3})Ca_2Al_2BSi_4O_{16}$; the small content of magnesium being ignored.

A series of Weissenberg photographs, namely the zero, first and second layers of [100], the zero, first, second and third layers of [010] and [001], the zero layer each of $[0\bar{1}1]$, [101] and [011] and the fourth layer of $[0\bar{1}1]$, were taken using Cu $K\alpha$ radiation ($\lambda = 1{\cdot}54$ Å) (for the setting of the axes see § 2). Intensities of reflexions were estimated visually and converted by the multiple-film technique into numerical values, which were later rendered comparable with the absolute values by multiplying by a proportionality factor that reduced the sum of differences of observed and calculated structure amplitudes of (200) and (040)* to a minimum. For the

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* Indices after another setting of the axes adopted for the convenience of analysis (see § 3).