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Extinction in a lithium fluoride sphere.

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Intensity measurements have been made on a sphere of lithium fluoride with Mo $K\alpha$ and Cu $K\alpha$ radiations. The sphere, of radius $2{\cdot}99 \pm 0{\cdot}03 \times 10^{-2}$ cm, was ground from a cleavage fragment of a synthetic crystal obtained from the Harshaw Company. The $\mu_0 R$ value was 0·11 for Mo $K\alpha$ and 0·96 for Cu $K\alpha$.

According to recent theory (Zachariasen, 1967) the observed structure factors, F_σ, are related to the calculated values, F_c, as follows (for unpolarized incident radiation):

$$\begin{aligned} F_\sigma &= CF_c y^{1/2}, \\ y &= (y_1 + K^2 y_K)/(1+K^2), \\ y_K &= (1+2X_K)^{-1/2}, \\ x_K &= r^* K^2 Q_0 \lambda^{-1} \bar{T}, \\ r^* &= r[1+(r/\lambda g)^2]^{-1/2}, \\ \bar{T} &= AdA^*/d\mu_0 . \end{aligned} \tag{1}$$

C is the scale factor while $K=1$ for the normal and $K=|\cos 2\theta|$ for the parallel component of polarization. The other symbols have their usual meanings.

It is sometimes convenient to use a simplified, but approximate form of equation (1), namely

$$\begin{aligned} y &= (1+2x)^{-1/2} \\ x &= r^* Q_0 \lambda^{-1} \bar{T} p_2/p_1 \end{aligned} \tag{2}$$

where

$$p_2/p_1 = (1+\cos^4 2\theta)/(1+\cos^2 2\theta) .$$

The intensities of all reflections with $2\theta < 90°$ were measured with molybdenum radiation, only the reflections ($HK0$) with $2\theta < 120°$ with copper radiation.

The stationary counter-crystal procedure was used with Zr or Ni filter. The counting rate was kept low by attenuating the beam with a set of carefully calibrated Ni foils. A balanced Y–Zr filter was used for background correction for the molybdenum data. In the copper case the background was measured at $2\theta \pm 2°$, and the mean value taken to be the background under the peak.

The intensities varied very little from plane to plane of a given form with an indicated accuracy of one per cent for the mean value. The F_σ values are given in Tables 1 and 2 (adjusted to ultimate C values of unity).

Table 1. *Structure factors.* Mo $K\alpha$

HKL	F_c	$F_c y^{\frac{1}{2}}$	F_σ
111	19·9	18·9	19·0
200	30·0	27·3	27·1
220	21·9	21·0	21·0
311	9·59	9·52	9·31
222	17·0	16·7	16·7
400	13·8	13·6	13·9
331	6·31	6·30	6·18
420	11·5	11·4	11·4
422	9·86	9·81	9·80
511	4·87	4·86	4·95
333	4·87	4·86	5·07
440	7·62	7·60	7·59
531	4·10	4·10	4·09
442	6·83	6·81	6·87
600	6·83	6·81	6·81
620	6·17	6·16	6·14
533	3·59	3·59	3·58
622	5·63	5·62	5·60
444	5·16	5·15	5·06
711	3·22	3·22	3·22
551	3·22	3·22	3·24
640	4·76	4·75	4·69
642	4·41	4·40	4·32
731	2·90	2·90	2·91
553	2·90	2·90	2·87

Table 1 *(cont.)*

Table 2. *Structure factors.* Cu $K\alpha$

HKO	F_c	$F_c y^{\frac{1}{2}}$	F_σ
200	30·0	23·9	23·7
220	21·9	19·4	19·7
400	13·8	13·1	13·3
420	11·5	11·2	11·0

In the interpretation of the data the f curves of Cromer & Waber (1964) for Li^+ and F^- were adopted, and the very small anomalous dispersion corrections were neglected.

The closest agreement between the sets F_σ and $CF_c y^{1/2}$ for the molybdenum data was sought as C, B_{Li}, B_F, and r^*_{Mo} were varied. For $r^*_{Mo} = 2{\cdot}2 \times 10^{-6}$ cm one finds $B_{Li} =$

$0{\cdot}90 \pm 0{\cdot}04$ Å^2, $B_F = 0{\cdot}63 \pm 0{\cdot}01$ Å^2, and, as seen from Table 1, the resulting R value is 0·008.

With these B values and $r^*_{Cu} = 4{\cdot}5 \times 10^{-6}$ cm one obtains the agreement shown in Table 2 for the copper data.

The two results $r^*_{Mo} = 2{\cdot}2 \times 10^{-6}$ cm and $r^*_{Cu} = 4{\cdot}5 \times 10^{-6}$ cm give $r = 1{\cdot}14 \times 10^{-5}$ cm and $g = 316$.

Since $r/\lambda g = 5{\cdot}1$ for Mo $K\alpha$ and 2·35 for Cu $K\alpha$, the lithium fluoride sphere approaches a type I mosaic crystal in which the width of the mosaic spread is much greater than that of the diffraction pattern from a single domain.

The writer is indebted to Miss H. A. Plettinger, who made most of the intensity measurements. The work was supported in part by the Advanced Research Projects Agency under Contract SD-89.

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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. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (G. Boom, Department of Metallurgy, University of Oxford, Parks Road, Oxford, England). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

International Union of Crystallography

International Tables for X-ray Crystallography

The Executive Committee of the International Union of Crystallography announces that from 1 April 1968 the price of each of the three Volumes of *International Tables for X-ray Crystallography* will be revised to £6.10*s*. The preferential price for *bona fide* crystallographers, who must give an undertaking when purchasing that the volume is for their *personal use only*, will be £3.15*s*. per volume. For prospectus and order forms write to the publishers, The Kynoch Press, Witton, Birmingham 6, England.

Volume II (*Mathematical Tables*) has just been reprinted with corrections. Stocks are available both of this and of Volume I (*Symmetry Groups*). Volume III (*Physical and Chemical Tables*) is being reprinted and will be available again shortly.

It is regretted that these slight price rises have occurred. They are due to the need to meet the costs of reprinting and increased distribution charges.

Denver Conference on Applications of X-ray Analysis Denver, USA, 21–23 August 1968

The annual Denver Conference on Applications of X-ray Analysis will be held from 21 to 23 August 1968 at Denver, U.S.A. The emphasis will this year be on Diffraction Metallography. The meeting will consist of invited lectures and contributed fifteen-minute papers on subjects relating to the application of diffraction methods to the characterization of materials. Proceedings of the conference will be published as *Advances in X-ray Analysis*, Volume 12.

Contributed papers are now invited. Three copies of titles and abstracts (about 300 words) should be sent before 8 April 1968 to G. R. Mallett or J. B. Newkirk, Department of Metallurgy, University of Denver, Denver, Colorado 80210, U.S.A. Final manuscripts are due on 15 July 1968.

The Precision of Determination of Molecular Geometry by Diffraction and Spectroscopic Techniques

Advanced course, Aarhus, 29 July – 7 August 1968

An advanced course on the determination of molecular geometry by diffraction and spectroscopic techniques will be held at Aarhus University, Denmark, from 29 July to 7 August 1968. The course is supported by NATO and is intended primarily for advanced students or young research workers with research experience in determining accurate geometric molecular parameters. Accommodation is available for 80 participants. There will be the opportunity of critically comparing the different methods, and ample time will be provided for discussion. The course will be followed by a symposium announced below.

A limited number of grants are available for applicants from NATO countries.

Enquiries should be addressed to Prof. S. E. Rasmussen, Department of Inorganic Chemistry, Institute of Chemistry, University of Aarhus, 8000 Aarhus C, Denmark, not later than 15 April 1968.

Symposium, Aarhus, 8–10 August 1968

An advanced symposium on the determination of molecular geometry by diffraction and spectroscopic techniques will be held at Aarhus University, Denmark, from 8 to 10 August 1968. The symposium is a continuation of the advanced course mentioned above. Attendance is limited to about 160 participants, including the participants in the course. It is intended to obtain a balanced participation of older and younger workers, and a reasonable spread among the different methods.

Enquiries should be addressed to Prof. S. E. Rasmussen, Department of Inorganic Chemistry, Institute of Chemistry, University of Aarhus, 8000 Aarhus C, Denmark, not later than 15 April 1968.