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Atomic scattering factor for O^{2-}.

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It is well known that the existence of the doubly charged negative oxygen ion in some oxide crystals is a useful working hypothesis, although the free O^{2-} ion is not confirmed experimentally. With the aid of the variational method Yamashita & Kojima (1952) first obtained the $2p$ wave function of the O^{2-} ion in the crystalline state of MgO. They found it possible that the O^{2-} ion can exist there by the stabilizing effects of the mutual interaction of ions. Recently Watson (1958) has calculated the wave functions of the O^{2-} ion in the additive potential wells of +1 and +2 charge by means of the self-consistent method.

Table 1. *f values for* O^{2-}

	f (total)		$f(2p)$		
$\sin\theta/\lambda$	+1 well	+2 well	+1 well	+2 well	MgO
0·00	10·000	10·000	1·000	1·000	1·000
0·05	9·491	9·551	0·926	0·937	0·932
0·10	8·357	8·475	0·769	0·789	0·768
0·15	7·027	7·159	0·592	0·616	0·580
0·20	5·802	5·908	0·439	0·459	0·418
0·25	4·789	4·857	0·321	0·334	0·296
0·30	3·994	4·028	0·234	0·241	0·208
0·35	3·383	3·394	0·170	0·173	0·145
0·40	2·918	2·916	0·123	0·124	0·100
0·50	2·298	2·287	0·063	0·062	0·044
0·60	1·938	1·929	0·029	0·028	0·016
0·70	1·721	1·714	0·012	0·010	0·002
0·80	1·578	1·574	0·002	0·001	−0·003
0·90	1·472	1·469	−0·002	−0·003	−0·005
1·00	1·382	1·381	−0·004	−0·004	−0·005
1·10	1·300	1·299	−0·004	−0·005	−0·005
1·20	1·221	1·220	−0·004	−0·004	−0·004
1·30	1·144	1·143	−0·004	−0·004	−0·003

Since the above wave functions are represented in analytical forms and the electron distribution of the O^{2-} ion can be safely assumed to be spherical, the atomic scattering factor of the O^{2-} ion can also be expressed by an analytical formulae. We have thus computed the f values of the O^{2-} ion in the +1 and +2 wells using the results of Watson. The scattering factor of a $2p$ electron in MgO has also been calculated on the basis of the wave function of Yamashita & Kojima. The results are summarized in Table 1. The difference in f values for the two models of the +1 and +2 wells in our procedure seems to be insignificant. The $f(2p)$ values of MgO deviate a little from that of the general models of Watson. The values of f(total) are reasonable in comparison with the f values of the other states of oxygen calculated by Freeman (1959).

The numerical computations were performed by the P–C–1 in the University of Tokyo. The author wishes to express his thanks to Mr M. Tokonami for his kindly help in this computation.

References

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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 (Dr D. W. Smits, Laboratory of Inorganic and Physical Chemistry, 10 Bloemsingel, Groningen, The Netherlands).

International Union of Crystallography

World Directory of Crystallographers

As announced earlier in this journal (see *Acta Cryst.* (1959), **12**, 826) a second edition of the *World Directory of Crystallographers* will be published before the forthcoming Fifth International Congress of the Union in August 1960. Questionnaires were distributed to crystallographers throughout the world, and national lists are now being prepared by Sub-Editors in the various countries.

The *Directory* will contain the names, addresses, and further biographical information concerning crystallographers and all other scientists who in their research make to a great extent use of crystallographic methods. This means that the booklet will also contain the names of a great number of solid-state physicists and chemists who are applying crystallographic and diffraction methods, of many mineralogists and geologists who are studying crystal minerals, *etc.*

Readers of this notice who feel that their names ought to be included in the *Directory*, but who have not received and returned a questionnaire, are urgently requested to write without delay to the General Secretary of the Union, Dr D. W. Smits, Laboratory of Inorganic and Physical Chemistry, 10 Bloemsingel, Groningen, The Netherlands. Please give the following details in your letter: full name, title, year of birth, highest degree (incl. year, University and field), present position, full address, and major crystallographic interests.

Copies of the first edition of the *World Directory* can still be obtained from the Polycrystal Book Service, G.P.O. Box 620, Brooklyn 1, N.Y., U.S.A., at the price of U.S. $1·50 per copy, postpaid, if payment accompanies order.

Summer School in Crystal-Structure Determination

A Summer School in Modern Methods of Crystal-Structure Determination will be held in the Manchester College of Science and Technology on 29th August–9th September, 1960. Amongst the lecturers will be the following:

Prof. W. T. Astbury, Leeds.
Dr C. A. Beevers, Edinburgh.
Dr E. F. Bertaut, Grenoble.
Prof. J. M. Bijvoet, Utrecht.
Prof. M. J. Buerger, Cambridge, Mass.
Dr W. Cochran, Cambridge.
Dr D. W. J. Cruickshank, Leeds.
Dr A. Hargreaves, Manchester.
Dr J. Karle, Washington.
Prof. H. Lipson, Manchester.
Dr A. L. Patterson, Philadelphia, Pa.
Prof. R. Pepinsky, University Park, Pa.
Dr M. F. Perutz, Cambridge.
Dr C. A. Taylor, Manchester.
Dr W. H. Taylor, Cambridge.
Dr V. Vand, University Park, Pa.
Dr M. M. Woolfson, Manchester.

The main topics dealt with, by lectures, practical work and discussions, will be direct methods, Fourier-transform and optical-transform methods, anomalous scattering, and refinement procedures. In addition there will be some lectures and discussions on recent results in various fields, with assessment of their implications.

The fee for the course will be £25, including accommodation in one of the University Halls of Residence. The fee for attendance without accommodation will be £5.

Further details and a form of application can be obtained from The Director, The Extra-Mural Department, The University, Manchester 13, to whom any enquiries should be addressed. The form of application should be returned before 27th May, 1960. If all the available places are filled, it may be possible to allow attendance at the lectures and discussions only at a reduced fee.

Special grants

NATO has granted recognition to this school and is prepared to give substantial travel and subsistence allowances to members of NATO countries. Enquiries about such grants should be made to Prof. H. Lipson, Physics Department, College of Science and Technology, Manchester 1.

Book Review

Works intended for notice in this column should be sent direct to the Editor (A. J. C. Wilson, Department of Physics, University College, Cathays Park, Cardiff, Great Britain). As far as practicable books will be reviewed in a country different from that of publication.

Vector Space and its application in crystal structure investigation. By M. J. Buerger. Pp. xiv+347 with many figs. and tables. New York: John Wiley. 1959. Price $12, £4·16*s*.

Patterson's announcement in 1934 of the discovery of his now-famous function aroused great excitement in the crystal-structure world; it seemed that the basic problem was now solved and that all crystal structures could be determined. Simple structures such as KH_2PO_4 responded directly; more complicated ones such as $CuSO_4.5\,H_2O$ were not quite so direct but were still fairly straightforward. Gradually, however, the realization came that our hopes (or fears according to one's point of view!) were not to be so simply fulfilled. The Patterson function certainly contained all the information about a crystal structure in the form of the vector distances between the atoms but to disentangle this information in general has proved so far to be an impossible task.

Nevertheless many crystallographers felt that the approach to the determination of crystal structures lay in the Patterson synthesis and therefore tried to find ways of transforming a pattern of vectors into a pattern of atomic positions. No one has contributed more to this task than the author of this book. He has, over the years, produced a number of ingenious approaches—such as 'implication theory' and the 'image-seeking function'—and these he has collected together in the first book entirely devoted to this subject.

As one would expect from the author, the account is comprehensive and is, in many ways, clearer than some of the original papers. He has set himself the task of catering for the student and those who wish to find out what Patterson methods can do need not look further than this book. Full theoretical details are given together with practical examples of their use in successful structure determinations.

Nevertheless, the reviewer laid down the book with a sense of dissatisfaction. It is expensive—it costs much more than some general books on X-ray diffraction—yet it deals with only one facet of the subject. It is comprehensive in its theory, but tends to be sparing in practical details. Examples of structure determination are given, but often they seem to depend upon evidence—presence of a heavy atom or isomorphous replacement—which lessens their illustrative value. The book certainly justifies its place on the shelf of the X-ray crystallographer, but it could have been a monograph rather than a full-sized book.

But perhaps the most trenchant criticism is that the name Crowfoot appears only once in the index and the name Hodgkin not at all!

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