from the *American Institute of Physics Handbook* (1963), with two exceptions: ordered Cu_3Au, from Flinn, McManus & Rayne (1960), and β-CuZn, from McManus (1963). The results for KCl and NaCl are in good agreement with the values given by Nilsson, but, contrary to Schwartz's results for Cu_3Au, no case was found for which $\mathscr{K}$ was less than $\mathscr{K}_a$. The discrepancy between $\mathscr{K}$ and $\mathscr{K}_a$ varies more or less systematically as a function of the anisotropy factor parameter, increasing with increasing departures from isotropy in either sense. The magnitude of the discrepancy is appreciable for very anisotropic materials.

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Location of the anomalous scatterer in neutron anomalous scattering studies.

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A method is suggested for obtaining a Patterson map which contains only vectors related to the atom giving rise to anomalous scattering. This map gives directly the position of the anomalous atom, and can be used in the first stage of the method suggested by Singh & Ramaseshan (1968) for the solution of the phase problem in neutron diffraction.

Singh & Ramaseshan (1968) have pointed out that in a structure determination by neutron diffraction, using the anomalous scattering of neutrons by nuclei such as Cd^{113} and Sm^{149} to phase the reflexions, there will be difficulty in locating the anomalous atom by the Patterson method. This arises because vectors $A-A$ between anomalously scattering atoms (A) are obscured by $N-N$ vectors between normal atoms (N), even if the $A-N$ vector peaks are removed by suitably combining the intensity measurements on either side of the resonance wavelength (λ_0). To overcome this difficulty Singh & Ramaseshan (1968) have suggested an analytical method which combines data at two wavelengths to give F_A^2, the contribution due to A atoms alone. The position of the A atom can then be determined by a Patterson synthesis with F_A^2 as coefficients.

In this note we show that a Patterson map can be obtained directly, from data collected at two wavelengths, which is completely free of both $A-N$ and $N-N$ interactions and contains only $A-A$ vectors. The Patterson map is based on the Fourier cosine synthesis proposed by Okaya & Pepinsky (1961). The location of the A atoms using this map is then straightforward.

In the case of a non-centric crystal containing atoms which scatter neutrons anomalously, the Patterson function is complex. Following Okaya & Pepinsky (1961), it can be written as

$$P(\mathbf{U}) = P_c(\mathbf{U}) - iP_s(\mathbf{U}) \quad \text{where}$$
$$P_c(\mathbf{U}) = \Sigma' \left(|F(\mathbf{H})|^2 + |F(\bar{\mathbf{H}})|^2\right) \cos 2\pi \mathbf{H} \cdot \mathbf{U} \quad \text{and}$$
$$P_s(\mathbf{U}) = \Sigma' \left(|F(\mathbf{H})|^2 - |F(\bar{\mathbf{H}})|^2\right) \sin 2\pi \mathbf{H} \cdot \mathbf{U} .$$

$\mathbf{H}$ is (h,k,l), $\mathbf{U}=(u,v,w)$, and Σ' is the summation over half of the reciprocal sphere.

Where there is only one type of anomalously scattering atom in the unit cell, it can be shown from equations (12) and (13) of Okaya & Pepinsky's paper that

$$|F(\mathbf{H})|^2 + |F(\bar{\mathbf{H}})|^2 = \sum_{\substack{A-A \\ \text{Pairs}}} (b_A'^2 + \Delta b_A''^2) \cos 2\pi \mathbf{H} \cdot \mathbf{U}_{AA} + \sum_{\substack{A-N \\ \text{Pairs}}} b_A' b_N' \cos 2\pi \mathbf{H} \cdot \mathbf{U}_{AN} + \sum_{\substack{N-N \\ \text{Pairs}}} b_N' b_{N'}' \cos 2\pi \mathbf{H} \cdot \mathbf{U}_{NN}$$

and

$$|F(\mathbf{H})|^2 - |F(\bar{\mathbf{H}})|^2 = \sum_{\substack{A-N \\ \text{Pairs}}} \Delta b_A'' b_N' \sin 2\pi \mathbf{H} \cdot \mathbf{U}_{AN}$$

where $\mathbf{U}_{AA}, \mathbf{U}_{AN}, \mathbf{U}_{NN}$ are vectors between AA, AN, NN atoms and the scattering factor of the anomalous scatterer

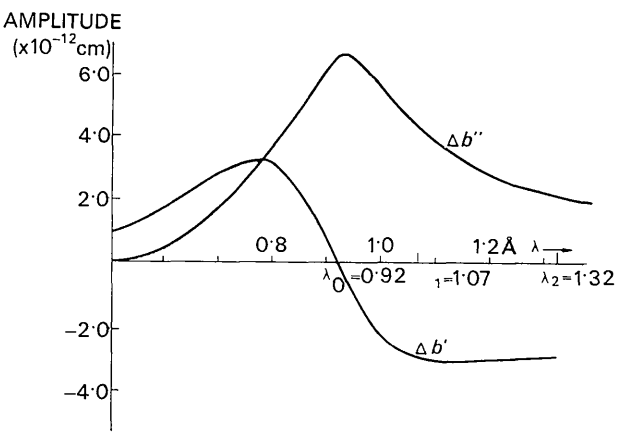

Fig. 1. Wavelength dependence of $\Delta b'$ and $\Delta b''$ for Sm^{149}.

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is of the form

$$b = b_0 + \Delta b' + i\Delta b'' = b' + i\Delta b'' .$$

b_0 is the potential term arising from hard-sphere scattering, and $\Delta b'$, $\Delta b''$ are the real and imaginary contributions from resonance scattering. For normal atoms (N), $\Delta b''$ is zero.

Thus a P_c map will contain $A-A$, $A-N$ and $N-N$ vectors with peak heights proportional to $b_A'^2 + \Delta b_A''^2$, $b_A' b_N'$, $b_N' b_N'$, respectively and will be as difficult to interpret as the ordinary Patterson function for normal scattering. On the other hand, the P_s map has only $A-N$ vectors with peak heights $+\Delta b_A'' b_N'$ at $\mathbf{U}_{AN}$ and $-\Delta b_A'' b_N'$ at $\mathbf{U}_{NA}$. In the X-ray case, since all the atoms have scattering factors with positive sign, P_s will contain clusters of peaks around the A atoms which are either positive or negative in sign and can be deconvoluted. For neutron scattering, the scattering amplitudes can be both positive and negative and so there will now be mixed clusters containing both positive and negative peaks, which for high overlap may obscure some of the vectors. Thus the P_s synthesis will be of limited application in neutron diffraction. However, if intensities of Bijvoet pairs are recorded at two wavelengths, λ_1, and λ_2, such that $b_A'(\lambda_1) = b_A'(\lambda_2)$ and a difference map plotted of $\Delta P_c = P_c(\lambda_1) - P_c(\lambda_2)$, then the $A-A$ vectors can be easily picked out. For $b_A'(\lambda_1) = b_A'(\lambda_2)$, the equations above show that $A-N$ vectors will vanish as well as the $N-N$ vectors in the ΔP_c Patterson. The only vectors remaining are $A-A$ with peak heights proportional to $\Delta b_A''^2(\lambda_1) - \Delta b_A''^2(\lambda_2)$.

The condition $b_A'(\lambda_1) = b_A'(\lambda_2)$ can be achieved readily in neutron diffraction as can be seen from Fig. 1, which gives the wavelength dependence of $\Delta b'$ and $\Delta b''$ for ^{149}Sm (Dale & Willis, 1966). Suitable values of λ_1 and λ_2 for ^{113}Cd and ^{149}Sm are 0·75, 0·90 Å and 1·07, 1·32 Å respectively, but other combinations are also possible. Both λ_1 and λ_2 lie well within the useful wavelength range for neutron diffraction. For one wavelength, $\Delta b_A''$ is large and for the other wavelength it is small, thus giving a large peak height for the $A-A$ vectors.

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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, Laboratorium voor Fysische Metaalkunde der Riiksuniversiteit, Universiteitscomplex Paddepoel, Groningen, The Netherlands). 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

Appointment of Executive Secretary

At their meeting of 29–30 June 1968, the Executive Committee of the International Union of Crystallography decided that a full-time salaried Executive Secretary should be appointed as soon as possible and applications were invited shortly afterwards. The decision was taken after discussions of reports by the (Honorary) General Secretary and the (Honorary) Treasurer, from which it was clear that the volume of daily work made it impossible for them, or indeed any successors, to continue with the present manner of operation. The Executive Secretary is to take over the day-to-day administration and will thus relieve the Honorary Officers of much of their work. The establishment of the new post is subject to confirmation by the Eighth General Assembly in August 1969.

The Executive Committee is glad to announce the appointment of Dr J. N King as Executive Secretary of the Union.

Dr King is British and was born in 1937. He studied physics at Imperial College, London, where he took his B.Sc., M.Sc. and Ph.D. (solid state physics) degrees. He went to Australia in 1963, where he worked on the preparation of thin metal films and their examination by electron diffraction and electron microscopy, at the Aeronautical Research Laboratories, Melbourne.

Dr King was Secretary of the Organizing Committee of the International Conference on Electron Diffraction and the Nature of Defects in Crystals, Melbourne 1965, which was sponsored jointly by the Union and the Australian Academy of Science, with the support of the Commission on the Solid State of IUPAP. He returned to England in September 1968.

Combined office accommodation is to be found in Chester, England, for the Executive Secretary and the Union's Technical Editor, Mr S. A. Bryant. Until further notice all correspondence for the Technical Editor should continue to be addressed to his present office at 1 Stanley Place, Chester, England.

Dr King started work on 1 February 1969, and will be visiting the General Secretary and the Treasurer before taking over the daily administration of the Union. Correspondence should *not* be directed to Dr King for action in his capacity as Executive Secretary until notice is given. However, it will be appreciated if information copies of appropriate correspondence are sent to Dr King at the Technical Editor's present address.