**Computer Program**

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**A general computer program for the analysis of X-ray diffraction data for liquids.** By G. LICHERI, G. PICCALUGA and G. PINNA, Istituto Chimico, Università di Cagliari, Via Ospedale 72, 09100 Cagliari, Italy

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A general computer program for the analysis of X-ray diffraction data for liquids is here described. It consists of a central part (main) and a number of subroutines, in which one single step of the elaboration of experimental intensities is performed. This arrangement allows the entire sequence of operations to be performed as far as the radial distribution functions; alternatively only a part can be performed, starting or stopping at any point. The program is flexible and easily modifiable for the user’s needs.

**Introduction**

The analysis of data in X-ray diffraction studies of liquids is not carried out in the same way by different authors. Therefore, it may be useful to have at one’s disposal a general computer program, which is also very adaptable to different requirements and easily modifiable.

The aim of data treatment is usually to evaluate a structural function, which is the Fourier transform of a radial distribution function as the incoherent intensity in electron units scaled to one structural unit containing m atomic species, and is the coherently scattered intensity in electron units scaled to one structural unit. Different choices of the function \( i(s) \) are possible with simple modifications in the program. Modifications are easily achievable for other steps in data treatment for which alternative solutions may be desired (e.g. absorption correction, scaling procedures, etc.)

**Program description**

The main program consists of input–output statements, control statements corresponding to different options contemplated and statements regarding some elementary operations. A number of subroutines are called and each one executes a single step of the elaboration of the experimental diffraction intensities. This general structure simplifies the understanding and the use of the program itself and makes easier eventual modifications of it. Most subroutines have been described in detail elsewhere (Licheri, Piccaluga & Pinna, 1974a, b). A description and list of the others is included in a technical report containing the list of the main program and the instructions for using it. This report is available on request.

The sequence of operations is here reported, associated with the names of the subroutines that execute them.

(i) **Subroutine SCATT** – The functions

\[
\frac{1}{\sum_{j=1}^{m} x_i f_j^2(s)} \left( \sum_{j=1}^{m} x_i f_j(s) \right)^2
\]

are computed where \( I_{inc}^j \) is the incoherent intensity of the \( j \)th species, \( R \) is the recoil Breit–Dirac correction and \( T \) is the monochromator transmission factor, which must be programmed by the user in the subroutine COMP called by SCATT.

(ii) **Subroutine CORR** – Evaluation of total intensity \( I_T(s) \), corrected for background, absorption and polarization and its associated statistical error \( \sigma_I(s) \) (Mikolaj, 1965; Licheri, Piccaluga & Pinna, 1973a). The absorption factors are calculated in the subroutine ABSOR which should be programmed by the user according to the experimental geometry used.

(iii) Smoothing of high-angle data and evaluation of a confidence interval \( \pm \mu_{0.9} \sigma_I(s) \) around the smoothed points (Mikolaj, 1965), which may show anomalous points to be
The constant \( u_o \) is the probability point of normal distribution, corresponding to significance level \( p \). The smoothing process is performed in a subroutine (Sub. SPLFN) which uses a spline function method (Galligani, 1971).

(v) Subroutine INTRP – Interpolation of the total intensity \( I_1 \) with constant step in the variable \( s \), useful to calculate integrals with quadrature formulæ.

(vi) Subroutine KRMOE – Evaluation of the normalization constant \( \alpha \) according to the method of Krogh-Moe (1956).

(vii) Subroutine STRUF – Evaluation of the function \( s . i(s) \) where \( i(s) \) is the structure function as defined in (2) and \( I_{\text{nu}}(s)=a I_1(s)-I_{\text{nu}}(s) \).  

(viii) Subroutine RAHMN – Test of the reliability of the structure function based on the integral equation written by Rahman (1965), providing a necessary (but not sufficient) condition which the structural function must satisfy.

(ix) Subroutine MOD – Evaluation of the so-called modification function (Waser & Schomaker, 1953) and multiplication by \( s . i(s) \). This is a dummy subroutine where any modification function may be programmed by the user.

(x) Subroutine DRADA – Evaluation of the radial distribution function \( D(r) \), of the correlation function \( G(r)=D(r)/4 \pi r^2 \varrho_0 \) and of the function \( Q(r)=D(r)/(4 \pi r^2-4 \pi r_0^2) \) where \( \varrho_0 \) is the average number density. The integrals are calculated using Filon’s (1928) quadrature formulæ.

Fig. 1. Flow chart of the program.

The flow chart of the program (Fig. 1) clearly shows the sequence of operations and the possibility of executing only some of them. Data processing can therefore be repeated from one point or another of the entire sequence, whenever examination of partial results shows the necessity of making changes.

The program consists of five sections that can be performed separately or one after the other (except Section 5), depending on the values of the codes punched on the first input card. The results obtained in each section can be loaded into a disc storage or punched on cards and used as input data for the subsequent sections.

Size and storage requirements

The physical size of the program is about 1200 cards. Storage requirements depend on the size of the arrays. In our conditions the occupancy is about 87000 bytes for an IBM 370 computer and the time required for the execution of all the steps is about 10 min for a typical calculation, depending mainly on the number of experimental data, and on the integration limits and steps for all the integrals computed.

The program has also been used on an IBM 1130 com-
puter. In this case small modifications in some statements are necessary in addition to an expedient to overcome the limitations of the core storage.

References


Laboratory Note


A miniature goniometer head*

A miniature, two-arc, lockable, nonmagnetic goniometer head with all movements confined within a cylinder of 1.5 cm diameter has been constructed. The upper and lower arcs are adjustable to ±10° and ±5° and the common center of arcs lies 0.95 and 1.6 cm above the top and bottom pedestals respectively. It has functioned satisfactorily, withstanding repeated thermal cyclings between 300–4°K and upholding the mounted ferromagnetic crystal exerting a large field-induced torque in the cryomagnetic neutron experiment.

In our instrumentation, the sample space in the cryostat tail situated between the magnet poles is about 1.8 cm in diameter. Three different goniometer heads for this configuration have been constructed and tested successfully. The smallest model is shown in Fig. 1 where A is an exemplary crystal holder; B, the upper cradle with two locking screws for A and a pair of curved grooves for the upper arc; C, the lower cradle with a pair of slide-guiding dowel pins and a locking screw for each of the mating grooves in B and D; D, the lower-arc grooved base with a press-fitting hole and a dowel pin for the mounting stud E. Steric clearance necessitates an intricate shaping of C. High thermal conductivity of the sample mount is preferable in our temperature-control monitoring and hence construction metals chosen were Ti–Zr null-matrix alloy for A and the locking screws, tempered aircraft aluminum alloy (7075, ASTM B211) for B, C, and D, copper for E and stainless steel for the dowel-pins. An auxiliary micrometer is used in the cradle positioning. The X-ray method is employed for the prealignment so as to attain the least correction in the multi-parameter angular settings of the neutron-scattering and magnetic-field vectors. The final translational alignment is made externally with the centering devices for the whole cryostat–magnet assembly (Atoji, 1965). A miniaturized model of the one-arc one-rotor goniometer head (Davies & Mathieson, 1965) is also being designed.

* Work performed under the auspices of the U. S. Atomic Energy Commission.

Fig. 1. An exploded view of the miniature goniometer head.

Crystalllographers

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

Professor Alexandru Codarcea died on 29 May 1974. He was Professor of Mineralogy at the Department of Geology of the Institutul Politehnic ‘Gh. Gheorghiu-Dej’, Bucharest, and a member of the Academy of the Romanian Socialist Republic. He had been President of the Republican Commission of Geological Reserves.

Professor G. V. Raynor, Professor of Physical Metallurgy at the University of Birmingham, is now in South Africa, where he has taken up the appointment of Royal Society Leverhulme Visiting Professor in the University of Witwatersrand.

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