Computer Program


LAZY PULVERIX, a computer program, for calculating X-ray and neutron diffraction powder patterns.

By Klaus Yvon, Wolfgang Jeitschko* and Erwin Parthé. Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24 quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland

(Received 8 September 1976; accepted 23 September 1976)

A computer program has been written with the aim of calculating powder patterns without the use of crystallographic tables. This has been achieved by deriving all symmetry information such as general equivalent positions from the Hermann–Mauguin space-group symbols, by calculating automatically the multiplicities of special positions and by storing the necessary constants, such as scattering factor tables, anomalous dispersion correction terms and X-ray wavelengths in the program. Owing to the very restricted amount of input data this program is especially suited for users with a limited knowledge of crystallography.

Introduction

The comparison of powder patterns is a standard procedure in the characterization of solid-state materials. The calculation of powder patterns is therefore frequently desired. It is a crystallographic problem which contains pitfalls for people who are not familiar with crystallographic nomenclature or who are not accustomed to the use of International Tables for X-ray Crystallography. It was therefore desirable to develop a computer program that does not rely on this knowledge and which nevertheless gives reliable results.

The present program has been written with this aim. It calculates powder patterns from the strictest minimum of information necessary to correctly describe a crystal structure. This information includes the lattice parameters, the space-group symbol and the coordinates and chemical symbols of the atoms contained in one asymmetric unit. Access to these data is easy since they can be taken directly from handbooks and original articles or can be generated from computer files containing pertinent structural information such as the TYPiX file (Portheine, Yvon & Parthé, 1977). Further, distinct from other powder intensity programs (as for example the one by Clark, Smith & Johnson 1973), it is not necessary to use separate code-number tables for the notation of space groups and atom kinds.

All other parameters which are necessary to perform a powder-pattern calculation often require a certain minimum of crystallographic knowledge and are more burdensome to retrieve (for example the general equivalent point positions, the multiplicities of atoms in special positions, the Laue symmetry and the scattering factors with the proper corrections for anomalous dispersion).

The main advantage of the present program is the fact that it either contains these parameters or that it derives them automatically from the space group and element symbols.

The program also allows a graphical representation of the powder pattern to be printed to any desired resolution.

Outline of the program

LAZY PULVERIX consists of two programs which are run one after the other. The first routine LAZY reads the data cards and prepares the input for the second routine, PULVERIX, which is the main routine for calculating powder patterns.

LAZY derives the equipoints, the Laue-group, the conditions for systematically absent reflexions, the atomic form factors and the coefficients for anomalous dispersion. The Hermann–Mauguin symbol for the space groups is used to derive the general positions corresponding to the settings of International Tables for X-ray Crystallography with a routine written by Böhme, Burzlaff & Gomm (1975). If two settings are given for a particular space group in these tables the program generates the one with a centre of symmetry at the origin. In the case of monoclinic groups only space-group settings with b as the unique axis are accepted. All other settings, however, can be used by explicitly specifying the symmetry operators on data cards.

Scattering factors are approximated by the analytical function

\[ f(\sin \theta / \lambda) = \sum_{i=1}^{4} a_i \exp (-b_i \sin^2 \theta / \lambda^2) + c. \]

The coefficients \(a_i, b_i\) and \(c\) (International Tables for X-ray Crystallography, 1974, Table 2.2B) are called up by the program through the element symbols.

The values for the dispersion corrections (International Tables, 1974, Table 2.3.1), the coherent neutron scattering lengths (International Tables, 1974, Table 2.6) and the more frequently used wavelengths (International Tables, 1974, Tables 1.1A and 2.1A) are also accessible to the program.

Provisions are made to account for a variety of experimental techniques such as diffractometers, Debye–Scherrer and different Guinier cameras.

PULVERIX is an extended version of an unpublished routine (Yvon, Jeitschko & Parthé, 1969). It calculates the position of the diffraction lines from Bragg’s law and their \(d\) spacings. The reflections are then ordered into decreasing values of \(d\) spacing. The diffraction intensity \(I_{hkl}\) is calculated as

\[ I_{hkl} = MLPF^2_{hkl}, \]

where \(M\) = multiplicity factor of a powder line, \(L\) = Lorentz factor and \(P\) = polarization factor. The structure factor \(F_{hkl}\) is defined by

\[ F_{hkl} = \sum_{T} f_{O_j} \exp \left[ 2\pi i (h x_j + k y_j + l z_j) \right] \exp \left( -B_j \frac{\sin^2 \theta}{\lambda^2} \right) \]

where \(f_j\) = atomic or nuclear scattering factor of atom \(j\), \(O_j\) = occupation factor of site \(x_j, y_j, z_j\) for atom \(j\) and \(B_j\) = Debye–Waller factor in \(\text{Å}^2\) for atom \(j\).

Program output

The output of the program consists of a tabular listing of \(hkl\), \(d\) spacings, \(\theta\) values, structure factors and intensities. Several

* Present address: Institute for Inorganic and Analytical Chemistry, University of Giessen, West Germany.
output modifications are available which allow the printing of normalized intensities, \(1/d^2\) and \(\sin^2 \theta\) values. If anomalous dispersion corrections are made for non-centrosymmetric structures, the Friedel pairs are listed separately.

As a special option a graphical representation of the powder pattern is printed (Fig. 1) to any desired resolution. The reflexions are identified by their \(hkl\) values. In complex powder patterns, where several reflexions may fall within a small interval, the number of the reflexions within the resolution interval and the \(hkl\) value of the strongest reflexions will be given.

**Hardware and software requirements**

The program requires 35 K words of computer memory (Univac 1108: 36 bits per word) and two scratch units. It is written in USA Standard Fortran language. The prescriptions of the X-RAY system (1976) for 'Pidgin' Fortran have been followed to a great extent. Exceptions are logical and relational expressions (OR, AND and LT, EQ) and TYPE statements, which are frequently used but in such a way that they do not cause problems to Fortran compilers of most medium or large-size computers.

The input to \textit{LAZY PULVERIX} has been made compatible with that of the X-RAY system whenever this was possible. All cards are therefore recognized by alphabetic labels in the first columns and may appear in any order for a given calculation.

The program has been debugged and tested on a CDC 3800 computer and has run successfully on a UNIVAC 1108 and IBM 360 computer. It is available upon request.

We thank Professor H. Burzlaff for a copy of his routine which interprets space-group symbols and Professor A. Guinier for a discussion concerning different formulae for Lorentz factors. Dr D. T. Cromer and Dr J.-L. Staudenmann kindly supplied the coefficients for atomic scattering factors and the correction terms for anomalous dispersion on computer cards.

**References**


