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Fortran90 sources of the subroutines of *UMWEG*. II. The subroutines providing crystallographic data

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The Fortran90 sources of the subroutines of the program *UMWEG* providing the crystallographic data necessary for intensity calculations have been deposited in the IUCr electronic archives.

1. Introduction

To make further developments and improvements of the analysis in the field of kinematical multiple diffraction possible and easy, the Fortran90 sources of the program *UMWEG* (Rossmanith 2003, 2006*a*) are given in a series of papers. The subroutine *UPFORM* for the determination of dispersion corrections and scattering factors for free atoms and ions was discussed by Rossmanith (2006*b*).

In the present paper, the deposited Fortran90 sources providing the crystallographic data necessary for intensity calculations are briefly described.[1] These subroutines can be called by any crystallographic program needing the data given in the DATA statements. It is also possible to extract the DATA statements for programs having other purposes. These subroutines are therefore given separately.

The *UMWEG*-specific subroutines will be presented and deposited together with the PostScript-plot software subroutines and the simple and short main program of the command line version of the program *UMWEG* in a forthcoming paper. The main intention of this forthcoming paper will be to explain the crystallographic background of the *UMWEG*-specific subroutines and to point out possible further developments and improvements.

In the last paper of this series, the main program of the Windows version of *UMWEG* will be presented and deposited together with the thesaurus, *i.e.* with the input files for many examples.

2. The subroutines of *UMWEG* providing crystallographic data

The Fortran90 sources of the following five subroutines of the program *UMWEG* can be downloaded from the IUCr electronic archives.

[1] Supplementary data for this paper are available from the IUCr electronic archives (Reference: FE5012). Services for accessing these data are described at the back of the journal.

ABSOR1.F90. The subroutine provides the absorption correction factor A^* for spherical samples according to Weber (1969). Table 2 given by Weber (1969) is used with two corrections: for $\mu R = 9.3$ and $\theta = 80^\circ$ the value for $A^* = 16.28$ has to be replaced by 26.28, and for $\mu R = 9.8$ and $\theta = 65^\circ$ the value for $A^* = 43.87$ has to be replaced by 34.87 (private communication).

MUE.F90. The subroutine returns the linear absorption coefficient and the density for a given wavelength and cell volume, calculated according to paragraph 3.2.2 of *International Tables for X-ray Crystallography* [1962, Vol. III, expression (2)]. The subroutine is a modified version of a program developed by Werner (1993). The linear absorption coefficient obtained with this subroutine is used in *UMWEG* in cases where the dispersion correction is not known for the particular wavelength.

RAUMGR.F90. For a given space-group number, the subroutine returns the space-group symbol, the number of symmetry operators and the symmetry operators according to *International Tables for Crystallography* (2005, Vol. A).

UPFORM.F90. The Fortran90 source of the subroutine *UPFORM*, which provides dispersion corrections and scattering factors for all free atoms and ions in the range $0 \leq \sin\theta/\lambda \leq 6\ \text{Å}^{-1}$ has been deposited (Rossmanith, 2006*b*).

UPFORM_N.F90. The subroutine returns the atomic weights and the scattering lengths for neutrons.

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