International Union of Crystallography

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Commission on Journals

Submission of Manuscripts Based on Powder Diffraction Profile Fitting or Refinement (Rietveld) Methods: Deposition of Data

A steadily increasing number of manuscripts that depend on the use either of powder diffraction profile fitting or refinement (Rietveld) methods are being submitted for publication. Commission policy has recently required that figures in such manuscripts that present the experimental and calculated diffraction profiles of the material studied should also contain the difference profile ($I_{obs}-I_{calc}$), as an aid to the reader. It is recognized that the primary diffraction data cannot be extracted satisfactorily from such figures. The Commission has now decided that, in addition to the figure, the authors of such manuscripts should deposit the numerical intensity of each measured point on the profile, as a function of scattering angle.

The attention of authors is also drawn to notices concerning stereofigures [*Acta Cryst.* (1978), B**34**, 3846], dimensions of material for deposition [*Acta Cryst* (1979), B**35**, 792], estimated standard deviations, SI units and anisotropic thermal parameters [*Acta Cryst.* (1979), B**35**, 1302], submission of connected computer output [*Acta Cryst.* (1979), B**35**, 2284–2285], chemical-connectivity relationships [*Acta Cryst.* (1980), B**36**, 1524], and estimated standard deviations with a zero value for varied parameters [*Acta Cryst.* (1980), B**36**, 2508], in addition to the information given in *Notes for Authors* [*Acta Cryst.* (1978), A**34**, 143–157].

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Commission on Journals

Standards for the Publication of Powder Pattern Data

Standards for the publication of powder patterns, originally compiled by a subcommittee of the American Crystallographic Association and published in *National Bureau of Standards* Special *Publication* 567 (1979), have been accepted by the Commission on Crystallographic Data and the Commission on Journals. Papers that present powder pattern data submitted for publication in IUCr journals are now required to follow these standards.

The information requested by the standard data-form, a completed example of which is given in Table 1, must be given as compactly as possible. Essential information is requested by the bold-face headings. The remaining information sought is highly desirable, although it is recog-

Table 1. *Example of completed data form: powder diffraction data for phase characterization*

Data from Swanson, H. E. *et al.* (1971). *NBS Monograph* No. 25, Section 9, p. 25.

Bold-face items are considered essential.

Sample characterization

Name (chemical, mineral, Trivial) **Magnesium Aluminum Oxide (Spinel)**

Empirical formula $MgAl_2O_4$

Chemical analysis No x **Yes**

Source/preparation Synthetic; fusion of binary oxides

Chemical Abstracts Registry No. 12068-51-8 Pearson phase designation cF56

Other **Index of Refraction = 1·718 (Isotropic)**

Technique

Radiation type, source X-rays, Cu **λ value used** 1·54056 Å $K\alpha_1$

λ Discrim. (Filters, mono, *etc.*) **Diffracted beam, curved LiF mono**

λ Detector (Film, Scint., Position-sensitive, *etc.*) **Geiger**

Instrument description (Type, Slits, *etc.*) **17 cm vertical diffractometer**

Div 1° **Rec** 0·003″

Soller Yes **No.** 1 **Position** Inc. **Aperture** q = 1·2

Instrumental profile breadth 0·10 °2θ **Temp. (°C)** 25 ± 1

Specimen form/particle size Edge loaded powder/ < 10 μm particle size for *I*'s, packed for 2θ's

Range of 2θ from 5 °2θ **to** 165·0 °2θ **Specimen motion** None

Internal/External 2θ std (if any) Ag (internal) **Lattice parameter of 2θ std** 4·08641 Å

2θ error correction procedure Linear interpolation from nearest 2θ's of std

Intensity meas. technique Strip chart record (peak heights) **Error (~)** 5%

Peak x **Integrated**

Minimum intensity threshold (in relative intensity units) 0·3

Intensity std used α-Al_2O_3 *hkl*'s of intensity std 113

Intensity ratio I/I_C 1·70 (5) Conversion factor if corundum not used

Resolution (FWHM) for this material: 0·10°2θ at 59·37°2θ

2θ reproducibility for this material: ±0·02°2θ at All °2θ

Unit-cell data

Method of cell detn. Cell and structure known from Bragg (1915)

Cell refinement method Least-squares. See Appleman & Evans (1975)

a = 8·0831 (1) Å; b = ( ) Å; c = ( ) Å

α = (°); β = (°); γ = (°)

Z = 8; D_m = ( ) Mg m^{-3}; D_x = 3·578 Mg m^{-3}; V = 528·1 Å^3; Formula Wt. = 142·25

Crystal sys. Cubic Space group *Fd*3*m* [227] Crystal data index No. 8·0831

Figure of merit type F_N. See Smith & Snyder (1979) Value F_{29} = 58 (0·015, 33)

( ) indicates standard deviation in least significant digit(s).