International Union of Crystallography

J. Appl. Cryst. (1981). **14**, 216

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).

nized that some may not be available in all cases. Powder data corresponding to the information given in Table 1 are given, in the preferred form, in Table 2. Partial omission of the optional data will not preclude publication of the paper. Reprints of the complete standard, including copies of the blank data-form, are available from any Co-editor. Guidance in filling out the form is available from the JCPDS International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA.

Among the requirements for reporting powder diffraction data are:

(*a*) The published powder pattern should be as complete as possible and should include weak as well as strong diffraction lines. Where possible, the data should extend to at least 100° 2θ(Cu $K\alpha$ radiation). Patterns with a small number of lines should extend to the limit of the experimental method used.

(*b*) The experimentally observed 2θ values should be given in degrees, corrected for systematic instrumental error.

(*c*) Intensities should be reported numerically, with the most intense line scaled to 100 and intensities less than 1 reported as decimal fractions. Intensity values reported should not imply a precision greater than that measured.

(*d*) The reproducibility of the measured values of 2θ and I should be indicated, as obtained by multiple mountings of the sample material.

(*e*) Indexing of the powder diffraction data is required for all but the rarest and best-defended cases. Authors should report a figure of merit based on the accuracy of the 2θ measurements and the completeness of their data.

(*f*) Information concerning line breadth of the sample should be supplied.

(*g*) Additional information of value to future users should be supplied, such as the standard deviations, Chemical Abstracts Service Registry number, Crystal Data index number, *etc.*

To justify being published, powder diffraction data must constitute an original contribution to the literature. As an original contribution, the data must be the first published for a well-characterized phase, must be a significant correction to or an improvement on published data, or must relate to the phase in a previously uncharacterized condition, *e.g.* at elevated temperatures or pressure. A powder pattern calculated from single-crystal structure data does not in itself meet the criterion of originality.

Table 2. *Powder data*

Information in the first two columns is essential, that in the remaining three columns is desired (see text).

2θ exp (°)	I/I_0	d_{exp} (Å)	*hkl*	$\Delta 2\theta$* ( )
19·02	35	4·66	111	+0·019
31·27	40	2·858	220	−0·003
36·84	100	2·437	311	−0·009
38·53	3	2·335	222	−0·021
44·83	65	2·020	400	+0·016
55·64	9	1·650	422	−0·020
59·37	45	1·5554	511	+0·008
65·24	55	1·4289	440	−0·001
68·64	3	1·3662	531	+0·006
74·13	3	1·2780	620	+0·003
77·32	8	1·2330	533	−0·029
78·40	1	1·2187	622	−0·013
82·64	5	1·1666	444	+0·006
85·76	2	1·1320	711	−0·012
90·97	5	1·0802	642	−0·009
94·10	12	1·0524	731	−0·005
99·34	7	1·0104	800	−0·006
107·90	2	0·9527	822	−0·020
111·22	8	0·93343	751	−0·014
112·32	1	0·92738	662	−0·035
116·91	6	0·90384	840	−0·025
120·50	1	0·88722	911	+0·004
121·69	0·9	0·88203	842	−0·021
126·76	0·8	0·86161	664	+0·013
130·74	8	0·84737	931	−0·011
138·07	17	0·82488	844	+0·033
142·97	0·4	0·81232	933	+0·024
152·70	2	0·79266	10,2,0	−0·033
160·65	11	0·78139	951	+0·025

*$2\theta_{exp}-2\theta_{calc}$

References

Appleman, D. E. & Evans, H. T. (1973). NTIS Document No. PB-216188.

Bragg, W. H. (1915). *Nature (London)*, **95**, 561.

Smith, G. S. & Snyder, R. L. (1979). *J. Appl. Cryst.* **12**, 60.

Communicated Abstracts

Twelfth International Congress of Crystallography, Carleton University, Ottawa 16–25 August 1981

The abstracts of papers communicated to the Congress will be published as a Supplement to *Acta Crystallographica*, Section A. The Supplement will contain abstracts directly reproduced from typescript copy furnished by the authors. Copies will be sent *gratis* to subscribers to Section A, but not to subscribers to Section B or to *Journal of Applied Crystallography*. However, copies may be ordered direct from the publishers, Munksgaard, 35 Nørre Søgade, DK-1370 Copenhagen K, Denmark, at a price of 170 Danish kroner.

Crystallographers

Dr **S. C. Abrahams**, of Bell Laboratories, Murray Hill, and Editor of *Acta Crystallographica*, will receive the degree of Doctor of Philosophy *honoris causa* from the University of Uppsala at a ceremony on 5 June 1981.

Professor **D. A. Bekoe,** Vice-Chancellor of the University of Ghana, was elected President of the International Council of Scientific Unions in September 1980. He had previously served as Treasurer and then Vice-President of the International Council of Scientific Unions.

Professor **Dorothy Hodgkin**, formerly head of the Laboratory of Chemical Crystallography at the University of Oxford, has been elected a foreign member of the Bayerische Akademie der Wissenschaften, where **Max von Laue** presented his well-known paper on the discovery of X-ray diffraction. Professor Hodgkin is the first lady to be so elected to the Akademie.

Dr **B. A. Joyce**, Philips Research Laboratories, Redhill, England, has been awarded the Duddell Medal and Prize of the Institute of Physics for his work on the growth of epitaxial semiconductor materials and related surfaces.

Professor **H. Lipson,** who was Professor of Physics at the University of Manchester Institute of Science and Technology until his retirement in 1977, will give the fifth Bragg Lecture at the Royal Institution, London, and at the University of Leeds on 28 and 29 October 1981. Professor **M. M. Woolfson**, of the Department of Physics at the University of York, will give the sixth Bragg Lecture in Manchester and Cambridge in October 1982. The Bragg Lectures were initiated in 1962 to commemorate the work of Sir **William** and Sir **Lawrence Bragg.** Previous lecturers were Professor **P. P. Ewald** (1962), Dame **Kathleen Lonsdale** (1965), Professor **Dorothy Hodgkin** (1968) and Professor **R. W. G. Wyckoff** (1973).

Dr **M. Schlenker,** Director of Laboratoire Louis Néel, CNRS, Grenoble, has been