Powder Diffraction notes for authors

I. SCOPE

Powder Diffraction is a quarterly journal publishing articles, both experimental and theoretical, on the use of powder diffraction and related techniques for the characterization of crystalline materials. It is published by Cambridge University Press (CUP) for the International Centre for Diffraction Data (ICDD).

II. CATEGORIES OF MANUSCRIPTS

Publications in *Powder Diffraction* should fall under one of the following categories:

(1) *Review Articles* may be voluntary or solicited and are intended to be an authoritative presentation of a significant subject in powder diffraction analysis. The material should be comprehensive, and the historical influence on the topic should be emphasized along with modern enhancements. A complete literature search is an important part of review articles.

(2) *Technical Articles* on original research may be either experimental or theoretical studies revealing new information on the applications of powder diffraction and related techniques for the characterization of materials. Topics may include, but are not limited to, qualitative and quantitative phase analysis, characterization of new materials, characterization of thin films, diffraction measurements coupled with computer analyses, instrumental techniques, assessment of precision and accuracy in data processing, indexing of powder data, crystal-structure determination or refinement of powder data, residual stress analysis, and microstructural measurements such as those for preferred orientation, crystallite size, microstrain and microstructure defects.

(3) *New Diffraction Data* are short articles which present powder diffraction patterns and associated experimental documentation on crystalline materials of interest to science and industry. The scientific and materials significance of the compounds should be described, and the documentation should follow the guidelines presented in section V (Manuscript Preparation) below.

(4) *Rapid Communications* are short articles on original research, usually limited to two printed pages of about 1000 words. They may include the same topics as in section (2), but are designed for rapid processing and publication. These may also include descriptions of new computer programs.

(5) *Laboratory Notes* are short articles on new techniques of diffraction analysis or modifications of equipment implemented in specific laboratories or for specific materials. They are usually limited to two printed pages of about 1000 words.

(6) *Crystallography Education* provides tutorial and instructional articles related to powder diffraction crystallography. The creation of educational materials about crystallography not found in books or manuals is encouraged. This section will publish invited and contributed articles, and will be subjected to the normal editing process before publication.

(7) *Letters to the Editor* is a forum for individuals to discuss material printed in *Powder Diffraction*. A letter will be reviewed by the editor-in-chief, who will suggest changes in presentation, if appropriate. A letter that refers to a specific publication will be sent to the author(s) of the article under discussion for a reply. Usually, the letter and the reply (if available) will appear in the same issue.

(8) *Erratum* is a forum to be used by the author to submit corrections to published papers in *Powder Diffraction*.

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(9) *International Reports* is a section of *Powder Diffraction* devoted to disseminating current information on activities of interest to the powder diffraction community. Submissions are solicited from anyone with appropriate information. Topics of interest include announcements, reviews of meetings, book reviews, educational activities, people working in the field of powder diffraction, especially their awards and honors, activities of any organization worldwide which pertain to powder diffraction, and very short descriptions of new products.

(10) *Calendar of Meetings and short Courses and Workshops* is a section listing meetings and workshops of interest to the powder diffraction community. Please do not use ScholarOne to submit a calendar notice. Please send notices by e-mail to the Calendar of Meetings and Workshops Editor (gangwang@ aphy.iphy.ac.cn).

III. SUBMISSION OF MANUSCRIPTS

All manuscripts must be submitted to ScholarOne online at http://mc.manuscriptcentral.com/pdj. This web-based manuscript submission and peer review system is hosted by Thomson Reuters on behalf of Cambridge University Press. ScholarOne is an editorial management service that provides electronic processing of manuscripts from author submission to manuscript review, revision, and final approval. Review the online submission guidelines and tutorials available at http://mchelp.manuscriptcentral.com/gethelpnow/training/author/before submitting your paper. Additional assistance is available from http://mc.manuscriptcentral.com/pdj under "Resources" in red at the top right corner of the screen.

Submission of a manuscript is considered an implicit guarantee that the paper has not been published previously in any language or concurrently submitted for publication to another journal. You will be asked to confirm this during submission. If accepted for publication in *Powder Diffraction*, a signed publishing agreement transferring full-term copyright to ICDD will be required. The copyright form is located at http://www.icdd.com/resources/pdj/authors.htm. You may mail, fax, or e-mail the signed agreement to the attention of the managing editor at:

Nicole M. Ernst Boris
Managing Editor, *Powder Diffraction*
12 Campus Blvd.
Newtown Square, PA 19073
Phone: 610-325-9814
Fax: 610-325-9823
E-mail: boris@icdd.com

IV. REVIEW OF SUBMISSIONS

Acceptance of manuscripts for publication is the responsibility of the editor-in-chief. Manuscripts are usually reviewed by two qualified individuals selected by an assigned editor. Referees will be asked to certify the appropriateness of the subject matter for *Powder Diffraction* and to comment on the technical merit and presentation of the article. Authors, not reviewers, are responsible for preparing the manuscript in readable English. Manuscripts too difficult to read will be returned to the authors without review.

The review process will be conducted anonymously unless a reviewer specifically instructs the editor to reveal his or her identity. Authors may request anonymity by selecting the appropriate option during submission and by preparing the manuscript so that the file and the paper itself do not identify the author(s). Authors may also suggest a specific individual to act as reviewer or indicate an individual who they do not want to review the paper. The author submitting the manuscript will be considered the corresponding author.

The review process will result either in acceptance of the manuscript, suggested modifications of the text prior to acceptance, or rejection of the manuscript. In cases where reviewers differ significantly in their evaluation of a paper, the editor may request a third review. When changes are required, the manuscript will be returned to the corresponding author for revision. If manuscripts returned to the author are not resubmitted within a reasonable time, the manuscript will be considered withdrawn, and a subsequent submission will be treated as a new article. All changes should be accompanied by a separate document/file detailing the responses to the reviewer's recommendations. Manuscripts which require major changes may be sent to the reviewers for their acceptance of the changes. When the assigned editor feels the paper is ready for publication, he or she will send the paper to the editor-in-chief for a final decision on publication. When the manuscript has been accepted for publication in *Powder Diffraction*, the author will be informed, and the manuscript will be passed on to the publisher. Rejected manuscripts will be returned to the author with comments and reasons for rejection.

Processing dates published with the manuscript will include the date the manuscript was submitted (received date) and the date of acceptance by the editor-in-chief (accepted date). The date of acceptance may be delayed until all requested revisions, figures, or other parts of the paper are received.

V. MANUSCRIPT PREPARATION

For categories (1) to (6) manuscripts, follow these manuscript preparation instructions.

Manuscripts must be written in English and will be published in English. Authors are expected to follow conventional writing, notation, and illustration style as prescribed in these notes. It is suggested that authors also examine the style of the appropriate article type as presented in a recent issue of *Powder Diffraction* and the CUP style guide located at: www.cambridge.org/us/notesforauthors/cambridge_style.doc. Abbreviations, symbols, and units should correspond with suggestions in these notes and examples of previous articles. It is strongly suggested that authors have a co-author or colleague not primarly responsible for the writing to review the manuscript before submission.

A. Text of paper

1. Abstract

An abstract must accompany all articles. The abstract should be double-spaced on the first page, separate from the rest of the manuscript. An abstract is a self-contained, brief summary of a paper. It is used to communicate complex research and findings efficiently. Because online search databases contain abstracts only, it is vital to write a complete, but concise, description of your work to encourage others into obtaining a copy of the full paper. The decision to read the entire paper is often predicated on what the reader finds in the abstract. An abstract is the most widely read portion of the paper; a well written abstract is often an indication that the entire paper meets the criteria and standards of a good scientific report.

Write the abstract after you have finished writing the entire paper, not before. One paragraph maximum or even two or three sentences are optimum lengths. However, the length depends upon the complexity of the subject matter. Fewer than 200 words are usually sufficient. Short papers like rapid communications, laboratory notes, and letters to the editor may have one-sentence abstracts, in which case the sole sentence would be the purpose of the paper.

The reader is looking for the purpose of the experiment, the plan, the most important findings, and conclusion, but the abstract must avoid anything not confirmed in the paper. The first sentence must state what you did in your experiment or the purpose of the paper; it must not be an introduction to a subject or a problem (as it does not tell the reader what was done or accomplished in your experiment); example of an appropriate first sentence: "Time-resolved synchrotron powder diffraction was used to follow the

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thermal transformation of cement-asbestos." The next sentences should give the principal results. Background information relating to why the study was done may be included; otherwise such information belongs in the introduction section. Experimental details, including instrumentation and parameters, should be in the experimental section of the paper. Because an abstract must stand alone from the rest of the paper, do not refer to equations, figures, tables, or cited sources. It is, however, the correct place to use abbreviations used later in the body of the paper.

2. Key words

Include a set of no note than six key words/terms below the abstract (on same page); not required for letters to the editor, erratum, contributions to international reports or to the calendar. Select the terms carefully as these will help researchers and readers locate your article during bibliographic searching and indexing. All words in the list should be lowercase (except proper names and chemical formulas) and separated by commas.

3. General format

The rest of the paper should include the usual sections appropriate for such a paper, including, but not limited to, an introduction, experimental, results and discussion, and conclusion section. Sections must be numbered as shown in Figure 1.

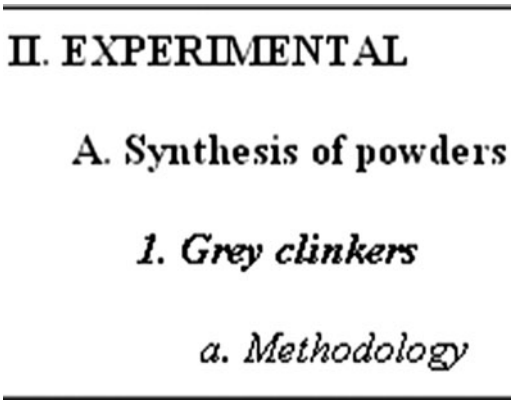

Figure 1. Levels of Section headings.

Shorter papers like rapid communications, laboratory notes, and letters to the editor may not have sections. Other notes about section headings are as follows:

- References and footnotes are not allowed in headings
- Rename any headers named CONCLUSIONS to CONCLUSION
- If acknowledging only one person or place the heading is left singular (ACKNOWLEDGMENT); if acknowledging more than one, it should be plural (ACKNOWLEDGMENTS)
- Do not number the acknowledgment(s) heading

Double space the text and number the sections as seen in this document. Use 12-point size Times or Times New Roman font; if special symbols or Greek letters are used, avoid using nonstandard fonts as this may lead to errors in transmission and conversion.

4. Style

Proper style according to the points below and the examples in Table I should be used. Be consistent throughout the paper. For more information please refer to the Cambridge University Press Style Guide: www.cambridge.org/us/notesforauthors/cambridge_style.doc.

Acronyms do not need to be defined, especially common ones like XRD. It is not necessary to change appropriate text throughout to its acronym, unless such presentation is distracting (like the text is too long).

Italics are used to denote text in foreign languages, variables in equations, and to distinguish between elements and non elements. Greek letters and foreign words, including species names in Latin, should be in italics. *Ab initio*, *in situ*, *in vitro*, *in vivo*, *ibid.*, and *et al.* should be in italics, but e.g., etc., i.e., viz., and vs. are not in italics. Single letter variables should be in italics ($x = 50$, not x = 50); *hkl* should be in italics. Letters in space groups should be in italics, but not numbers ($P2_1/c$). Use of letters to denote a series of elements or something other than an element should in general be in italics. This is important as some authors like to use the letter B to denote something other than boron. Letters A, M, and R are also frequently used to denote a series of elements (note that these letters are not assigned in the periodic table). For example, consider $A_2BV_3O_{11}$ (A = Mg, Zn and B = Ga, Fe, Cr)—letter A is not an assigned letter in the periodic table and letter B does not refer to boron. Cu$K\alpha$ is written as such because letter K does not refer to potassium and α is a Greek letter.

Figure and table should be spelled out, but not Equation (Eq.). Space group should not be abbreviated SG.

Pay special attention to the presentation of units of measure. These, if preceded by a number, should be abbreviated. There should be a space between the number and units (10 mm, not 10mm), except for the percent sign (22%) and degrees sign without Celsius of Fahrenheit (84°). Do not repeat the units if only a word separates two numbers of the same unit (10 and 14 mm, not 10 mm and 14 mm). Variables and their units in table column headings or figure axis labels should be written like x (%), not $x/\%$.

TABLE I. Examples of style errors corrected.

Not acceptable	Acceptable
β	β
Homo sapiens	*Homo sapiens*
Fm***	*Fm****
I_{obs}	I_{obs}
B_{iso}	B_{iso}
R_p	R_p
$NdMMgMn_2O_6$ (M = Li,Na,K,Cs)	$NdMMgMn_2O_6$ (M = Li,Na,K,Cs)
CuKα	Cu $K\alpha$
Fig. 1a	Figure 1(a)
Figures 1a, b	Figures 1(a) and 1(b)
Table 1	Table I
S.G.	space group
60 hours	60 h
600°C	600 °C
3GPa	3 GPa
22 %	22%
84 °	84°
14.842(4)Å	14.842(4) Å
V/Å^3	V (Å^3)
Melting point/°C	Melting point (°C)
between 2–6 mm	between 2 and 6 mm
from 8°C-10°C	from 8 to 10 °C
Equations 2–5	Eqs. (2)–(5)
(see Eq. (2))	[see Eq. (2)]

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A hyphen/minus (−) or en dash (–) should not be used to denote a range in running text; for example use between *x* and *y*, not between *x*–y; use from *x* to *y*, not from *x*–y; using an en dash is acceptable for dates, to denote a range of figures, tables, or equations, or when space is an issue like in table columns. Note that when a dash is to be used to denote a range, use en dash (–) not hyphen/minus (−).

The exact symbol or special character must be used—correct any substitutions. For example, authors will commonly superscript small letter o to mimic the degrees symbol. This is unacceptable—the real degrees symbol must be used. See Table II for examples. Since it is difficult to see the difference in many cases, it's suggested that anytime you come across a special character, insert the proper symbol as if the original were incorrect.

TABLE II. Misuse of simple characters as substitution for special characters corrected.

Not acceptable	Acceptable
°C [using superscript letter o for degrees]	°C
um [substituting letter u for Greek letter mu]	μm
x [using letter x for multiplication or dimensions]	×
≤ [underlining < for less-than or equal to]	≤
e [using small letter e without the acute]	é

5. Mathematics

Mathematical expressions introduced in your paper must be on a separate line and numbered:

$$\text{[Equation]} \tag{1}$$

$$\text{[Equation in appendix]} \tag{A1}$$

Do not use mathematical derivations when they are easily located elsewhere in the literature, but merely cite the appropriate reference(s).

6. Acknowledgement(s)

If you wish to acknowledge specific people, state their affiliation. Do not just state their name; an affiliation will help identify the acknowledged if unknown to the reader. Do not acknowledge reviewers or the staff of this journal. Place the acknowledgements section after the running text but before the references, and do not number the section with a Roman numeral.

B. References

References must be cited in text using the author's last name and year of publication (do not use the numerical format). For example, a reference with one author would be cited in text like this: (de Wolff, 1968); with two authors: (Smith and Snyder, 1979); with three or more authors: (McMurdie *et al.*, 1986). Use a semicolon (;) to separate multiple references in the same sentence: (de Wolff, 1968; Smith and Snyder, 1979; McMurdie *et al.*, 1986). If you mention the authors name as part of the sentence, then only the year is in parenthesis: McMurdie *et al.* (1986).

In referring to two or more of the same author's works published in the same year, distinguish between them in text and in the references list with a lowercase letter after the year (2000a, 2000b, 2000c…). This is important so the reader knows exactly which citation is being referenced. The citation noted as "a" is the one that comes before "b" in the references list in proper order—it is not necessarily the first one cited in text.

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References must include the names of all authors, the title of any journal or book article and must be listed alphabetically by the last name of the first author in a separate section at the end of the text. The order of presentation generally should be author(s)' last names, including the initials of given names, year of publication, article title, journal, volume, and inclusive pages. Examples of citations in proper format follow. More can be found at: http://www.icdd.com/resources/pdj/Commonly%20Cited%20Sources.doc

1. Journal article

Shannon, R. D. (**1976**). "Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides," Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Gen. Crystallogr. **32**, 751–767.

Shannon, R. D. (**1976**). "Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides," Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Gen. Crystallogr. **32**, (In press).

Shannon, R. D. (Submitted). "Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides," Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Gen. Crystallogr.

Shannon, R. D. (In progress). "Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides," Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Gen. Crystallogr.

2. Book

Buhrke, V. E., Jenkins, R., and Smith, D. K. (Eds.) (**1998**). *A Practical Guide for the Preparation of Specimens for X-ray Fluorescence and X-ray Diffraction Analysis* (Wiley, New York).

Klug, H. P. and Alexander, L. E. (**1974**). *X-ray Diffraction Procedures for Polycrystalline and Amorphous Materials* (Wiley, New York), 2nd ed., p. 966.

3. Selection from an anthology

Snyder, R. and Bish, D. L. (**1989**). "Quantitative analysis by X-ray powder diffraction," in *Modern Powder Diffraction*, edited by D. L. Bish and J. E. Post (Mineralogical Society of America, Washington), Vol. 20, pp. 101–144.

4. Report

Larson, A. C. and Von Dreele, R. B. (**2000**). *General Structure Analysis System (GSAS)* (Report LAUR 86-748). Los Alamos, New Mexico: Los Alamos National Laboratory.

5. Computer program

Coelho, A. A. (**2007**). TOPAS-Academic, version 4.1 (Computer Software), Coelho Software, Brisbane.

A list of notable and commonly referred to citations is located at http://www.icdd.com/resources/pdj/authors.htm. A few references also appear at the end of this document.

6. Databases and Powder Diffraction File

The format for citing a database is as follows:
First, A. A. (**Year**). Name of database (Database), Company Name
City, State, Country.
First, A. A. and Second, B. B. (**Year**). Name of database (Database), Company Name
City, State, Country.
Company as author (**Year**). Name of database (Database), edited by A. A. First, City, State, Country.

When referring to Powder Diffraction File (PDF) numbers please refer to the source in text as "PDF XX-XXX-XXXX (ICDD, Year)".

To cite the PDF Data Book, follow the format for citing a book. For example, cite the Data Book issued in 2010 as follows:

ICDD (**2010**). *Powder Diffraction File Inorganic and Organic Data Book*, edited by Dr. Soorya Kabekkodu (International Centre for Diffraction Data, Newtown Square, PA USA), Set 60.

To cite the PDF relational databases, follow the format for citing a database. For example, cite the PDF-4/Organics 2011 database released in 2010 as follows:

ICDD (**2010**). PDF-4/Organics 2011 (Database), edited by Dr. Soorya Kabekkodu, International Centre for Diffraction Data, Newtown Square, PA, USA.

Please cite the PDF-4+ 2010 database as follows:

ICDD (**2010**). PDF-4+ 2010 (Database), edited by Dr. Soorya Kabekkodu, International Centre for Diffraction Data, Newtown Square, PA, USA

For questions regarding citing PDF products in *Powder Diffraction*, please contact the managing editor, Nicole M. Ernst Boris (boris@icdd.com) or 610-325-9814.

C. Tables

Extensive numerical material should be presented in tables rather than in the body of the text. Each table should be numbered with a Roman numeral (I, II, III. . .) and produced at the end of the running text (after references). Each table must have a caption that makes the data in the table intelligible without reference to the text. Avoid complicated column headings. If necessary, use symbols that are explained in the caption or in the table footnotes. Place the caption above the table, and single space the table and caption (do not double space). Each table should be listed under the heading "Tables" after the references list.

D. Figures

Figures published in the journal are received electronically from the author, and integrated with the text of the article, creating completely electronic pages. Please adhere to the following guidelines when preparing your illustrations so that the files are of production quality.

Figure files must be in encapsulated postscript (EPS) or tagged image file (Tif/Tiff). No other format is acceptable, including JPEG, JPG, GIF, PDF or application files such as Corel Draw. Images embedded in word processor files cannot be accepted. Please see http://dx.sheridan.com/guidelines/digital_art.html for more information.

Create illustrations using these settings:

Line artwork
Format: tif or eps
Colour mode: black and white (also known as 1-bit)
Resolution: 1200 dpi

Combination artwork (line/tone)
Format: tif or eps
Colour mode: grayscale (also known as 8-bit)
Resolution: 800 dpi

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Black and white halftone artwork
Format: tif
Colour mode: grayscale (also known as 8-bit)
Resolution: 300 dpi

Colour halftone artwork
Format: tif
Colour mode: CMYK colour
Resolution: 300 dpi

Make sure there is one figure per file. Each figure file should include all parts of the figure but without figure caption. For example, if Figure 1 contains three parts [(a), (b), (c)], then all of the parts should be combined in a single file for Figure 1. The parts should be label as such. The captions of all figures should be listed together in a separate page after the tables. When submitting your paper, do not embed the figures with the text of the paper inside the word processor file. Upload the individual figure files as noted in the submission guide.

E. Supplemental Data

Supplemental data should be submitted via ScholarOne along with your manuscript and figure files. CUP will assign one digital object identifier (DOI) to the published article. Supplemental material now gets deposited and linked with the DOI for the article, allowing easier access to all material by one click of the mouse. These data are also deposited with ICDD and are subject to the same copyright laws as the manuscript.

Please note that the supplemental data of the digital form of each experimental diffraction pattern used in a new-diffraction-data paper are now required to be submitted via ScholarOne along with its article and figure files. Submission of the supplemental data of each digital observed XRD pattern used in a crystal-structure article is also encouraged.

To submit supplemental data, simply choose "Supplementary Material (online publication only) when uploading those files. It is recommended to use of common file types, such as .DOC and .PDF, to provide simplistic retrieval. Once the manuscript is approved, all files are forwarded by the managing editor to CUP.

For assistance or questions regarding supplemental data, please contact the managing editor at boris@icdd.com.

For technical assistance, please use the 'Get Help Now' link on your ScholarOne Manuscripts site to submit a support case or follow this link: http://mchelp.manuscriptcentral.com/gethelpnow/question.htm.

VI. PROOFS

A. Process

Page proofs of articles will be sent by CUP directly to the corresponding author by e-mail. Notification may take several weeks after the paper is received by CUP. All corrections, revisions, and additions must be communicated by a single e-mail reply. The proof should be checked with the utmost care, especially tables, equations, formulas, and symbols. Check the last page of the proof for notes and requests from CUP. Ultimate responsibility for detecting errors resides with the author. Proofs should be done in a timely manner so that there will be no production delays.

B. Free color figures online

If authors supply usable color graphics files in time for the production process, color will appear in the online journal free of charge. Usable color graphics files must be created by the authors as described above. Figures will continue to appear in black and white in the print version with a notation "(Color online)" in the caption to alert readers that color is available online.

Authors may not submit two versions of the same illustration (for example, one in color and another in black and white). When preparing illustrations that will appear in color in the online journal and in black and white in the printed journal, authors must ensure that colors chosen will reproduce well when printed in black and white, and descriptions of figures in text and captions will be sufficiently clear for both print and online versions. This is the author's responsibility.

If color figures submitted are of acceptable quality, authors will see color versions of those illustrations when viewing their author proofs. At the proof stage and if not already included, authors must insert the phrase "(Color online)" into the captions of color figures. Authors can simply state in the reply e-mail which figures are color online, but this must be done by the author (color online notation may also be included in the figure caption prior to submission). Example of an amended figure caption: Figure 10. (Color online) Experimental (dotted curve) and simulated (solid curve) X-ray diffraction spectra.

VII. NOMENCLATURE

In general, the nomenclature should conform to recommendations established by the appropriate international body. Crystallographic nomenclature should follow the recommendations of the International Union of Crystallography (IUCr). The naming of compounds should conform to the recommendations of the International Union of Pure and Applied Chemistry (IUPAC), International Union of Biochemistry (IUB), or other appropriate bodies. Mineral names should conform to the recommendations of the International Mineralogical Association (IMA). Any accepted trivial name, trademark, recommended International Non-Proprietary Name, United States Adopted Name, or British Pharmacopoeia Approved Name may be retained, but the corresponding systematic IUPAC name should always be provided. For complex organic compounds, a figure containing the structural formula of the molecule(s) is recommended. Nomenclature for X-ray emission lines is in a state of transition. For new compounds, the author should obtain the CAS (Chemical Abstract Service) number assigned to that compound.

VIII. DATA PRESENTATION AND DOCUMENTATION

For papers that include powder diffraction data, follow these guidelines.

A. Introduction

The introduction section should discuss the reasons for scientific or industrial interest in the crystalline phase(s). It should note any existing powder diffraction patterns, especially those in the PDF. A figure showing a structural formula is requested for all but the simplest organic molecules in a phase.

B. Experimental methods

1. Sample

If synthesized, describe procedure; include any specimen pre-treatment. If a mineral, give locality and any associated minerals and physical description (color, hardness, optical data, etc.).

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2. Specimen preparation

Describe the procedure used for powdering the specimen (mortar and pestle grinding, filing for metals followed by annealing, etc.), and give an indication of grain size. Note the type of specimen [smear on glass slide; front-loaded pressed powder; side-drifted in Al well (McMurdie *et al.*, 1986)].

3. Standard

Indicate whether external or internal. Give name and origin of standard. Give unit-cell parameter(s) used in calibrations to full precision. For quantitative analyses using an internal standard, give details of the amount of internal standard added and the method used to ensure total mixing of the sample with the internal standard.

4. Data collection

Include the following information:

1. Radiation and values of wavelength(s) used in angle-to-*d* conversions; *Powder Diffraction* now uses 1.5406 Å (or 0.15406 nm) for Cu $K\alpha_1$ radiation for all purposes, except when the author makes a case for the use of an alternate value.
2. Instrument power: kV, mA.
3. Mean temperature of measurement.
4. For diffractometer data, providing the name and model of the instrument is encouraged because of the information this conveys to knowledgeable readers about instrument resolution, sensitivity, etc.
5. Theta compensating slit? If so, equivalent fixed-slit *I*s must be reported.
6. Filter or monochromator—diffracted beam or incident beam.
7. 2θ scan range.
8. If an automated powder diffractometer was used, give step size and count time at each step, and note whether smoothing or α_2 stripping was performed (it is important to report whether α_2 stripping was done, because relative intensities will differ markedly from the intensities where stripping has not been done).
9. Camera data: diameter and other camera particulars; incident beam monochromator or filter; shrinkage and absorption corrections performed.

5. Data reduction

Include the following information:

1. Peak finding program, peak finding method, or both.
2. Least-squares refinement program used and other particulars on the refinement.
3. Source of initial cell (crystallographic database, single-crystal technique, etc.) or indexing program [give programs and FOMs of indexing, for example F_N (Smith and Snyder, 1979) and M_{20} (de Wolff, 1960)].

C. Results and discussion

A figure with a complete diffraction pattern, or a selected range, is desirable in many papers, because of the information conveyed in the profiles that is lost during numerical data reduction. The ICDD is now archiving digital diffraction patterns for possible future publication as a supplement to the numerical PDF entry. With the knowledge of the instrument and data reduction given in the manuscript, the ICDD will be able to convert most file formats into archival format.

In most articles, especially those for new diffraction data, a table for powder diffraction data should be included. The data columns listed in the table are: $2\theta_{obs}$, d_{obs}, I_{obs}, (hkl), $2\theta_{cal}$, d_{cal}, I_{cal} and $\Delta 2\theta$ (i.e., $2\theta_{obs}$ - $2\theta_{cal}$). Values of $2\theta_{obs}$, d_{obs} and I_{obs} are determined from the experimental diffraction pattern, while values of $2\theta_{cal}$, d_{cal} and I_{cal} are calculated from refined unit-cell parameters and Miller indices

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(hkl). The I_{calc} column can be omitted if calculated intensities are unavailable. The submitted powder diffraction data will be checked by an editorial and database building code known as SQLAIDS. When this program indicates problems with the powder data, authors will be provided with a copy of the program output.

The angle 2θ is the preferred entry to the computer database, and from it d_{obs} will be calculated from the wavelength value given for the X-ray source. The 2θ reported are the values after correction for systematic errors, providing the d_{obs} data used in the least-squares refinement permits an additional editorial check. Note: authors should be aware of a small systematic error in some computer peak-finding programs where the α doublet is not resolved. By converting to d with a single wavelength (either α or α_1), a systematic error is introduced. Because SQLAIDS uses only one wavelength, all peak 2θ positions read as α values should be converted to the α_1 values corresponding to d_{obs} in the submitted data table. Note that this problem is eliminated when α_2 stripping is performed and all angle-to-d conversions are done with a single wavelength.

Crystal data for the refined unit-cell parameters [unit-cell parameters with estimated standard errors, space group, formula units/unit cell (Z), and calculated density (ρ_x)] may be included in the abstract without repetition in the text. F_N (Smith and Snyder, 1979) and/or M_{20} (de Wolff, 1960) should be included too.

The corundum reference intensity ratio (I/I_c) is a desirable component of a powder diffraction data article, because it is useful for semi-quantitative estimation of the amounts of phases in mixtures. The computer pattern modeling code POWD by Smith *et al.* (1983) provides a calculated I/I_c, which can be included for comparison to the observed value.

In the case that the powder pattern for the phase has been previously published in the literature, in the PDF, or both, a discussion of the improvements provided by the new powder pattern should be given.

Here are a few preferred terms for powder diffraction pattern papers: *sample* for the aliquot of the phase before grinding, *specimen* for the material placed in the diffractometer or camera, *reflection* when referring to a Bragg reflection with a specific (*hkl*), *peak* when referring to a peak in a diffraction pattern, which may consist of several overlapped, but not resolved, reflections, and *unit-cell parameters* instead of lattice constants or lattice parameters.

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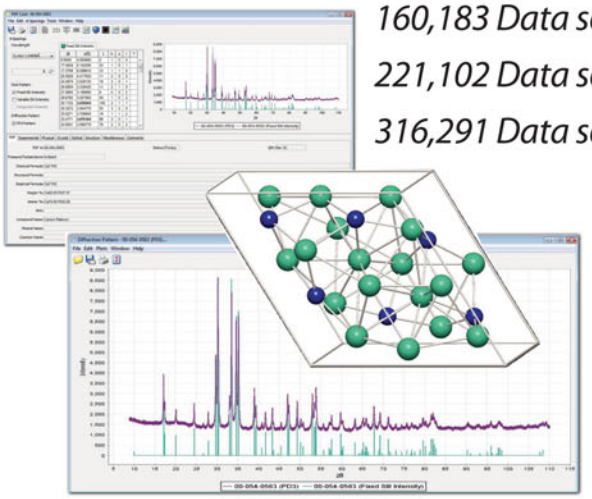

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