

International Union of Crystallography

Acta Crystallographica Section D

Notes for Authors

1. Scientific scope of Section D

Section D of *Acta Crystallographica* welcomes the submission of papers covering any aspect of biological crystallography, particularly structures of biological macromolecules. In addition to new structural determinations, preliminary data on unit-cell dimensions and space groups will be considered for publication, provided suitable diffraction photographs (or their equivalent), together with an estimate of resolution, are included. Also, articles on crystal growth of biological macromolecules are welcomed, and refinements of known structures may be published if the information content warrants it. For all structural papers, sufficient evidence should be provided to convince the referees that the interpretations of the diffraction data and electron-density maps are correct, within the resolution of the analysis.

2. Categories of contributions

2.1. Research Papers

Full-length *Research Papers* should not normally exceed 15 journal pages (about 15 000 words or 60 double-spaced manuscript pages). They should be submitted to one of the **Co-editors**.

2.2. Short Communications

Short Communications are intended for the presentation of topics of limited scope, or for preliminary announcements of novel research findings. They are not intended for interim reports of work in progress, and must report results that are of scientific value in their own right.

Short Communications must not exceed two journal pages (about 1500 words or six double-spaced manuscript pages). A maximum of two figures and two tables of appropriate size are permitted. Figures should be clearly lettered. If the paper is available on diskette, this should be sent with the manuscript, together with details of the word-processing package used (see §3.4); complicated tables should be submitted as camera-ready copy.

All *Short Communications* should be submitted to the **Section Editor**. They will be refereed rapidly and printed as quickly as possible, using desktop publishing methods or prioritized typesetting.

2.3. Lead Articles

Lead Articles are authoritative, comprehensive and forward-looking reviews of major areas of research interest. They are always **commissioned by the Section Editor**, on the advice of the Editorial Board. Suggestions for suitable topics and of potential author(s) are welcomed by the Section Editor for discussion with the Board.

The Editor will discuss the treatment of the topic, the length of the *Article* and the delivery date of the manuscript with invited author(s); completed manuscripts will be refereed in the normal manner. *Lead Articles* will be highlighted on the cover of the relevant issue, clearly identified within the journal and will carry brief biographical details of their author(s), which should be provided by the author(s) on submission of the article.

2.4. Topical Reviews

A *Topical Review* is a short, highly focused survey covering a relatively narrow area of current research interest. It should be written so as to benefit both subject experts and also a more general audience of interested research scientists. A *Topical Review* should not aim to be comprehensive, but a brief introduction should provide historical perspective and a brief conclusion should indicate likely future directions. It is hoped that a less formal style of scientific writing can prevail in these articles.

Topical Reviews will be limited to about ten journal pages (10 000 words or 40 double-spaced manuscript pages) except in special agreed circumstances. They will be **commissioned by the Section Editor** either personally, or following a **formal proposal by prospective author(s)**. A letter of intent should be sent (faxed or e-mailed), giving the proposed topic, its importance and an indication of the material to be covered. This letter may be sent to one or more members of the Editorial Board for comment before the full article is commissioned. Once commissioned, author(s) will have priority in their topic within an agreed submission deadline. *Topical Reviews* will be refereed in the normal way, be highlighted within the journal issue, and carry brief biographical details of their author(s), which should be provided by the author(s) on submission of the article. It is hoped that direct contributions by prospective author(s) will become the norm for *Topical Reviews*.

2.5. Letters to the Editor

These may deal with non-technical aspects of crystallography, its role, its propagation, the proper function of its Societies etc., or may make a technical observation that would usefully be brought to a wider audience. Letters should be sent to the **Section Editor** or to the **Editor-in-Chief** of *Acta Crystallographica* only. They will not be formally refereed.

3. Submission and handling of manuscripts

3.1. Submission

Manuscripts should be prepared on one side of the paper in **double-spaced** format. All contributions should be submitted in **triplicate** and authors are reminded to keep an exact copy of the submission for later editorial adjustments and for checking proofs. Machine-readable submissions are encouraged (see §3.4).

Every issue of the journal contains the names and addresses of the Section Editor, the Co-editors of *Acta Crystallographica Section D* and of the Managing Editor. Contributions should be submitted as follows:

Research Papers: to any of the Co-editors.

Short Communications: to the Section Editor

Lead Articles and *Topical Reviews*: these will be handled by the Section Editor as described in §2 of these Notes.

3.2. Languages of publication

Acta Crystallographica Section D will publish papers in English, French, German and Russian. All contributions must be accompanied by an English language *Abstract* and synopsis.

3.3. *Handling of manuscripts*

All contributions will be seen by referees (normally two) before they can be accepted for publication. The editor to whom the manuscript is sent is responsible for choosing referees and for accepting or rejecting the paper. This responsibility includes decisions on the final form of the paper and interpretation of these Notes when necessary.

For accepted papers, it is the responsibility of the Managing Editor to prepare the paper for printing. This may involve correspondence with the authors and/or the responsible editor in order to resolve ambiguities or to obtain satisfactory figures or tables. The date of acceptance that will appear on the published paper is the date on which the Managing Editor receives the last item required. Proofs will be sent to the author who signed the letter of submission unless the Managing Editor is informed of some other suitable arrangement.

On rare occasions an editor may consider that a paper is better suited to a section of *Acta Crystallographica* other than that specified by the author(s), to the *Journal of Applied Crystallography* or to the *Journal of Synchrotron Radiation*. Alterations to the section or journal of publication will only be made after full discussion with the communicating author.

3.4. *Machine-readable submissions*

Authors who have used \TeX , \LaTeX , WordPerfect or Word to prepare their manuscripts should send a machine-readable version with their submission. The following formats may be used: 3.5 and 5.25 in IBM-compatible and 3.5 in Apple Macintosh diskettes. *Short Communications* should be accompanied by a diskette whenever possible. It would be appreciated if all machine-readable submissions were accompanied by an ASCII dump of the file(s), to aid possible troubleshooting, and details of the word-processing package used.

After acceptance of the paper for publication, authors may also send the version of the paper accepted by the Co-editor to the editorial office by e-mail or ftp (see §13).

3.5. *Author's warranty*

The submission of a paper is taken as an implicit guarantee that the work is original, that it is the author(s) own work, that all authors concur with and are aware of the submission, that proper credit is given to others, that the manuscript has not already been published (in any language), and that it is not being considered and will not be offered elsewhere while under consideration for an IUCr journal. For these reasons, the submission must be made over the signature of at least one author.

3.6. *Copyright*

Except as required otherwise by national laws, an author must sign and submit a copy of the Transfer of Copyright Agreement form (given at the end of these Notes) for each manuscript before it can be accepted.

3.7. *Author grievance procedure*

An author who believes that a paper has been unjustifiably rejected by the Co-editor may appeal initially to the Section Editor and then to the Editor-in-Chief if still aggrieved by the decision.

3.8. *Contact e-mail address*

The contact author should, where possible, provide an e-mail address. This will be used for editorial communications and will normally appear in the published paper.

4. **Layout and typography**

Contributions should be prepared on one side of the paper in **double-spaced** format with wide margins, and should conform to the general editorial style of IUCr journals.

4.1. *Type style*

The editorial staff in Chester will indicate to the printer the style of type to be used. It is better that authors should not indicate type style at all rather than do so in a way different from that used by the printers. However, it is helpful if authors indicate vectors and tensors by a wavy underline.

4.2. *Mathematics and letter symbols*

The use of the stop (period) to denote multiplication should be avoided except in scalar products. Generally no sign is required but, when one is, a multiplication sign (\times) should be used.

Greek letters should not be spelled out except in marginal notes of clarification.

Care should be taken not to cause confusion by using the same letter symbol in two different meanings.

Gothic, script or other unusual lettering should be identified in marginal notes. The printer may be instructed to use another type face if that indicated by the author is not readily available.

Equations, including those in published Appendices, should be numbered in a single series.

5. **Abstract and synopsis**

All contributions must be accompanied by an English language *Abstract* and a one or two sentence synopsis of the main findings of the paper for inclusion in the Table of Contents for the relevant issue. The *Abstract* should state as specifically and as quantitatively as possible the principal results obtained.

The *Abstract* should be suitable for reproduction by abstracting services without change in wording. It should not repeat information given in the title. Ordinarily 200 words suffice for *Research Papers*, *Lead Articles* and *Topical Reviews* and 100 words for *Short Communications*. It should make no reference to tables, diagrams, atom numbers or formulae contained in the paper. It should not contain footnotes. Numerical information given in the *Abstract* should not be repeated in the text. It should not include the use of 'we' or 'I'.

Literature references in an *Abstract* are discouraged. If a reference is unavoidable, it should be sufficiently full within the *Abstract* for unambiguous identification, e.g. [Terwilliger (1994). *Acta Cryst.* D50, 17–23].

6. **Diagrams and photographs ('figures')**

6.1. *Design*

The choice of tables and figures should be optimized to produce the shortest printed paper consistent with clarity. Duplicate presentation of the same information in both tables and figures is to be avoided, as is redundancy with the text.

Supplementary diagrams may be deposited (see §12.1).

Authors of protein structure papers are requested to submit a picture of the $C\alpha$ chain trace. This will be helpful for referees and may be deposited. In addition, a diagram of the fit of a side chain is helpful to the reader in terms of assessing the resolution and map quality.

File data should contain appropriate information such as a photograph of the data. As primary diffraction data cannot be satisfactorily extracted from such figures, the basic digital diffraction data should be deposited.

6.2. Quality

Diagrams must be provided in 'hard-copy' form, that is, as careful drawings in black ink or as high-quality photographic copies (glazed prints, not mounted). An individual hard-copy diagram must be provided for each figure.

6.3. Colour figures

Figures in colour are accepted **at no cost to the author** provided that the editor agrees that they improve the understanding of the paper. They should be provided as glossy prints or slides; laser printer or photocopier output will generally be unsatisfactory for colour reproduction. Slides should be accompanied by a photocopy showing the required figure layout.

6.4. Size

Diagrams should be as small as possible consistent with legibility. If possible, each diagram should be provided on a separate sheet of about A4 International Paper Size (210 × 297 mm). They will normally be further reduced by the printer, generally so that the greatest width including lettering is less than the width of a column of the journal (approximately 80 mm). Figures at greater than column width are allowed at editorial discretion.

6.5. Stereofigures

Stereofigures are welcomed in *Section D*. Atom labelling when included should be on both left and right views in stereo perspective.

6.6. Lettering and symbols

Fine-scale details and lettering must be large enough to be clearly legible (not less than 1.2 mm in height) after the whole diagram has been reduced to one column (80 mm) width.

Lettering should be kept to a minimum; distances, bond angles and torsion angles should be given as tables and descriptive matter should be placed in the legend.

6.7. Numbering and legends

Diagrams and photographs are to be numbered as figures in a single series, normally in the order in which they are referred to in the text. A list of the legends ('figure captions') is to be attached to the manuscript.

6.8. Electronic submission of figures

After acceptance of the paper for publication, authors may send figures direct to the editorial office by e-mail or ftp (see §13).

Figures may be sent as HPGL, or PostScript files. A complete list of file formats that are supported can be obtained from the editorial office. Hard-copy figures must be provided in all cases.

7. Tables

7.1. Economy in use of tables

Numerical information is generally most economically presented in tables. Text and diagrams should not be redundant with the tables.

Small tables will normally be set in type while large tables may be photographically reproduced or deposited.

Where possible, e.s.d. values should be provided for all numerical data e.g. unit-cell dimensions. Atomic coordinates and structure factors of macromolecular structures should be deposited.

7.2. Design, numbering and size

Tables must be numbered in a single series of arabic numerals, normally in the order in which they are referred to in the text. They should be provided with a caption either at the top or, if the table is to be photographed, on a separate sheet.

Tables should be carefully designed to occupy a minimum of space consistent with clarity. Tables to be photographed should be prepared in single spacing, without excessive space between columns.

8. Nomenclature

8.1. Crystallographic nomenclature

Atoms of the same chemical species within an asymmetric unit should be distinguished by an appended arabic numeral. **Chemical and crystallographic numbering should be in agreement wherever possible.** When it is necessary to distinguish crystallographically equivalent atoms in different asymmetric units the distinction should be made by lower-case roman numeral superscripts (*i.e.* i, ii, iii *etc.*) to the original atom labels.

Space groups should be designated by the Hermann-Mauguin symbols. Standard cell settings, as listed in **Volume A of International Tables for Crystallography**, should be used unless objective reasons to the contrary are stated. When a non-standard setting is used, the list of equivalent positions should be given. Hermann-Mauguin symbols should also be used for designating point groups and molecular symmetry. It is helpful if the origin used is stated explicitly where there is a choice.

The choice of axes should normally follow the recommendations of the Commission on Crystallographic Data [Kennard, Speakman & Donnay (1967). *Acta Cryst.* **22**, 445-449].

A symbol such as 123 or *hkl* without brackets is understood to be a reflection, (123) or (*hkl*) a plane or set of planes, [123] or [*uvw*] a direction, {*hkl*} a form and ⟨*uvw*⟩ all crystallographically equivalent directions of the type [*uvw*]. Other bracket notations should be explicitly defined.

For the nomenclature of crystal families, Bravais-lattice types and arithmetic classes see de Wolff *et al.* [*Acta Cryst.* (1985), **A41**, 278-280].

For symbols for symmetry elements and symmetry operations see de Wolff *et al.* [*Acta Cryst.* (1992), **A48**, 727-732].

8.2. Nomenclature of chemical compounds etc.

Chemical formulae and nomenclature should conform to the rules of nomenclature established by the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry and Molecular Biology (IUBMB), the International Mineralogical Association and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name.

Any accepted trivial or non-systematic name may be retained, but the corresponding systematic (IUPAC) name should also be given.

If help on assigning systematic names is sought from advisory sources, authors are requested to indicate the source consulted.

8.3. Units

The SI system of units is to be used except that the ångström (symbol Å, defined as 10¹⁰ m) is preferred to the nanometre (nm) or picometre (pm). Recommended prefixes of decimal multiples should be used rather than '× 10ⁿ'.

9. References

References to published work must be indicated by giving the authors' names followed immediately by the year of publication, e.g. Neder, Frey & Schulz (1990) or (Neder, Frey & Schulz, 1990). Where there are six or more authors the reference in the text should be indicated in the form Smith *et al.* (1989) or (Smith *et al.*, 1989) *etc.* (all authors should be included in the full list).

At the end of the paper a list giving full details of all references should be appended separately. In the reference list, entries for journals [abbreviated in the style of *Chemical Abstracts* (the abbreviations *Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.* are exceptions)], books, multi-author books, computer programs, personal communications and undated documents should be arranged alphabetically and conform with the following style:

- Arnoux, B., Ducruix, A. & Reiss-Husson, F. (1996). In preparation.
 Bricogne, G. (1993). *Acta Cryst.* D49, 37–60.
 Carter, C. W. Jr (1990). *Methods: a Companion to Methods in Enzymology*, Vol. 1, pp. 12–24. New York: Academic Press.
 Collaborative Computational Project, Number 4 (1994). *Acta Cryst.* D50, 760–763.
 Chiang, L.-C., Cabezas, E., Calvo, J. C. & Satterthwait, A. C. (1994). In *Peptides: Chemistry, Structure and Biology. Proceedings of the 13th American Peptide Symposium*, edited by R. Hodges & J. A. Smith. Leiden: ESCOM.
 Crowther, R. A. (1972). *The Molecular Replacement Method*, edited by M. G. Rossmann, pp. 173–178. New York: Gordon and Breach.
 Brünger, A. T. (1992a). X-PLOR. Version 3.1. A System for X-ray Crystallography and NMR. Yale University, Connecticut, USA.
 Brünger, A. T. (1992b). *Nature* (London), 355, 472–474.
 Jancarik, J. & Kim, S.-H. (1991). *J. Appl. Cryst.* 24, 409–411.
 Matthews, B. W. (1968). *J. Mol. Biol.* 33, 491–497.
 Olsnes, S. & Pihl, A. (1982). *Molecular Action of Toxins and Viruses*, edited by P. Cohen & S. Van Heyningen, pp. 51–105. New York: Elsevier.
 Schuller, D. J. (1996). *Acta Cryst.* In the press.
 Strong, R. K. (1990). PhD thesis, Harvard University, USA.
 Vogel, A. (1978). *Textbook of Practical Organic Chemistry*, 4th ed. London: Longman.
 Wang, B.-C. (1985). *Methods Enzymol.* 115, 90–112.
 Yariv, J. (1983). Personal communication.

Note that **inclusive** page numbers must be given.

10. Evaluation criteria

The criteria by which papers are evaluated are based on recommendations of the Commission on Biological Macromolecules.

10.1. Unrefined structures

Adequate experimental details should be provided to convince referees that the interpretation is correct, within the resolution of the analysis. If heavy-atom derivatives were used, sufficient data should be provided for evaluation of the quality of those derivatives. The fit of the model to the electron-density maps used to determine the structure should be shown or described by quantitative indicators, such as real-space residuals.

10.2. Refined structures

For refined structures the data required depend on the effective resolution of the analysis. It would be helpful to include the following.

Effective resolution should be described clearly, by giving the percentage of data recorded in the various resolution ranges;

the internal agreement of the data in each of these ranges; the percentage of data considered observable in each of the resolution ranges, along with the specific criteria that were used to select observable data; and the average $I/\sigma(I)$ value for each range.

The crystallographic R index should be tabulated as a function of resolution. The value for all reflections should be given along with any other values based on selected data. R_{free} should also be included.

A final Ramachandran plot or related conformational analysis should be given, with favourable energy regions indicated. Distributions of χ_1 , χ_2 values for side chains might be presented along with an analysis of deviations from expected minimum-energy ranges.

The r.m.s. deviations in B values within each residue's main-chain and side-chain atoms should be included.

Adequate details should be provided regarding the steps followed in constructing the model and refining the structure. The number of solvent atoms should be given along with information regarding solvent B values, and the approach that was used to identify solvent sites. The report should include the history and salient details of the refinement methods employed, including the resolution ranges that were used at various stages of refinement; the restraints used; a description of how the thermal parameters were treated; and how the solvent sites were selected and handled during refinement. It should be clear if van der Waals distances were restrained, either explicitly or by energy-minimization methods.

Hydrogen-bonding patterns within the protein should be described. The number of hydrogen-bond donors that are not involved in hydrogen bonding should be given with particular attention to unsatisfied buried main-chain hydrogen bonds.

Deviations of bond lengths, bond angles and planes from ideal geometries should be given. Close intramolecular and intermolecular van der Waals contacts should be described. The character and stereochemistry of major crystal contacts should be discussed.

Any structural features that are considered somewhat unusual should be described. Examples include *cis* peptide bonds; unoccupied volume inside the protein, buried charge groups that are not involved in salt bridges or reasonable hydrogen-bonding environments; unusual locations of glycine and proline residues; and unusual distributions of polar and hydrophobic groups within the molecule.

11. Crystal structure determinations

Papers which report the results of crystal structure determinations of small molecules must report the associated numerical data as required in Notes for Authors for *Section C* of *Acta Crystallographica*. These data should be supplied in a machine-readable file in CIF format. All numerical data will be checked in Chester for internal consistency.

12. Supplementary publication procedure (deposition)

12.1. Purpose and scope

Parts of some papers are of interest to only a small number of readers, and the cost of printing these parts is not warranted. Arrangements have therefore been made for such material to be deposited with the IUCr, with the Protein Data Bank at Brookhaven and the ICDD as appropriate.

The information to be deposited is **at the discretion of the editor** and may include:

Details of the experimental procedure.

Details of the stages of structure refinement.

Details of mathematical derivations given only in outline in the main text and in mathematical Appendices.

Lengthy discussion of points that are not of general interest or that do not lead to definite conclusions but that do have significant value.

Additional diagrams.

For papers reporting results of crystal structure determinations the following additional items are required:

Normal intermolecular distances.

Structure factors; weak reflections classified as unobserved should be included.

Anisotropic displacement parameters where relevant, including e.s.d.'s.

Least-squares planes and deviations from them.

Calculated H-atom coordinates if relevant.

All material to be deposited should be clearly so marked; it will be subject to the usual refereeing procedure.

12.2. Preparation of material for deposit

Material for deposit should:

be of a quality such that photocopies of it are completely legible;

have dimensions for text and tables not exceeding A4 International Paper Size (210 × 297 mm) (larger dimensions may be acceptable in exceptional circumstances);

not be photographically reduced so that character heights are less than 1.2 mm;

contain the title page of the paper to which it relates (including the *Abstract*);

have pages clearly numbered to ensure the correct sequence;

be sent in **triplicate** with the paper when it is submitted (but note that only one copy of the structure factors is required).

After acceptance of the paper for publication, material for deposition may be sent direct to the editorial office by e-mail or ftp (see §13).

12.3. Macromolecular structures

Data deposited should correspond to the level of detail described in the structural paper. For all structural studies of macromolecules, coordinates and structure factors must be deposited with the Protein Data Bank at Brookhaven National Laboratory if a total molecular structure has been reported. Authors should supply the Protein Data Bank reference codes for inclusion in the published paper.

An author may request that the structure factors be given a privileged status for a period of no longer than four years and

for atomic coordinates no longer than one year from the date of publication. Earlier release would require the specific consent of the author.

13. File transfer

After acceptance of the paper for publication, authors with computer access to the *Internet* may use anonymous file transfer protocol (ftp) to transfer large electronic files to the editorial office in Chester. Files larger than 70K bytes should be transferred in this way, smaller files can be sent by e-mail to **med@iucr.ac.uk**.

The procedure for transferring files by ftp is described below. Files need to be deposited in a directory called 'incoming' with a filename constructed from the *reference number* supplied by the Co-editor. Files containing text in $\text{T}_{\text{E}}\text{X}$ or $\text{L}_{\text{A}}\text{T}_{\text{E}}\text{X}$ should be given the extension **.tex**, and WordPerfect or Word files should be given the extensions **.wp** or **.doc**, respectively. Files containing diagrams in HPGL, or PostScript format should be given the extensions **.hpg**, or **.ps**, respectively. Multiple files for the same submission should be identified by filenames constructed as *ref.id.ext* where *id* indicates the contents, e.g. *xz1087.fig1.ps* and *xz1087.fig2.ps*.

The procedure for transferring files is given below.

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(i) On your workstation enter:      ftp ftp.iucr.ac.uk
(ii) Wait for Name ...: prompt and enter:      anonymous
(iii) Wait for Password: prompt
and enter:                                  your e-mail address
(iv) Wait for ftp> prompt and enter:      cd incoming
(v) Transfer a file from your account
(e.g. j29.ps) as an identifiable name
(e.g. ja0325.ps):                          put j29.ps ja0325.ps
(vi) Wait for ftp> prompt before sending another file
(vii) Finish off the ftp session by entering:      bye
(viii) Send an e-mail to Chester (med@iucr.ac.uk) with a
list of the files transferred by ftp
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14. Electronic status information

Authors may obtain information about the current status of their papers *via* the world-wide web at the address **http://www.iucr.ac.uk/docs/status.html/** (authors will need to provide the Co-editor reference number of their paper and the last name of one of the authors) or by e-mail by sending an e-mail message to **status@iucr.ac.uk** with the Co-editor reference number and the name of one of the authors as the subject line (e.g. JA0325 Smith). The body of the message should be empty. A status report will be returned by e-mail.

15. Reprints

Twenty-five reprints of each published article will be provided to a nominated author free of charge.

International Union of Crystallography Transfer of Copyright Agreement

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Authors (*Please type or use capital letters*)

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- (3) In the case of 'work for hire', the right of the employer to incorporate all or part of this article in future works.
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Name and position, if not author Name and position, if not author

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Date Date

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By signing this form you certify that your contribution is your original work, has not been published before and is not being considered for publication elsewhere; that you have obtained permission for and acknowledged the source of any excerpts from other copyright works; and that to the best of your knowledge your paper contains no statements which are libellous, unlawful or in any way actionable.

The signed statement must be received before the article can be accepted for publication. Requests for further information should be sent to the Executive Secretary of the Union.

* In this case please give further details overleaf.

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M. E. Ref.	Co-editor Ref.	Issue	Journal
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