Acta Cryst. (1991). C**47**, 2266–2275

International Union of Crystallography

Acta Crystallographica – Section C
Notes for Authors

1. Introduction

These Notes for Authors for contributions to *Acta Crystallographica* Section C replace all previous versions. These Notes embody the policy of the Commission on Journals of the International Union of Crystallography towards the publication of crystal structure analyses, as described in *Acta Cryst.* (1991). C**47**, 2263–2265. Major changes introduced here are:

All papers for Section C (but **not** for Sections A or B) must be submitted to the Chester office.

Normal Section C papers will all be printed in a common format – there is no distinction between a 'Full' paper and a 'Short-Format' paper.

Authors are encouraged to submit their work in machine-readable form. Machine-readable manuscripts should be encoded in the formats of the Crystallographic Information File [CIF: Hall, Allen & Brown (1991). *Acta Cryst.* A**47**, 655–685].

Conventional hard-copy manuscripts must have the numerical details of crystal data, experimental conditions and refinement procedures encoded on a simple standard form which accompanies these Notes.

The new submission procedures are linked to semi-automated data-checking software and an increasing degree of desktop journal production in the Editorial Office. The procedures are designed to improve the throughput of manuscripts and the accuracy of the printed contents of Section C.

2. Submission of contributions

2.1. *Address for submissions*

All new contributions to *Acta Cryst.* Section C should be sent to:

The Technical Editor,
International Union of Crystallography,
5 Abbey Square,
Chester CH1 2HU,
England

e-mail: teched@iucr.ac.uk
Telephone: 44 (0)244 342878
Fax: 44 (0)244 314888.

2.2. *Languages of submission*

The languages of publication are English, French, German and Russian.

2.3. *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 proper credit is given to others, that the manuscript has not 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 this reason, the submission must be made over the signature of at least one author.

2.4. *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.

2.5. *Categories of submission*

(*a*) The primary purpose of Section C is to publish short *Structural Papers* that report the results of one or more crystal structure determinations. *Structural Papers* will now be printed in a new format which is fully described in §3 of these Notes. §3 indicates clear guidelines for the tabular material, illustrations and text comment that may appear in a Section C *Structural Paper*. Submissions which exceed these guidelines may either be shortened for publication in Section C or be transferred to Section B at the discretion of the Co-editor and referees.

A supplementary publication (deposition document) will normally be associated with each *Structural Paper*. The information content of a supplementary publication is summarized in §4.

(*b*) Section C also publishes *Short Communications*. These are normally used (i) for reporting errata in an existing Section C publication or (ii) for brief comments (*e.g.* space-group revisions) on existing structural results. *Short Communications* should not exceed 1000 words, are printed in smaller type and are handled as rapidly as possible. They are refereed in the normal way and are *not* intended for interim reports of work in progress.

2.6. *Methods of submission*

Contributions may be submitted to the Chester office in one of three ways:

(*a*) As a machine-readable file (CIF format) *via* e-mail, together with certain additional material (letter of submission, Transfer of Copyright Agreement form, illustrations and structure factor lists) by normal postal communication. (See details in §5.)

(*b*) As a machine-readable file (CIF format) on diskette or magnetic tape, together with additional material (as above) by post. (See details in §5.)

(*c*) As a 'conventional' hard-copy manuscript (by post), but with certain numerical data items encoded on the 'Experimental Data' form provided at the end of these Notes. (See details in §6.)

2.7. *Handling of manuscripts*

Once a paper has been received in Chester the numerical data will be checked for internal consistency and to ensure that all the required information is included. Checks will also be made for previous publication of the structure(s) contained in the paper.

Incorrectly constructed CIF files, poorly completed forms or any submission not containing the appropriate minimum information will be returned to the author for revision at this stage.

The paper together with a report on the checks carried out will be forwarded to one of the Co-editors, who may send it to referees and is responsible for accepting or rejecting the paper.

If the paper is accepted, it is the responsibility of the Technical Editor to prepare the paper for printing; he may have to correspond with authors and/or the Co-editor involved in order to resolve ambiguities or to obtain satisfactory figures or tables. The date of acceptance that will appear on the published paper will be the date on which the Technical Editor receives the last item needed.

2.8. *Selection of Co-editor*

Authors may indicate, in a covering letter or in the CIF submission, the name of their preferred Co-editor. The new procedures are designed to permit regulation of Co-editorial workloads, hence it may be necessary to transfer the submission to another Co-editor.

2.9. *Author grievance procedure*

An author who believes his paper has been unjustifiably rejected by the Co-editor may appeal initially to the Editor for a new review and, finally, to the Editor of *Journal of Applied Crystallography* if the author is still aggrieved by the decision.

3. Presentation of *Structural Papers*

The printed material for all structural papers in Section C will now be presented in a single-column format. The categories of text, tables and illustrations within this format follow.

3.1. *Title and author list*

The *Title* should be both short and informative. Complicated IUPAC names should be avoided in the *Title*.

3.2. *Abstract*

The *Abstract* must be written in English and should summarize the most important structural features. It should **not contain the crystal data**. The systematic IUPAC name should be given here if it is not included in the *Title*.

3.3. *Comment*

This should state the reason for undertaking the structure determination and give brief details of the origin of the specimen. Comment should be made on any unusual features of the coordination, bonding, geometry, conformation, crystal packing *etc.* There is no formal length restriction on this section.

3.4. *Acknowledgements*

3.5. *References*

References to published work must be cited as described in §9

3.6. *Experimental*

Routine experimental details will be tabulated under the headings *Crystal data*, *Data collection* and *Refinement*. Discussion of the experimental procedure should be limited to any novel or unusual features and should be given in grammatically correct text.

A list of experimental details to be included is given in Appendix 1.

3.7. *Atomic coordinates for non-*H *atoms*

Equivalent isotropic values for the anisotropic displacement parameters should be given where appropriate. H atoms may be printed at the Co-editor's discretion.

3.8. *Table of selected geometrical data*

The **most important** bond distances, interatomic contacts, bond angles and torsion angles should be selected. This selection may be amended by the Co-editor.

3.9. *Chemical structural diagram*

Papers reporting structures of organic or metal-organic compounds should normally contain a chemical structural diagram.

3.10. *Crystallographic diagram(s)*

Usually one per structure; additional diagrams are at the Co-editor's discretion.

4. Supplementary publications

Each *Structural Paper*, and some *Short Communications*, must be accompanied by a *Supplementary Publication* which will be deposited at the British Library Document Supply Centre. The following categories of information are required for deposition.

4.1. *Table of* H*-atom coordinates*

These may be printed in special circumstances at the Co-editor's discretion.

4.2. *Table of anisotropic displacement parameters*

These may be printed at the Co-editor's discretion.

4.3. *Complete geometry tables*

A complete list of interatomic distances should be provided. Valence and torsion angles may be included if desired.

4.4. *Tables of structure factors*

These should always be provided in hard-copy form and **never** included in machine-readable submissions. Weak reflections classified as unobserved should be included.

4.5. *Miscellaneous data*

Other miscellaneous items of information (including diagrams) may be deposited at the discretion of the Co-editor. Such material **must** be provided in hard-copy form.

4.6. *Powder diffraction data*

For papers that present the results of powder diffraction profile fitting or refinement (Rietveld) methods, the primary diffraction data, *i.e.* the numerical intensity of each measured point on the profile as a function of scattering angle, will be deposited.

Co-editors will send powder diffraction data (reported either in the paper or in the deposited material) to the International Centre for Diffraction Data (ICDD), 1601 Park Lane, Swarthmore, PA 19081–2389, USA. These data will then be checked and assigned an ICDD reference number which will, where possible, be published in the paper.

5. Submission in machine-readable (CIF) format

5.1. *General principles*

The crystallographic information file [CIF: Hall, Allen & Brown (1991). *Acta Cryst.* A**47**, 655–685] provides a common format for the transmission of the numerical results of a crystal structure determination. Each data item has a corresponding CIF data name; the data names corresponding to those data items that normally form part of a Section C *Structural Paper* are identified below and in Appendix 1. It is expected that the bulk of the numerical data in a CIF will be generated by the relevant structure solution package. [The present CIF represents a core format for single-crystal structure determinations; data names for powder diffraction and protein structure determinations are under active development.]

The CIF format also provides fields for the transmission of text information, *e.g. Abstract*, *Comment*, *References*, and for the inclusion of the necessary submission details. These fields should be added to a machine-generated CIF using a suitable text editor.

The submitted CIF may contain extra fields that will not form part of a Section C presentation. These fields will be ignored during processing at the Editorial Office.

Note that the CIF can also be used to transmit much of the supplementary publication information. However, **structure factor tables should not be included in the CIF.** Their inclusion will often cause problems in e-mail transmission and may exceed the capacity of some diskettes.

At present the CIF **cannot** be used to transmit graphical information.

Thus a CIF submission is in two parts: (*a*) a machine-readable file containing the information of §§3.1–3.8 and 4.1–4.3 and (*b*) hard-copy material including the information of §§3.9, 3.10, 4.4 and 4.5 together with a letter of submission and a signed Transfer of Copyright Agreement form.

The CIF may be transmitted *via* e-mail or by diskette or magnetic tape as described in §§5.9 and 5.10.

The printed manuscript will be generated directly from the CIF using software available in the Editorial Office. Illustrations will be added during page make-up. The supplementary publication will be constructed from the CIF content and the hard-copy material supplied.

5.2. *Submission information in the CIF*

This should be included as free text in the CIF under the following self-explanatory data names [see the *CIF Dictionary* given by Hall, Allen & Brown (§5.1) for complete details]:

```
_publ_contact_author
_publ_contact_author_email
_publ_contact_author_fax
_publ_contact_author_phone
_publ_contact_letter
_publ_requested_coeditor_name
_publ_requested_journal
```

5.3. *Text information*

The following CIF fields are provided to carry the necessary text information

```
_publ_section_title
_publ_author_name
_publ_author_address
_publ_section_abstract
_publ_section_comment
_publ_section_experimental (see §5.4 for use)
_publ_section_acknowledgements
_publ_section_references
_publ_section_figure_captions
_publ_section_table_legends
```

CIF files contain plain ASCII text and can be edited by any text editor. Authors should adhere to the following simple guidelines when entering information **in the free text fields**

do not enter any non-printing characters

do not indicate italic typeface

do not indicate bold typeface

enter Greek characters as \a for α, \b β, \g γ, \d δ, \e ϵ, \z ζ, \h η, \q θ, \i ι, \k κ, \l λ, \m μ, \n ν, \x ξ, \o o, \p π, \r ρ, \s σ, \t τ, \u υ, \f φ, \c χ, \y ψ, \w ω and \A for A, \B B, \G Γ *etc.*

enclose superior characters within the symbols '^'; *e.g* enter Csp^3 as Csp^3^ and 10^{12} as 10^12^

enclose inferior characters within the symbols '~'; *e.g.* enter U_{12} as U~12~

enter é as \'e [*e.g.* Universit\'e for Université]

enter à as \`a [*e.g.* Universit\`a for Università]

enter â as \^a [*e.g.* Ch\^atanay for Châtanay]

enter ç as \, [*e.g.* re\,cu for reçu]

enter ü as \"u [*e.g.* f\"ur for für]

enter $P\bar{1}$ as P -1

enter ° as \%

enter Å as \%A

indicate any other accents on a separate sheet to accompany the hard-copy material

Typesetting flags will not normally be used in non-text CIF data items such as `_chemical_formula_` or `_symmetry_space_group_name_`.

5.4. *Experimental information*

Appendix 1 lists the items essential for the critical assessment of Section C *Structural Papers*, together with their CIF names. Note particularly that the *CIF Dictionary* provides a number of *standard codes* to describe certain experimental procedures; these should be used and will be listed in that form in the paper. Examples are `_exptl_absorpt_correction_type`, `_refine_ls_hydrogen_treatment`. Special features of the experimental procedure should be encoded in plain text under `_publ_section_experimental`.

5.5. *Atomic coordinate data*

This should be provided as a CIF looped structure and the looped list should contain at least:

```
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
```

the rules on atom labelling in the *CIF Dictionary* should be adhered to throughout.

5.6. *Geometrical data*

The `_geom_` data names permit the inclusion of interatomic distances, valence angles and torsion angles in the CIF as

```
_geom_bond_distance
_geom_contact_distance
_geom_angle
_geom_torsion
```

A `_geom_*_publ` flag is associated with each value (`yes` or `no`) to indicate whether it is selected for inclusion in the printed tables.

5.7. *Supplementary material in the CIF*

The H-atom coordinates, anisotropic displacement parameters and full geometrical data may be transmitted in the CIF format or supplied as hard copy (see below). Structure factors should **not** be included in the CIF.

5.8. *Associated hard-copy material*

This material must contain:

(*a*) a signed copy of the letter of submission;

(*b*) a signed Transfer of Copyright Agreement form;
(*c*) the chemical structural diagram (three copies);
(*d*) crystallographic illustrations prepared as described in §7 (three copies);
(*e*) structure factor listing (three copies);
(*f*) other supplementary material if not present in CIF (three copies).

Supplementary material should be prepared as described in §6.4.

5.9. *CIF submission via electronic mail*

The CIF file for a *Structural Paper* should be sent to the following e-mail address:

teched@iucr.ac.uk

Receipt will be acknowledged *via* e-mail and a reference number assigned. After receipt has been acknowledged, associated hard-copy material should be sent **quoting the reference number** to: The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

5.10. *CIF submission via diskette or magnetic tape*

The electronic CIF file for a *Structural Paper* and the associated hard-copy material (see §5.8) should be sent to the Technical Editor at the postal address above. Receipt will be acknowledged.

The following formats may be used
3.5" IBM-compatible diskettes.
5.25" IBM-compatible diskettes.
3.5" Apple Macintosh diskettes.
3.5" Sun OS diskettes (cpio format).
0.5" 1600/6250 bpi magnetic tape.

6. Submission in hard-copy form

One standard printed form for each structure and **three** copies of the manuscript should be submitted.

6.1. *General layout*

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 the journal. The text and tables should be set out under the standard subheadings of §3.

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.

6.2. *Standard printed form for experimental data*

The numerical and text description of the experimental procedures must be encoded on the standard form (Appendix 2). The form covers all of the quantities listed in Appendix 1. The purpose of the form is twofold. Firstly it is input by editorial staff to create a CIF file which, together with the tabulated data of §6.3, can be input to automated checking routines and used to prepare camera-ready copy for printing. Secondly it ensures that authors do not accidentally omit essential information when preparing their manuscript.

Data names for powder diffraction (and protein) determinations are under development. In the meantime, authors of papers reporting the results of powder diffraction determinations should only complete the Crystal Data part of the form; details of the data collection and refinement should be given in grammatically correct text.

6.3. *Tabulated data*

The atomic coordinate table should show atom label, x, y, z and U_{eq} (together with associated e.s.d.'s in parentheses) for non-H atoms (for H atoms see §4.1). The geometry table should show only those parameters which are of maximum interest. Geometrical details of *e.g.* peripheral phenyl rings should be omitted. Data from these tables, together with material retrieved from the deposition document will be input by editorial staff.

6.4. *Supplementary material*

Material for deposit (§4) 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.

7. Diagrams and photographs ('figures')

7.1. *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.

In structural papers it is preferred that (i) distances and angles be given in tabular form and (ii) that a chemical structural diagram be included for organic and metal-organic compounds.

7.2. *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.

7.3. *Colour plates*

Plates in colour are accepted **at no cost to the author** if the Co-editor considers them essential for a clear understanding of the paper.

7.4. *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 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.

7.5. *Stereofigures*

The recommended limit on stereofigures is one per structure; more than one per structure may be included if the Co-editor and referees feel that this is necessary for understanding the paper. Authors are reminded that a non-stereoview (half a pair) is often an acceptable alternative. Stereoviews should ordinarily fit into a single column (80 mm wide), the centre-to-centre separation

(after reduction to 80 mm width) should be in the range 40 to 55 mm and atom labelling should be included on both left and right views in stereo perspective.

7.6. *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.

On diagrams and figures, the author's own lettering ready for photographing is preferred; if necessary, lettering will be added by the printer if a photocopy showing the required lettering is supplied with an unlettered original.

7.7. *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 included in the CIF submission or attached to the hard-copy manuscript.

8. Nomenclature

8.1. *Crystallographic nomenclature*

In 'conventional' hard-copy submissions, 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), A**41**, 278–280].

For the nomenclature of polytypes see Guinier *et al.* [*Acta Cryst.* (1984), A**40**, 399–404].

For the nomenclature of inorganic structure types see Lima-de-Faria *et al.* [*Acta Cryst.* (1990), A**46**, 1–11].

8.2. *Nomenclature of chemical compounds etc.*

Names of chemical compounds and minerals are not always unambiguous. Authors should therefore quote the chemical formulae, **including chemical structural diagrams for organic and metal-organic compounds**, of the substances dealt with in their papers.

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) and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name.

Any accepted trivial or nonsystematic 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 10^{-10} m) is preferred to the nanometre (nm) or picometre (pm). Recommended prefixes of decimal multiples should be used rather than '$\times 10^{n}$'.

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.* and *J. Appl. Cryst.* are exceptions)], books, multi-author books, computer programs, personal communications and undated documents should be arranged alphabetically and conform with the following style:

Bürgi, H.-B. (1989). Acta Cryst. B45, 383–390.
Hervieu, M. & Raveau, B. (1983a). Chem. Scr. 22, 117–122.
Hervieu, M. & Raveau, B. (1983b). Chem. Scr. 22, 123–128.
Hummel, W., Hauser, J. & Bürgi, H.-B. (1990). In preparation.
Jones, P. T. (1987). Personal communication.
McCrone, W. C. (1965). Physics and Chemistry of the Organic Solid State, Vol. 2, edited by D. Fox, M. M. Labes & A. Weissberger, pp. 725–767. New York: Interscience.
Perkins, P. (undated). PhD thesis. Univ. of London, England.
Sheldrick, G. M. (1976). SHELX76. Program for crystal structure determination. Univ. of Cambridge, England.
Smith, J. V. (1988). Chem. Rev. 88, 149–182.
Smith, J. V. & Bennett, J. M. (1981). Am. Mineral. 66, 777–788.
Vogel, A. (1978). Textbook of Practical Organic Chemistry, 4th ed. London: Longman.

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

When more than ten references are taken from a data base (usually for a structural paper), a condensed reference notation of the Coden type should be used.

APPENDIX 1
Items for inclusion in the *Experimental* Section

In order that a thorough critical assessment (and repetition of the work) may be made, the items in the following table must be included unless they are inappropriate for a particular determination. Additionally, a **chemical structural diagram** must be provided for all organic and metal-organic compounds. This diagram may be omitted only if the compound is simple (benzene, methanol *etc.*).

Essential items	CIF data names
Crystal data	
Source of material	`_chemical_compound_source`

Crystal shape and size	`_exptl_crystal_description`
	`_exptl_crystal_colour`
	`_exptl_crystal_size_max`
	`_exptl_crystal_size_mid`
	`_exptl_crystal_size_min`

Chemical formula	`_chemical_formula_analytical` or `_chemical_formula_moiety` or `_chemical_formula_structural`
Formula weight	`_chemical_formula_weight`
Crystal system	`_symmetry_cell_setting`
Space group	`_symmetry_space_group_name_H-M`

Unit-cell dimensions	`_cell_length_a`
	`_cell_length_b`
	`_cell_length_c`
	`_cell_angle_alpha`
	`_cell_angle_beta`
	`_cell_angle_gamma`

Number and θ range of reflections used for measuring lattice parameters	`_cell_measurement_reflns_used`
	`_cell_measurement_theta_min`
	`_cell_measurement_theta_max`

Volume of unit cell	`_cell_volume`
Z	`_cell_formula_units_Z`
D_x	`_exptl_crystal_density_diffrn`
D_m	`_exptl_crystal_density_meas`
Radiation and wavelength	`_diffrn_radiation_type` `_diffrn_radiation_wavelength`
Linear absorption coefficient	`_exptl_absorpt_coefficient_mu`
Temperature of measurement	`_cell_measurement_temperature`
Data collection	
Diffractometer	`_diffrn_measurement_device`
Method used to measure diffraction data	`_diffrn_measurement_method`

Absorption correction type (maximum and minimum transmission values)	`_exptl_absorpt_correction_type`
	`_exptl_absorpt_correction_T_min`
	`_exptl_absorpt_correction_T_max`

Number of reflections measured	`_diffrn_reflns_number`
Number of independent reflections	`_reflns_number_total`
Number of observed reflections	`_reflns_number_observed`
Criterion for recognizing unobserved reflections	`_reflns_observed_criterion`
R_{int}	`_diffrn_reflns_av_R_equivalents`
Maximum value of θ	`_diffrn_reflns_theta_max`

Range of h, k and l	`_diffrn_reflns_limit_h_min` `_diffrn_reflns_limit_h_max`
	`_diffrn_reflns_limit_k_min` `_diffrn_reflns_limit_k_max`
	`_diffrn_reflns_limit_l_min` `_diffrn_reflns_limit_l_max`

Standard reflections and their variation	`_diffrn_standards_number`
	`_diffrn_standards_interval_count`
	`_diffrn_standards_interval_time`
	`_diffrn_standards_decay_%`

APPENDIX 1 (*cont.*)

Essential items	CIF data names
Refinement	
Use of F, F^2 or I	`_refine_ls_structure_factor_coef`
$R\ [= \sum(\|\|F_o\| - \|F_c\|\|)/\sum\|F_o\|]$	`_refine_ls_R_factor_obs`
$wR\left\{= \left[\sum\left(w\|Y_m - Y_c\|^2\right)/\sum\left(wY_m^2\right)\right]^{1/2}\right\}$ [where Y_m and Y_c are the measured and calculated coefficients specified above (*i.e.* F, F^2 or I)]	`_refine_ls_wR_factor_obs`
Method of refining and locating H atoms	`_refine_ls_hydrogen_treatment`
Number of reflections used in refinement	`_refine_ls_number_reflns`
Number of refined parameters	`_refine_ls_number_parameters`
$S\left\{= \left[\sum w(\|Y_m\| - \|Y_c\|)^2/(m-n)\right]^{1/2}\right\}$	`_refine_ls_goodness_of_fit_obs`
Definition of w	`_refine_ls_weighting_scheme`
Maximum Δ/σ	`_refine_ls_shift/esd_max`
Maximum and minimum $\Delta\rho$ in final difference electron density map	`_refine_diff_density_max` `_refine_diff_density_min`
Extinction correction method (if applied)	`_refine_ls_extinction_method`
Primary- and secondary-extinction values	`_refine_ls_extinction_coef`
Source of scattering factors	`_atom_type_scat_source`

All computer programs used	`_computing_data_collection`
	`_computing_cell_refinement`
	`_computing_data_reduction`
	`_computing_structure_solution`
	`_computing_structure_refinement`
	`_computing_molecular_graphics`
	`_computing_publication_material`

Discussion of experimental procedure (see §3.6; including method to measure density, discussion of absolute structure and justification of any unusually high R values or shift-to-e.s.d. ratios >1.0)	`_exptl_crystal_density_method`
	`_refine_ls_abs_structure_details`
	`_publ_section_experimental`

APPENDIX 2
Experimental form to be completed for each structure (hard-copy submission)

EXPERIMENTAL DETAILS E.s.d.'s should be given where appropriate.. Please complete separate form for each compound studied	
Compound [*e.g.* (1), (2) *etc.*]	
CRYSTAL DATA	
Chemical formula	Crystal system
M_r	Space group
a (Å)	α (°)
b (Å)	β (°)
c (Å)	γ (°)
Z	D_m (Mg m^{-3})
V (Å^3)	D_x (Mg m^{-3})
Radiation	No. of reflections for lattice parameters
Wavelength (Å)	θ range for lattice parameters (°)
Absorption coefficient (mm^{-1})	Temperature (K)
Crystal source	
Crystal colour	Crystal description
Crystal size (mm)	
DATA COLLECTION	
Diffractometer type	Collection method
Absorption correction type (circle appropriate description) analytical integration empirical refdelf sphere cylinder none	Absorption correction (T_{min}, T_{max})
No. of reflections measured	R_{int}
No. of independent reflections	θ_{max}(°)
No. of observed reflections	No. of standard reflections (and interval)
Criterion for observed	Variation of standards
h_{min}	h_{max}
k_{min}	k_{max}
l_{min}	l_{max}

EXPERIMENTAL DETAILS (*continued*)	
REFINEMENT	
Treatment of hydrogen atoms (circle appropriate entry, or describe in box below) refall refxyz refU noref	F, F^2 or I
R	No. of parameters refined
wR	No. of reflections used in refinement
S	Weighting scheme w=
$(\Delta/\sigma)_{max}$	$(\Delta\rho)_{min}$ (e Å^{-3})
Extinction correction method (if applied)	$(\Delta\rho)_{max}$ (e Å^{-3})
Primary- and secondary-extinction values	Source of atomic scattering factors
Please enter below, in grammatically correct text, details of any novel or unusual features of the experimental procedure; method used to measure density, discussion of absolute structure and justification of unusually high R values or shift-to-e.s.d. values >1.0 should be included (attach extra sheet if necessary)	
A chemical structural diagram should be attached to this form.	
The remainder of the manuscript should consist of (i) double-spaced typed text and tables set out under the standard subheadings of §3 of the full Notes, (ii) figures and figure legends, (iii) supplementary data for deposition (see §4), (iv) signed Transfer of Copyright Agreement form, and (v) letter of submission.	

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