International Union of Crystallography

Acta Crystallographica Section C
Notes for Authors

1. Introduction

These Notes for Authors provide detailed information on the submission and publication procedures of *Acta Crystallographica Section C: Crystal Structure Communications*. They embody the latest policy of the IUCr Commission on Journals on the rapid publication of crystal structure studies and supersede those of *Acta Cryst.* (1995). C51, 159–174.

Authors are expected to submit *Section C* papers in Crystallographic Information File (CIF) format. Hard-copy submissions of manuscripts will not normally be accepted.

The Notes are divided into the following sections:

§2. Publication requirements
§3. Published material
§4. Supplementary material
§5. Submission procedure
§6. Diagrams
§7. Nomenclature
§8. References
§9. File transfer
§10. Electronic status information
§11. Reprints

Appendix 1. Guidelines for editing CIF text
Appendix 2. Essential items for the *Experimental* section
Appendix 3. Transfer of Copyright Agreement form
Appendix 4. Annotated example of a *Section C* paper

2. Publication requirements

2.1. *Address for submissions*

All papers submitted to *Section C* should be sent to the IUCr Offices in Chester.

Publication material submitted electronically in CIF format on magnetic media, or as hard-copy (diagrams and Transfer of Copyright Agreement form), should be sent by airmail or courier to:

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

Telephone: 44 1244 342878
Fax: 44 1244 314888

E-mailed manuscripts and data in CIF format should be sent to:

med@iucr.ac.uk

or, for large data files, transmitted by ftp (see §9) to:

ftp.iucr.ac.uk (192.70.242.1)

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 all authors concur with and are aware of the submission, 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 these reasons, 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 (*Appendix* 3) for each manuscript before it can be accepted.

2.5. *Categories of submission*

Section C publishes two categories of papers:

(i) The primary purpose of *Section C* is to publish papers that report the results of one or more crystal structure determinations. The format of these papers is described in §3. Submissions which exceed these guidelines will, at the discretion of the Co-editor and referees, be shortened for publication in *Section C*, or be transferred to *Section B*.

(ii) *Section C* also publishes *Addenda and Errata* to previously published papers. These are used for reporting additions to, comments on, or errata in existing *Section C* publications and are *not* intended for interim reports of work in progress. These manuscripts should not exceed 1000 words and, while being refereed as for (i), will be processed as rapidly as possible.

2.6. *Method of submission*

Manuscripts should be submitted to the Chester office electronically in CIF format. E-mail or magnetic media submission is accepted.

2.7. *Handling of manuscripts*

A paper submitted to Chester will be first checked for completeness (note the availability of a CIF pre-checking facility discussed in §5.1). If the material is incomplete or inadequate it will be returned to the author for correction. Numerical data are then checked for internal consistency, correct symmetry and cell dimensions, and sensible structural geometry. Checks will also be made for previous publication of the structure(s) contained in the paper. The results of these checks are summarized in a *Check Report*.

The paper, together with the *Check Report*, is forwarded to a Co-editor, who is in charge of the reviewing steps and future communications with the authors, up to the acceptance stage.

If a paper passes the checking process without significant fault it may be designated as a *fast-track submission* and sent, with a full advance proof, to a Co-editor for rapid reviewing. If the paper is accepted without significant change, the advance proof will be forwarded to the author for final approval. The fast tracking of papers offers significantly shorter publication times to authors who submit well prepared and carefully checked

manuscripts. This service is possible because of the reductions in workload that such submissions afford the editorial staff.

If changes to a manuscript requested by the editorial staff or the Co-editor are not received within six months of transmittal to the author, the submission will automatically be withdrawn. Any subsequent communication of the material will be treated as a new submission in the editorial process.

Once a paper is accepted, it is the responsibility of the Managing Editor to prepare the paper for printing and to correspond with the authors and/or the Co-editor to resolve publication ambiguities or inadequacies. The date of acceptance that will appear on the published paper will be the date on which the Managing Editor receives the last item needed.

2.8. Selection of Co-editor

Co-editors are assigned to a paper according to their current workload and expertise. Authors may indicate a preference for a particular Co-editor but the editorial staff reserve the right to make the final choice.

2.9. 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. Published material

The following material is required for publication in Section C. Details of these categories are given in §4. An example of a published paper is shown in Appendix 4.

3.1. Title and authors

The Title should be both short and informative. Avoid complicated IUPAC names and redundant phrases such as 'The Structure of ...' or 'Crystal Structure of ...' should be removed. It is preferred that the full first name of each author be used. 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.

3.2. Abstract

The Abstract must be written in English and should summarize only the most important aspects of the study. It should **not contain the crystal data**. The systematic IUPAC name and the chemical formula should be given here, if they are not included in the Title.

3.3. Comment

The Comment section should contain:

(i) Concise reasons why the structure determination was undertaken.

(ii) The origin of the material studied. General chemical background material and references should be included. Details of the chemical extraction, synthesis and crystallization processes should be given in the Experimental section (see §3.6).

(iii) Any novel and unusual features of the coordination, bonding, geometry, conformation, crystal packing, etc. Avoid discussions of geometry data which agree with established values (see Volume C of International Tables for Crystallography, pp. 681–791).

3.4. Acknowledgements

3.5. References

References to published work must be cited in the format detailed in §8. If reference is made to unpublished work, prior consent must be first obtained from the authors.

3.6. Experimental

Experimental details will be tabulated under the subheadings Crystal data, Data collection and Refinement. Any discussion of experimental procedure is to be limited to novel or unusual features and should be given in grammatically correct text.

A list of experimental data requested is provided in Appendix 2. These represent the primary information about the structure. If they are incomplete or inconsistent the manuscript will be returned to the authors as being inadequate. Authors should take particular note of the following editorial acceptance criteria.

(i) The chemical formula, chemical formula weight, volume of unit cell, space group and formula units per cell, Z, must be consistent with the atomic sites (see §§3.7 and 4.1).

(ii) The cell and space group must encompass the highest symmetry permitted by the diffraction intensities. Special care is needed if Z exceeds the number of general equivalent positions for a space group, e.g. check if multiple diffraction has affected the systematically absent intensities.

(iii) The precision of a structure is determined largely by the number and the reliability of the diffraction measurements. Unless there are mitigating circumstances, diffraction data should extend to at least $\sin\theta/\lambda = 0.6$ Å^{-1} (i.e. $\theta_{max} \geq 25°$ for Mo $K\alpha$; $\theta_{max} \geq 68°$ for Cu $K\alpha$).

(iv) Absorption corrections must be appropriate to the crystal and the precision of the analysis. If μ is less than 0.3 mm^{-1} and the crystal is regular, absorption corrections are usually unnecessary. Refined absorption techniques (based on ΔF) should be employed only if analytical or ψ-scan methods cannot be applied. The calculated maximum and minimum transmission values should be physically sensible with respect to the material and the crystal shape.

(v) An R value calculated with partial reflection data is not a good measure of structure reliability. The precision of a structure is better gauged from the estimated standard deviations of the parameters. These e.s.d.'s are critically dependent on the number and the reliability of the measured structure factors used in the refinement process. Usually, a low 'observed' threshold (see items 20 and 21 in Appendix 2) means that more reflections are used in the refinement (see item 30). This is more important to structure reliability than raising this threshold in order to lower the R value. Provided that the least-squares weights incorporate the e.s.d.'s of the measured intensities, low thresholds of say $\sigma(I)$ or $2\sigma(F)$ are recommended. For most analyses there are advantages in using all data in the least-squares refinement.

3.7. Table of atomic sites

A table containing atomic site data will be published. This will include the e.s.d.'s of the coordinates and displacement parameters. Information about hydrogen-atom sites will be printed only at the Co-editor's discretion. (See §§5.5 for submission details.)

3.8. Table of selected geometrical data

A table of the bond distances, interatomic contacts, bond angles and torsion angles **of special importance to the structure** and relevant to the discussion in the Comment section will be published. All other geometrical data will be archived. The data to be published may be amended by the Co-editor. (See §5.6 for submission details.)

3.9. Chemical structural diagram

Papers reporting the structure of a molecular compound must contain a chemical structural diagram (see §6 and the example in *Appendix* 4).

3.10. Crystallographic diagram(s)

Papers should contain one crystallographic diagram of each structure. For papers reporting molecular structures this should be a molecular diagram; otherwise it should be a packing or polyhedron diagram. Unique atom sites should be identified with labels as specified in §7.1. The atom labels used in the diagram should be consistent with those in the table of atom coordinates (§3.7). Additional diagrams are at the Co-editor's discretion.

The importance of high quality diagrams is detailed in §6. A clear, well presented crystallographic diagram is an essential component of the published material. It encapsulates information about the stereochemistry, the geometry, and, if it is a displacement ellipsoid plot, about the structural disorder and thermal motion. A displacement ellipsoid diagram is required, either for publication or as supplementary material to be used in the review process.

3.11. Contents requirements

The Table of Contents of the journal will list each paper with the title and author(s), a chemical structural diagram for molecular compounds, and a written synopsis for compounds which cannot be shown as a chemical structural diagram. A synopsis should be one or two sentences (less than 40 words) in length.

4. Supplementary material

Supplementary material is required for reviewing and checking the submission. This material will be archived but is not usually published. The following categories of data are requested.

4.1. Hydrogen-atom sites

Hydrogen-atom sites may, at the Co-editor's discretion, be published in the paper.

4.2. Anisotropic displacement parameters

Anisotropic displacement parameters (preferably as U_{ij}'s) may, at the Co-editor's discretion, be published in the paper. If parameters other than U_{ij}'s are used, the exact form of the temperature factor expression must also be indicated.

4.3. Geometrical data

A list of the important interatomic bond lengths and intermolecular non-bonded contact distances must be provided for checking purposes. Valence and torsion angles may be included if desired. Selected intermolecular distances and torsion angles may, at the Co-editor's discretion, be published in the paper.

4.4. Reflection data

A list of the reflection data h, k, l, Y_{meas}, Y_{calc}, σY_{meas} (where Y is F, F^2, or I), must be submitted. Where possible, this should be supplied as a single electronic file in CIF format (see §§5.7 and 9), otherwise as a hard-copy listing. Authors should indicate if the Y values have been corrected for absorption and extinction effects.

4.5. Miscellaneous data

Miscellaneous data (including diagrams) may be deposited at the discretion of the Co-editor. If the submitted crystallographic diagram (see §3.10) does not show the displacement-parameter ellipsoids, such a diagram is required for the checking and reviewing process.

Details of the parameter constraints and restraints applied to the refinement process must be supplied as supplementary material unless they are described in the experimental refinement procedure (see item 40 in *Appendix* 2).

4.6. Powder diffraction data

For papers that present results based on powder diffraction data, the numerical intensity of each measured point on the profile (as a function of scattering angle) will be deposited with the IUCr and sent by the Co-editor to the International Center for Diffraction Data (ICDD), 12 Campus Boulevard, Newton Square, PA 19073-3273, USA. These data will be checked and assigned an ICDD reference number which will, where possible, be published in the paper. Papers reporting Rietveld refinements should include a figure showing the diffraction profile and the difference between the measured and calculated profiles.

5. Submission procedure

5.1. General information

Authors are required to submit papers electronically in CIF format. The required data items are described briefly below and in *Appendix* 2. Detailed descriptions of these items are given in the *CIF Core Dictionary* [Hall, Allen & Brown (1991). *Acta Cryst.* A47, 655–685]. The special requirements for text items in a CIF are summarized in *Appendix* 1, and an example of a published paper is given in *Appendix* 4. Authors are also referred to the *Guide to CIF for Authors*, which is available free of charge from the Editorial Office.

It is anticipated that the bulk of the numerical data in a CIF will be generated by standard software, whereas the fields containing text for the sections *Abstract*, *Comment*, etc. (see §5.3) will be added by the author using a text editor.

The data items listed below, and summarized in *Appendix* 2, will be extracted automatically by the CIF-handling software in Chester. Authors who wish to include data items not listed below should identify these in the contact letter field (see §5.2). Otherwise these data items will be ignored by the extraction process. (The present *CIF Core Dictionary* contains only data names for conventional single-crystal structure studies. Data names for powder diffraction and protein structure items are available from the Managing Editor.)

Note that a CIF may also be used to transmit supplementary publication information. Authors are advised, however, **not to transmit** reflection data or diagrams as part of the standard CIF, as the size of these items may cause e-mail problems or exceed the capacity of some diskettes. Nevertheless, authors are requested, whenever possible, to submit these data electronically using the procedures described in §§5.7 and 9.

The submission of a manuscript will normally be in two parts: (i) a machine-readable file or files containing data items from §§3 and 4 and (ii) a signed Transfer of Copyright Agreement form accompanied by the balance of items as hard-copy material.

A CIF pre-checking facility is provided by the Editorial Office. Authors are encouraged to check a CIF, prior to submission, by sending it, without any attachments, such as the sender's signature script, to the e-mail address

checkcif@iucr.ac.uk

Tests will be made automatically for file integrity, mandatory data and sensible cell, symmetry and geometry information, and a *Check Report* will be returned to the sender's e-mail address. The tests are less extensive than those applied during

checking of a paper submitted for publication, but pre-checking will significantly reduce the delays which occur with incorrect or inadequate CIF submissions.

The Editorial Office also provides a manuscript previewing facility for authors. Following an error-free *Check Report* from **checkcif** (see above), authors are encouraged to e-mail the same CIF to

printcif@iucr.ac.uk

which will return a PostScript file of the paper in the form that is sent to the Co-editors for reviewing. This file can be printed locally so that authors can make final checks on the text and tables, prior to submission.

On submission of the CIF for publication, the numerical data, diagrams and text are checked for completeness and a printed copy of the paper is forwarded to a selected Co-editor for use in the review process. Any amendments to the paper during this review **must be indicated on the printed manuscript**, as this document is used by the editorial staff to update and revise the archived CIF. An author-modified CIF should *not* be resubmitted **except at the explicit request of the Co-editor**. Such a request will be made *only* if there are major changes to the data (*e.g.* re-refinement of the structure). In such cases the resubmitted CIF should be sent to Chester and must contain a `_publ_contact_letter` field stating the Co-editor's manuscript reference code.

5.2. *Initial publication request*

Details of the contact author and requested journal should be entered into the submitted CIF as the data items:

```
_publ_contact_author
_publ_contact_author_email (see §3.1)
_publ_contact_author_fax
_publ_contact_author_phone
_publ_contact_letter (include the date of submission)
_publ_requested_coeditor_name
_publ_requested_journal
```

5.3. *Manuscript text*

The manuscript text information is entered as the data items:

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

These text items are entered with a standard ASCII text editor. Guidelines for entering text are given in *Appendix* 1.

5.4. *Experimental data*

The experimental data should be submitted as the specific data items listed in *Appendix* 2. Most of these items are numerical values (with the estimated standard deviations appended in parentheses, if applicable) but some are descriptive text. Several require the use of standard codes from the *CIF Core Dictionary*; these items are flagged with a † in *Appendix* 2.

The two new data items in this section `_publ_section_exptl_prep` and `_publ_section_exptl_refinement` are intended for detailed descriptive text. The former should give sufficient information on the chemical and crystal preparation and

identification (*e.g.* on melting points and densities), to reproduce the experiment, and the latter should detail any special aspects of the structure determination and refinement. The older `_publ_section_experimental` field may be used if the experimental discussion cannot be categorized in this way.

5.5. *Atomic site data*

Atomic site information is entered as a list of data items. The following items must be supplied:

```
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
```

Additional items can be included where appropriate *e.g.* site occupancies as `_atom_site_occupancy` or disorder flags as `_atom_site_disorder_group`. The rules for labelling atom sites are detailed in §7.1.

5.6. *Geometrical data*

Structural geometry data (distances and angles) are entered as separate lists, in the data item *categories*:

```
_geom_bond_*
_geom_contact_*
_geom_angle_*
_geom_torsion_*
```

The data item `*_publ` associated with each distance or angle value that is **to be published in a table** must be set as `yes`.

5.7. *Supplementary material*

Supplementary data, as specified in §4, are needed for the checking and reviewing process. Reflection data and diagrams (as HPGL or PostScript files) can be sent as a separate e-mail, or transferred using the ftp procedures described in §9

5.8. *Non-CIF material*

A signed Transfer of Copyright Agreement form must be sent to Chester by post or fax. If diagrams and supplementary data cannot be transmitted by ftp (see §9) the following items should to be sent as hard-copy by post or courier:

(i) a chemical structural diagram, *in triplicate* (see §3.9);
(ii) a crystallographic diagram, *in triplicate* (see §§3.10 and 6);
(iii) a single listing of reflection data (see §4.4);
(iv) other supplementary material, *in triplicate* (see §6.4).

5.9. *CIF submission by Internet*

A CIF submission by network transmission should be directed to the Managing Editor's e-mail address (see §2.1). Receipt will be acknowledged by e-mail and a *reference number* assigned.

Associated hard-copy material (as per §5.8) should be sent, quoting this *reference number*, by post or courier to the Managing Editor's postal address (see §2.1).

5.10. *CIF submission by magnetic media*

A CIF submission by diskette or magnetic tape should be sent, along with the associated hard-copy material (see §5.8), to the Managing Editor's postal address (see §2.1). Receipt will be acknowledged. The following media formats may be used:

3.5 in IBM-compatible diskettes.
5.25 in IBM-compatible diskettes.
3.5 in Apple Macintosh diskettes.
3.5 in Sun OS diskettes (cpio format).
0.5 in 1600/6250 bpi magnetic tape.

6. Diagrams

6.1. Design

The choice of figures, and the associated tables, should be optimized to produce the shortest possible printed paper consistent with clarity. Duplicate presentation of the same information in tables and figures is to be avoided, as is redundancy within the text. Distances and angles should be given as a table rather than displayed in the crystallographic diagram.

A chemical structural diagram must be included for molecular compounds (see *Appendix* 4 for a typical example).

6.2. Quality

It is essential that diagrams be of *publication* quality (see §§3.9 and 3.10). If diagrams are submitted as hard copy, rather than electronically (see §§5.8 and 9), they must be high-resolution black and white originals or very good photocopies. Submissions containing diagrams of poor quality will not be processed until this is rectified.

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

Each diagram should be provided on a separate sheet of about A4 size (210 × 297 mm). These will normally be reduced by the printer to fit one-column width (80 mm). Authors are requested not to make this reduction, but should take care that the orientation and labelling of the diagram is optimal for a one-column presentation. Figures at two-column width will be at Co-editorial discretion.

6.5. Lettering and symbols

Fine-scale details and lettering must be large enough to be clearly legible (not less than 1.2 mm in height) when the diagram is one column (80 mm) in width. Lettering should be kept to a minimum. Atom site labels in crystallographic diagrams should match labels used in the atom site lists and text. Distance, bond angle and torsion angle values should be given as tables and **not appear in a diagram**. Descriptive matter should be placed in the legend. If a packing diagram is submitted it must show clearly the cell axes and orientation.

Author generated lettering is preferred on diagrams and figures. If necessary, lettering can be added by the printer if a photocopy showing the required lettering is supplied with an unlettered original.

6.6. 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') should be included in the CIF. Legends of figures containing displacement ellipsoids must state the probability limit used.

7. Nomenclature

7.1. Crystallographic nomenclature

Atoms of the same chemical species within an asymmetric unit should be identified by unique labels composed of a number appended to the IUPAC chemical symbol (*e.g.* C5, C7 *etc.*).

These numbers need not be placed in parentheses. Chemical and crystallographic numbering should be in agreement wherever possible. Crystallographically equivalent atoms in *different* asymmetric units should be identified with lower-case roman numeral superscripts appended to the original atom labels (*e.g.* $C5^i$ and $C7^{iv}$).

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].

7.2. Nomenclature of chemical compounds

Names of chemical compounds and minerals are sometimes ambiguous. Authors should therefore give the molecular formula and the chemical structure diagram for each molecular compound referred to in the manuscript.

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 systematic usage.

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.

7.3. 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 '$\times 10^n$'.

8. 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.*

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:

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. (1996). 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, University of London, England.

Sheldrick, G. M. (1976). SHELX76. Program for Crystal Structure Determination. University 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.

9. File transfer

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.

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 Chester on receipt of the initial CIF submission. Files containing reflection data in CIF format should be identified by the filename extension `.hkl`. 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 shown in Fig. 1.

10. 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.

11. Reprints

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

(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.* b28.cif) as an identifiable name (*e.g.* zb1032.hkl):	`put b28.cif zb1032.hkl`
(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	

Fig. 1. Procedure for transferring files.

APPENDIX 1
Entry guidelines for CIF text

The text data items in a CIF must be entered as standard ASCII printable characters (those with decimal integer values of 32 to 126). Non-printing characters should not be used. No attempt should be made to indicate *italic* or **bold** characters.

Superscript characters should be bounded by the symbol '^'; *e.g.* enter C5^ii^ for $C5^{ii}$, 10^-2^ for 10^{-2}.

Subscript characters should be bounded by the symbol '~'; *e.g.* enter U~12~ for U_{12}.

Greek characters may be entered as digraphs in which the backslash character '\' is used to signal that the next character should be treated as a special symbol.

\a 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 \A A \B B \G Γ *etc.*

Accented characters are represented in a similar way to Greek characters:

\'e é \'a à \^a â \,c ç \"u ü \~n ñ \<c č \;c ç \=g ḡ
\.z ż \/o ø \/O Ø \/l ł \/L Ł \?i ı \?j ȷ \&s ß \(u ŭ
\>o ő \% ° \%a å \%A Å

If other accents need to be indicated for characters used in CIF text, supply these as a separate hard-copy sheet.

Note that special characters will normally only be used in _publ_ **data items**. Do not use them in _chemical_formula_ or _symmetry_space_group_name_ data items.

APPENDIX 2
CIF data items included in the *Experimental* section

The following data should be submitted as discrete CIF data items and **not** as text items, with the exception of the data items _publ_section_exptl_prep and _publ_section_exptl_refinement (see §5.3). The items flagged with a † should be supplied as one of the standard codes listed in the *CIF Core Dictionary*.

CIF data names

Crystal data

1. Chemical and crystal source or preparation (see §5.3)	_publ_section_exptl_prep
2. Chemical formula	_chemical_formula_sum _chemical_formula_moiety
3. Chemical formula weight M_r (Da)	_chemical_formula_weight
4. Cell setting†	_symmetry_cell_setting
5. Space group	_symmetry_space_group_name_H-M
6. Unit-cell dimensions (Å, °)	_cell_length_a _cell_length_b _cell_length_c _cell_angle_alpha _cell_angle_beta _cell_angle_gamma
7. Volume of unit cell V (Å^3)	_cell_volume
8. Formula units per cell Z	_cell_formula_units_Z
9. Density calculated from formula and cell D_x (Mg m^{-3})	_exptl_crystal_density_diffrn
10. Density from independent measurements D_m (Mg m^{-3}) and measurement method	_exptl_crystal_density_meas _exptl_crystal_density_method
11. Radiation type and wavelength λ (Å)	_diffrn_radiation_type _diffrn_radiation_wavelength
12. No. of reflections for cell measurement and θ range (°)	_cell_measurement_reflns_used _cell_measurement_theta_min _cell_measurement_theta_max
13. Linear absorption coefficient μ (mm^{-1})	_exptl_absorpt_coefficient_mu
14. Measurement temperature (K)	_cell_measurement_temperature
15. Crystal shape, colour and size (mm)	_exptl_crystal_description _exptl_crystal_colour _exptl_crystal_size_max _exptl_crystal_size_mid _exptl_crystal_size_min _exptl_crystal_size_rad

APPENDIX 2 (*cont.*)

CIF data names

Data collection

16. Diffractometer type and data-collection method

`_diffrn_measurement_device`
`_diffrn_measurement_method`

17. Absorption correction type,† and maximum and minimum transmission values (permitted range 0.0–1.0)

`_exptl_absorpt_correction_type`
`_exptl_absorpt_correction_T_min`
`_exptl_absorpt_correction_T_max`

18. No. of reflections measured

`_diffrn_reflns_number`

19. No. of independent reflections

`_reflns_number_total`

20. No. of observed reflections

`_reflns_number_observed`

21. Criterion for observed reflections

`_reflns_observed_criterion`

22. R_{int}

`_diffrn_reflns_av_R_equivalents`

23. Maximum value of θ (°)

`_diffrn_reflns_theta_max`

24. Range of h, k and l for measured intensities

`_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`

25. No. of standard reflections, interval and intensity decay (%)

`_diffrn_standards_number`
`_diffrn_standards_interval_count`
`_diffrn_standards_interval_time`
`_diffrn_standards_decay_%`

Refinement

26. Use of F, F^2 or I†

`_refine_ls_structure_factor_coef`

27. $R \left[= \sum (||F_o| - |F_c||)/ \sum |F_o|\right]$

`_refine_ls_R_factor_obs`

28. $wR \left\{= \left[\sum \left(w|Y_m - Y_c|^2\right)/ \sum \left(wY_m^2\right)\right]^{1/2}\right\}$
[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`

29. $S \left\{= \left[\sum w(|Y_m| - |Y_c|)^2 /(n_h - n_p)\right]^{1/2}\right\}$

`_refine_ls_goodness_of_fit_obs`

30. Number of reflections used in refinement n_h

`_refine_ls_number_reflns`

31. Number of parameters refined n_p

`_refine_ls_number_parameters`

32. Method of refining and locating H atoms†

`_refine_ls_hydrogen_treatment`

33. Weighting scheme†

`_refine_ls_weighting_scheme`

34. Maximum Δ/σ

`_refine_ls_shift/esd_max`

35. $\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e Å^{-3})

`_refine_diff_density_max`
`_refine_diff_density_min`

36. Extinction correction method (if applied), and primary- and secondary-extinction values

`_refine_ls_extinction_method`
`_refine_ls_extinction_coef`

37. Source of atomic scattering factors

`_atom_type_scat_source`

38. Absolute structure details (if applicable)

`_refine_ls_abs_structure_details`

39. 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`

40. Discussion of structure determination and refinement procedure (see §5.3)

`_publ_section_exptl_refinement`

APPENDIX 3

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Authors (*Please type or use capital letters*)

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APPENDIX 4
Annotated example of a *Section C* paper

The First Dinuclear Cobalt–Rhenium Cluster Compound: Hexacarbonylbis(μ-dicyclohexylphosphanido)cobaltrhenium

The title should be concise yet descriptive. It must include the chemical name or the formula. Because all papers in Acta C describe structures, phrases such as 'Structure of' may be omitted.

ULRICH FLÖRKE AND HANS-JÜRGEN HAUPT

Anorganische und Analytische Chemie, Universität-GH Paderborn, Warburgerstrasse 100, D-4790 Paderborn, Germany. E-mail: floe@mvaxac.uni-paderborn.de
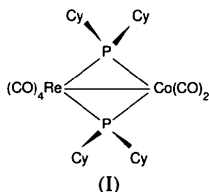
The authors' names should, where possible, include the full first name.

Abstract

The title compound [hexacarbonyl-$1\kappa^4C,2\kappa^2C$-bis(μ-dicyclohexylphosphido-$1:2\kappa^2P$)cobaltrhenium(Co—Re) 0.5-methanol solvate, [CoRe($C_{12}H_{22}P$)$_2$(CO)$_6$].0.5(CH$_3$-OH), belongs to a type of edge-linked tetrahedron–octahedron coordination complex. The molecule has local C_{2v} symmetry with ecliptic conformation of the carbonyl ligands at both metal centres, and a Co—Re single-bond length of 2.786 (1) Å.

The Abstract should contain the full IUPAC chemical name and formula (if it is not present in the title), and basic data which identify the type of chemistry and structure studied. Any special geometry should be highlighted.

Comment

In the course of our work on phosphanido-bridged homo- and heteronuclear metal-atom cluster compounds (Haupt, Balsaa & Flörke, 1988; Haupt, Heinekamp & Flörke, 1989; Flörke & Haupt, 1993), we isolated the title compound (I) in which a Co—Re bond is symmetrically bridged by two dicyclohexylphosphanido groups.

The Comment section should start with background information on the chemical, mineralogical and/or crystallographic origins of the material reported. The reasons why the structure was studied should be explained carefully. References to related studies should be included.

(I)

A chemical diagram is mandatory for molecular structure studies. This diagram will also be used for the Contents section of the journal (a synopsis will appear in the Contents listings for non-molecular structures).

The Co atom has distorted tetrahedral coordination from two carbonyl ligands and the bridging P atoms. These bridging atoms and four of the carbonyl groups give rise to distorted octahedral coordination at the Re atom. The central CoReP$_2$ ring is nearly planar; the maximum deviation from the best plane is 0.02 Å with a dihedral angle of 2.2°. With respect to the different metal atomic radii, the ring may be regarded as regular. It shows two equal M—P bond lengths for Co [2.111 (1) and 2.116 (1) Å] as well as for Re [2.541 (1) and 2.544 (1) Å]. The enclosed ring angles at both P atoms are acute [72.8 (1) and 72.9 (1)°] and the P—M—P angles reflect the distorted coordination polyhedron of each metal atom

Only the novel aspects of the structural geometry should be emphasized. These should be related to studies of similar structures and to studies of the compound using other techniques (NMR, IR, etc.). Any unusual geometry should be compared with the standard data listed in §9 of International Tables for Crystallography, Volume C.
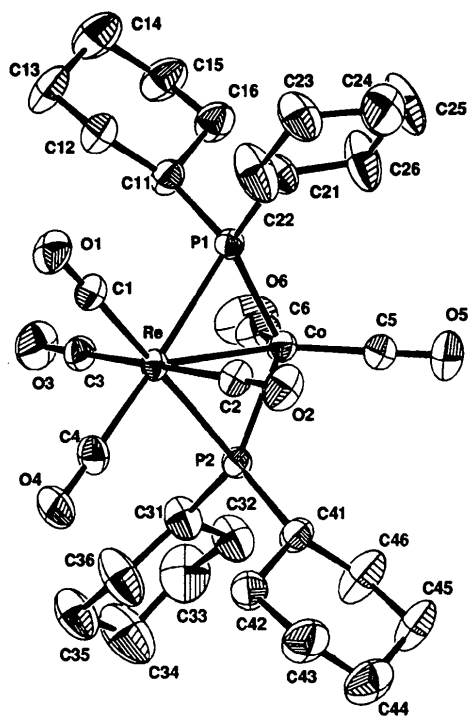
Fig. 1. Molecular structure showing 30% probability displacement
ellipsoids. H atoms are omitted for clarity.

A good molecular diagram is essential for a structural paper and it must be oriented to show the most important geometry. The atom labels must be readable when the diagram is reduced to one-column width (80 mm). Labels should clearly identify the atom sites and must match those listed in the table of atom coordinates and U values. Ellipsoid plots are preferred to line, ball-and-stick or CPK plots because they aid visualization of the atomic displacements and hence provide disorder and thermal-motion information. Unrefined H-atom sites may be omitted, or shown as balls. Distance and angle values should not be placed on the diagram.
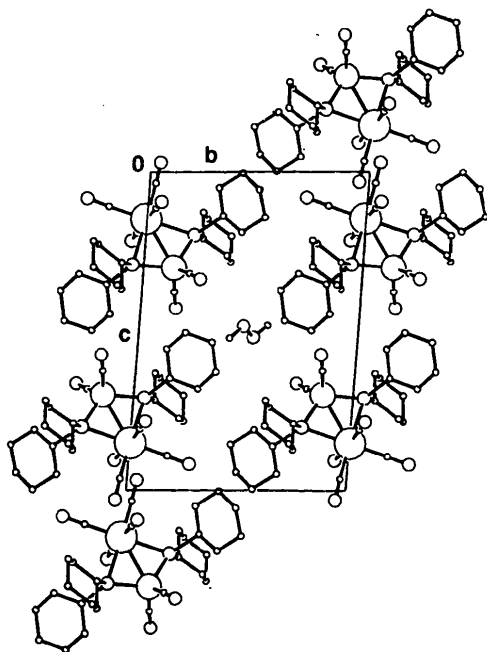
Fig. 2. Packing diagram viewed down the *a* axis. Note the solvent
molecule in the centre of the cell.

A cell plot is useful if hydrogen bonding, solvent molecules or close van der Waals contacts need to be shown. This diagram can be stylized to emphasize packing information. The orientation of the cell must be displayed with respect to a set of right-handed axes. Hydrogen bonds are normally shown as dashed lines with the donor and acceptor sites suitably labelled.

[121.3 (1) and 92.9 (1)° for Co and Re, respectively]. The most interesting structural feature is the Co—Re single bond which meets the requirement of 18 valence electrons for each metal atom and has a length of 2.786 (1) Å. We have established, by use of the Cambridge Structural Database (Allen *et al.*, 1979), that the only other cobalt–rhenium cluster reported so far is [Co$_2$Re(μ_3-CC$_6$H$_4$Me$_4$)(CO)$_{10}$] (Jeffery, Lewis, Lewis & Stone, 1985), with Co—Re bond lengths of 2.686 (1) and 2.720 (1) Å. This triangular cluster has distinctly different bonding and bridging patterns, so direct comparison of the heteronuclear bond lengths of both compounds is not possible. However . . .

Experimental

Synthesis was carried out by reaction of Re$_2$(CO)$_{10}$, Co$_2$(CO)$_8$ and HP(C$_6$H$_{11}$)$_2$ (molar ratio 1:1:2) in xylene solution for 10 h at 423 K in a glass tube. Recrystallization was from MeOH.

Crystal data

[CoRe(C$_{12}$H$_{22}$P)$_2$(CO)$_6$].-0.5CH$_3$OH	Mo $K\alpha$ radiation
M_r = 823.7	λ = 0.71073 Å
Triclinic	Cell parameters from 40
$P\bar{1}$	reflections
a = 10.452 (3) Å	θ = 7–16°
b = 11.664 (4) Å	μ = 4.07 mm^{-1}
c = 15.641 (4) Å	T = 293 K
α = 94.37 (2)°	Prism
β = 89.75 (2)°	0.50 × 0.34 × 0.28 mm
γ = 111.87 (2)°	Red
V = 1763.8 (8) Å^3	
Z = 2	
D_x = 1.551 Mg m^{-3}	
D_m not measured	

Data collection

Siemens $R3m/V$ diffractometer	R_{int} = 0.022
	θ_{max} = 27.5°
ω–2θ scans	h = −13 → 13
Absorption correction:	k = −15 → 15
empirical *via* ψ scans	l = −21 → 21
T_{min} = 0.690, T_{max} = 0.894	4 standard reflections
15 189 measured reflections	monitored every 400
8161 independent reflections	reflections
6813 observed reflections	intensity decay: none
[$F > 4\sigma(F)$]	

Refinement

Refinement on F	w = 1/[$\sigma^2(F)$ + 0.0001F^2]
R = 0.038	$(\Delta/\sigma)_{max}$ = 0.001
wR = 0.034	$\Delta\rho_{max}$ = 0.95 e Å^{-3}
S = 1.583	$\Delta\rho_{min}$ = −0.80 e Å^{-3}
6813 reflections	Extinction correction: none
379 parameters	Atomic scattering factors
H-atom parameters not refined	from *SHELXTL-Plus* (Sheldrick, 1990)

If there is more than one structure, each experimental data set should be identified with a sequence code [e.g. (1), (2), ... or (I), (II), ...].

A brief summary of the chemical and crystal preparation should be given in sufficient detail to reproduce these aspects of the experiment.

The wavelength λ refers to the radiation used to measure intensities (i.e. mean $K\alpha$ rather than $K\alpha_1$).

The absorption coefficient μ is in mm^{-1} not cm^{-1}.

The calculated density, D_x, must be supplied; D_m should be measured if at all possible and details of the method given.

θ_{max} refers to the diffraction angle θ not 2θ.

The absorption transmission factors T should range from 0.0 to 1.0. T_{min} must be $\leq T_{max}$. Co-editors will query T_{max} values that exceed 1.1, or T_{max}/T_{min} ratios that are inappropriate for the crystal under study.

The observed reflection threshold should be as low as possible so as not to bias the structure refinement. Use thresholds of $2\sigma(I)$ [or $4\sigma(F)$], or lower, to ensure that the number of reflections used in the least-squares refinement is as large as possible.

The R value is always calculated on F, whereas wR is calculated with the coefficient used in the least-squares refinement (F, F^2 or I).

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters ($\mathring{A}^2$)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Re	0.2227 (1)	−0.0032 (1)	0.1460 (1)	0.042 (1)
Co	0.2347 (1)	0.1392 (1)	0.2992 (1)	0.046 (1)
P1	0.3589 (1)	0.2221 (1)	0.1970 (1)	0.044 (1)
P2	0.1068 (2)	−0.0511 (1)	0.2891 (1)	0.046 (1)
C1	0.3087 (6)	0.0299 (6)	0.0346 (4)	0.057 (4)
O1	0.3569 (5)	0.0449 (5)	−0.0308 (3)	0.079 (3)
C2	0.0662 (6)	0.0396 (6)	0.1118 (4)	0.056 (4)
O2	−0.0268 (5)	0.0626 (5)	0.0927 (3)	0.087 (4)
C3	0.3789 (7)	−0.0423 (6)	0.1896 (4)	0.063 (4)
O3	0.4690 (5)	−0.0639 (5)	0.2137 (4)	0.109 (4)
C4	0.1264 (7)	−0.1761 (6)	0.1055 (4)	0.062 (4)
O4	0.0725 (5)	−0.2773 (4)	0.0804 (3)	0.082 (4)
C5	0.1174 (8)	0.2127 (6)	0.3180 (5)	0.074 (5)
O5	0.0439 (7)	0.2631 (6)	0.3357 (5)	0.132 (5)
C6	0.3598 (7)	0.1483 (7)	0.3744 (4)	0.067 (4)
O6	0.4420 (6)	0.1602 (6)	0.4263 (4)	0.113 (5)
C11	0.5479 (6)	0.2618 (6)	0.2073 (4)	0.056 (4)
C12	0.6243 (6)	0.2560 (7)	0.1253 (4)	0.069 (4)
C13	0.7736 (7)	0.2760 (8)	0.1443 (5)	0.087 (6)
C14	0.8445 (8)	0.3902 (9)	0.2000 (6)	0.095 (7)
C15	0.7702 (7)	0.3955 (8)	0.2803 (5)	0.080 (5)
C16	0.6220 (7)	0.3776 (7)	0.2601 (5)	0.072 (5)
C21	0.3424 (7)	0.3479 (6)	0.1367 (4)	0.066 (4)
C22	0.2909 (12)	0.3202 (8)	0.0493 (5)	0.115 (8)
C23	0.2763 (10)	0.4240 (7)	0.0032 (5)	0.101 (6)
C24	0.2284 (11)	0.5054 (9)	0.0555 (6)	0.136 (8)
C25	0.2913 (13)	0.5398 (8)	0.1420 (6)	0.127 (8)
...	...	...	...	...

Table 2. *Selected geometric parameters ($\mathring{A}$, °)*

Re—Co	2.786 (1)	Co—P1	2.111 (1)
Re—P1	2.544 (1)	Co—P2	2.116 (1)
Re—P2	2.541 (1)		
Co—Re—P1	46.4 (1)	Re—Co—P2	60.6 (1)
Co—Re—P2	46.5 (1)	P1—Co—P2	121.3 (1)
P1—Re—P2	92.9 (1)	Re—P1—Co	72.9 (1)
Re—Co—P1	60.8 (1)	Re—P2—Co	72.8 (1)

The enclosed CH_3OH solvent molecule had a site occupation factor of 0.5. Cyclohexyl H atoms were fixed at ideal positions with common isotropic displacement parameters ($U_{iso} = 0.08$ $\mathring{A}^2$). Structure solution and refinement used *SHELXTL-Plus* (Sheldrick, 1990). Other programs include *PARST* (Nardelli, 1983).

References

Allen, F. H., Bellard, S., Brice, M. D., Cartwright, B. A., Doubleday, A., Higgs, H., Hummelink, T., Hummelink-Peters, B. G., Kennard, O., Motherwell, W. D. S., Rodgers, J. R. & Watson, D. G. (1979). *Acta Cryst.* **B35**, 2331–2339.

Flörke, U. & Haupt, H.-J. (1993). *Acta Cryst.* **C49**, 374–376.

Haupt, H.-J., Balsaa, P. & Flörke, U. (1988). *Inorg. Chem.* **27**, 280–286.

Haupt, H.-J., Heinekamp, C. & Flörke, U. (1989). *Inorg. Chem.* **29**, 2955–2963.

Jeffery, J. C., Lewis, D. B., Lewis, G. E. & Stone, F. G. A. (1985). *J. Chem. Soc. Dalton Trans.* pp. 2001–2007.

Nardelli, M. (1983). *Comput. Chem.* **7**, 95–98.

Sheldrick, G. M. (1990). *SHELXTL-Plus. Structure Determination Software Programs.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Equivalent isotropic displacement parameters are calculated as follows:

From U_{ij}

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

From B_{ij}

$$U_{eq} = (1/24\pi^2)\Sigma_i\Sigma_j B_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

$$B_{eq} = (1/3)\Sigma_i\Sigma_j B_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

From β_{ij}

$$U_{eq} = (1/6\pi^2)\Sigma_i\Sigma_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

$$B_{eq} = (4/3)\Sigma_i\Sigma_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

Note that hydrogen-atom data should only be included in the table of coordinates if they have been refined. They will be published at the Co-editor's discretion.

Only geometric data (distances and angles) that need to be drawn to the special attention of the reader should be listed. Torsion angles, intermolecular contact distances and/or deviations from planes that are needed to describe novel features of the structure should be included.

The text of the Experimental *section should report specific technical data about the tables and details of the software used in the structure calculation and presentation. These details should be sufficient that, given access to the supplementary data, the presented results could be reproduced.*

Reference information must be submitted in the Acta style. First and last page numbers are mandatory.