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. These supercede those of *Acta Cryst.* (1993). C49, 194-204.

Authors are strongly encouraged to submit *Section C* papers in Crystallographic Information File (CIF) format. CIF submissions will be rewarded with faster publication. Hard-copy submissions must be keyboarded as a CIF by the editorial staff and this inevitably slows down the processing of a paper.

The Notes are divided into the following sections:

§2. Submission policies for papers
§3. Format and contents of published material
§4. Supplementary material for checking and archiving
§5. Requirements for papers submitted electronically
§6. Requirements for papers submitted as hard-copy
§7. Requirements for diagrams
§8. Nomenclature
§9. References
§10. Large data transfer

Appendix 1. Text entry requirements for electronic submissions
Appendix 2. Essential items for the *Experimental* section
Appendix 3. *Experimental Details* hard-copy submission form
Appendix 4. Transfer of Copyright Agreement form
Appendix 5. Annotated example of a *Section C* paper

2. Submission of papers

2.1. *Address for submissions*

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

Publication material submitted as a CIF on magnetic media, or as hard-copy, should be sent by airmail or courier to:

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

Telephone: 44 244 342878
Fax:　　　44 244 314888

Material submitted as a CIF should normally be e-mailed to:

med@iucr.ac.uk

or, for large data files, transmitted by FTP (see §10) to:

ftp.iucr.ac.uk (192.70.142.1)

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* 4) 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. *Methods of submission*

Papers may be submitted to the Chester office:
(i) as a CIF sent either by e-mail or by post on magnetic media (see §5),
(ii) as hard-copy material sent by post or courier (see §6), or
(iii) as a combination of (i) and (ii).

2.7. *Handling of manuscripts*

A paper submitted to Chester as a CIF will be first checked for completeness. If it is incorrectly constructed or incomplete it will be returned to the author for revision. A paper submitted as hard-copy is first keyboarded into CIF format and thereafter handled in the same way as an author-generated CIF. 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, and is a CIF submission, the Managing Editor may class it as a *fast-track submission.* These submissions will be 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.

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 §§5 and 6. An example of a published paper is shown in *Appendix 5*.

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 ...*'. The first name of each author should appear in full.

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.* Little or no discussion is required of geometrical data which agrees 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 §9. 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 headings *Crystal data*, *Data collection* and *Refinement*. Any discussion of *experimental procedure* should be given in grammatically correct text. A list of experimental data requested is provided in *Appendices* 2 and 3.

3.7. Atomic site data

A table containing site information for non-hydrogen atoms must be provided. Information about hydrogen-atom sites will be printed only at the Co-editor's discretion (see §§5.5 and 6.3).

3.8. Selected geometrical data

A tabulation of the most important bond distances, interatomic contacts, bond angles and torsion angles should be submitted, *e.g.* details of peripheral phenyl rings should be omitted. This material may be amended by the Co-editor (see §§5.6 and 6.3).

3.9. Chemical structural diagram

Papers reporting the structure of a molecular compound must contain a chemical structural diagram (see §7 and the example in *Appendix 5*).

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. Diagrams with atom sites displayed as displacement ellipsoids are preferred. Unique atom sites should be identified with labels as specified in §8.1. The atom labels must be used consistently in the diagram and the table of atom coordinates (§3.7). Additional diagrams are at the Co-editor's discretion. The required quality of diagrams is detailed in §7.

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 10), 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 requested for the checking and reviewing process.

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)*, 1601 *Park Lane, Swarthmore, PA* 19081-2389, *USA*. These data will be checked and assigned an *ICDD* reference number which will, where possible, be published in the paper.

5. CIF submission

5.1. General approach

Authors are strongly encouraged to use the CIF format to submit papers to *Section C*. In a CIF each data item is identified by a corresponding data name. The data items requested are described briefly below and in *Appendix 2*. More detailed descriptions of these items are given in the *CIF Core Dictionary* [Hall, Allen & Brown (1991). *Acta Cryst.* A47, 655-685]. The requirements for text items in a CIF are summarized in *Appendix 1*, and an example of a published paper is given in *Appendix 5*.

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 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 under active development.)

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 10.

The CIF 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 printed manuscript is generated from the submitted CIF using software at Chester. This will be forwarded to the Co-editor for use in the review process. Any amendments to the

paper during the 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
_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
_publl_section_comment
_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*. Two data items in this section, _chemical_compound_source and _publ_section_experimental are intended for detailed descriptive text. The former should give a summary of the chemical and crystal preparation in sufficient detail to reproduce the experiment, and the latter should detail any special aspects of the structure determination and refinement.

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.* disorder flags as _atom_site_disorder_group. The rules for labelling atom sites are detailed in §8.1.

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_*
```

Each distance or angle value must be tagged with a *_publ flag value of yes if it is to be published in a table.

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 (file transfer protocol) procedures described in §10.

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 §10) 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 7);
(iii) a single listing of reflection data (see §4.4);
(iv) other supplementary material, *in triplicate* (see §6.4).

5.9. *CIF submission by network transmission*

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″ 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. Hard-copy submission

If a paper cannot be prepared in CIF format, three copies of the hard-copy manuscript should be submitted along with **one** *Experimental Details* form *for each structure*. Supplementary material should be submitted, in triplicate, except for a single copy of the reflection data.

6.1. *General layout of the manuscript*

Papers 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.

6.2. *Experimental Details*

The numerical and text description of the experimental procedures must be submitted on a completed *Experimental Details* form (*Appendix* 3). The text description of the experimental procedures should be included on, or attached to, this form and *not given or repeated elsewhere in the paper*. The form covers all of the quantities listed in *Appendix* 2.

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, will be input to automated checking routines and used to prepare camera-ready copy of the *Experimental* section for printing (**there is thus no need for authors to write a separate** *Experimental* **section**). Secondly, it ensures that authors do not accidentally omit essential information when preparing their manuscript.

Data items required for powder diffraction studies will be published shortly. In the meantime, authors of these papers 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*

A table of site data for non-hydrogen atoms should include *atom label, fractional x, y, z* and *U* (together with associated e.s.d.'s in parentheses). The equivalent isotropic displacement value U_{eq} for the anisotropic displacement parameters should be given where appropriate (see *Appendix* 5 for definitions). If possible authors should supply displacement parameters as *U*'s rather than *B*'s. For hydrogen-atom site data see §4.1.

A table of intramolecular geometry for publication should contain only those distances and angles (together with associated e.s.d.'s in parentheses) that are of **maximum** interest.

6.4. *Supplementary material*

Supplementary material (see §4) submitted as hard-copy must:

(i) be sent, **in triplicate** (except for reflection data), with the submitted paper;
(ii) start with a page containing the *Title* and *Abstract* of the paper;
(iii) be of sufficient clarity for good quality photocopying;
(iv) be on paper not exceeding A4 size (210 × 297 mm);
(v) have lettering that is not less than 1.2 mm in height;
(vi) be clearly numbered to ensure the correct page sequence.

7. Diagrams

7.1. *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* 5 for a typical example).

7.2. *Quality*

If diagrams are submitted as hard-copy, rather than electronically (see §§5.8 and 10), they should be high-quality black and white originals or good photocopies. High-resolution laser printouts are acceptable.

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*

Where possible each diagram should be provided on a separate sheet of about A4 size (210 × 297 mm). These will normally be scaled by the printer so that the greatest width, including

lettering, will be one-column width (80 mm). Figures at two-column width will be at Co-editorial discretion.

7.5. *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.

7.6. *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') is to be included in the CIF submission or attached to the hard-copy manuscript.

8. Nomenclature

8.1. *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 in hard-copy manuscripts or diagrams 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].

8.2. *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.

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.*

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. (1994). 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.

10. Large data transfer

Authors with computer access to Internet (a primary e-mail route) may use anonymous file transfer protocol (FTP) to transfer large electronic files to the *Acta* 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 as follows:

(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

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 ŏ \% ° \%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 (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

	CIF data names
1. Chemical and crystal source or preparation	`_chemical_compound_source`
2. Chemical formula	`_chemical_formula_sum` `_chemical_formula_moiety`
3. Chemical formula weight M_r (Da)	`_chemical_formula_weight`
4. Crystal system†	`_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`

APPENDIX 2 (*cont.*)

CIF data names

| 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` |

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 variation (%)

`_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. $R [= \sum (||F_o| - |F_c||)/ \sum |F_o|]$ `_refine_ls_R_factor_obs`

28. $wR \left\{ = \left[\sum \left(w|Y_m - Y_c|^2\right)/ \sum \left(wY_m^2\right)\right]^{1/2} \right\}$ `_refine_ls_wR_factor_obs`
[where Y_m and Y_c are the measured and calculated coefficients specified above (*i.e.* *F*, F^2 or *I*)]

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

30. Number of reflections used in refinement   `_refine_ls_number_reflns`

31. Number of parameters refined   `_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 §3.6)

`_publ_section_experimental`

APPENDIX 3
Experimental form for hard-copy submission

E.s.d.'s should be given where appropriate. Please complete in the language of submission, ticking boxes as appropriate. A separate form should be provided for each compound studied.

Compound identifier [*e.g.* (1), (2) ... or (I), (II) ...] _____

Crystal data

1. Chemical and crystal source or preparation (append separate sheet if needed)

2. Chemical formula (sum) (*e.g.* C18 H19 N7 O8 S) _____

   (moiety) (*e.g.* C18 H17 N7 O7 S, H2 O) _____

3. Chemical formula weight M_r (Da) _____

4. Crystal system   ☐ Triclinic   ☐ Monoclinic   ☐ Hexagonal   ☐ Orthorhombic
                     ☐ Tetragonal   ☐ Cubic   ☐ Rhombohedral   ☐ Trigonal

5. Space group _____ (give details for non-standard settings) _____

6. Unit-cell dimensions (Å, °) a _____ b _____ c _____

   α _____ β _____ γ _____

7. Volume of unit cell V (Å^3) _____   8. Formula units per cell Z _____

9. Density calculated from formula and cell D_x (Mg m^{-3}) _____

10. Density from independent measurements D_m (Mg m^{-3}) _____

    Measurement method ☐ None ☐ Pycnometry ☐ Flotation in _____ ☐ Other_____

11. Radiation type   ☐ Mo $K\alpha$ ☐ Cu $K\alpha$ ☐ Ag $K\alpha$ ☐ Other_____

    Wavelength λ (Å) ☐ 0.71073 ☐ 1.54184 ☐ 0.5608 ☐ Other_____

12. No. of reflections for cell measurement _____ θ range (°) _____ to _____

13. Linear absorption coefficient μ (mm^{-1}) _____ 14. Measurement temperature (K) _____

15. Crystal shape _____ Colour _____

    Size (mm) ☐ Max. _____ Mid. _____ Min. _____ ☐ Radius _____

APPENDIX 3 (*cont.*)

Data collection

16. Diffractometer type _____

    Data-collection method ☐ ω scans ☐ $\omega/2\theta$ scans ☐ $\theta/2\theta$ scans ☐ Other _____

17. Absorption correction type   ☐ Analytical   ☐ Integration   ☐ Empirical   ☐ Refined from ΔF
                                ☐ Spherical   ☐ Cylindrical   ☐ None   ☐ Given in §40

                                  ☐ Other _____

    Minimum and maximum transmission values (permitted range 0.0-1.0) T_{min} _____ T_{max} _____

18. No. of reflections measured _____   19. No. of independent reflections _____

20. No. of observed reflections _____

21. Criterion for observed reflections   ☐ $I > n\sigma(I)$, n = _____   ☐ $F > n\sigma(F)$, n = _____

                                 ☐ Other _____

22. R_{int} _____   23. Maximum value of θ (°) _____

24. Range of h, k, l h_{min} _____ h_{max} _____ k_{min} _____ k_{max} _____ l_{min} _____ l_{max} _____

25. No. of standard reflections _____   ☐ Interval (No. of reflections) _____

    Intensity variation (%) _____   ☐ Interval (time) (min) _____

Refinement

26. Use of   ☐ F ☐ F^2 ☐ I ☐ Other _____

27. R _____   28. wR _____   29. S _____

30. No. of reflections used in refinement _____   31. No. of parameters refined _____

32. Method of refining and locating H atoms   ☐ All H-atom parameters refined   ☐ Only H-atom coordinates refined
                                       ☐ H atoms refined isotropically   ☐ Not refined
                                       ☐ Given in §40

                                       ☐ Other _____

33. Weighting scheme   ☐ Based on measured e.s.d.'s   ☐ Unit or no weights   ☐ Calculated weights

                         ☐ Other _____

     ☐ $w = 1/\sigma^2(F)$ ☐ Other w = _____

34. Maximum Δ/σ _____

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

36. Extinction correction method (if applied) _____

    Primary- and secondary-extinction values _____

APPENDIX 3 (*cont.*)

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37. Source of atomic scattering factors ☐ *International Tables for X-ray Crystallography* Vol. IV
☐ *International Tables for Crystallography* Vol. C
☐ Cromer & Waber (1974)

☐ Other _____

38. Absolute structure details (if applicable) _____

_____

39. All computer programs used [include name (date) reference, full reference to be given in the reference list]

Data collection _____

_____

Cell refinement _____

_____

Data reduction _____

_____

Structure solution _____

_____

Structure refinement _____

_____

Molecular graphics _____

_____

Preparation of material for publication _____

_____

40. Discussion of structure determination and refinement procedure (append separate sheet if needed)

APPENDIX 4

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APPENDIX 5
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

The authors' names should include the full first name.

Abstract

The title compound [hexacarbonyl-1$\kappa^4 C$,2$\kappa^2 C$-bis(μ-dicyclohexylphosphido-1:2$\kappa^2 P$)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.

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 a 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

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.
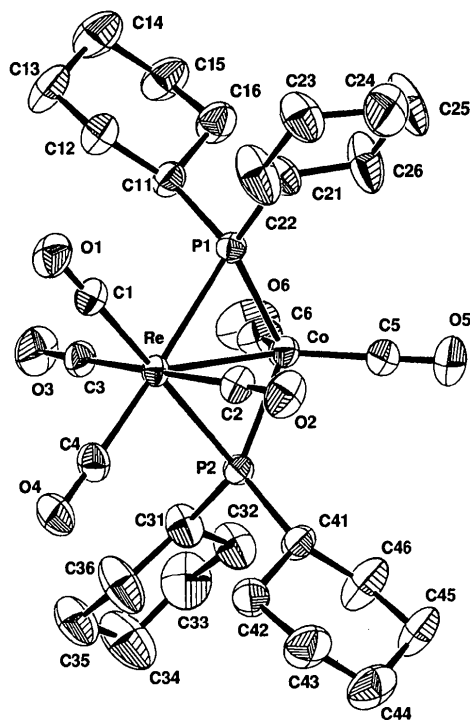
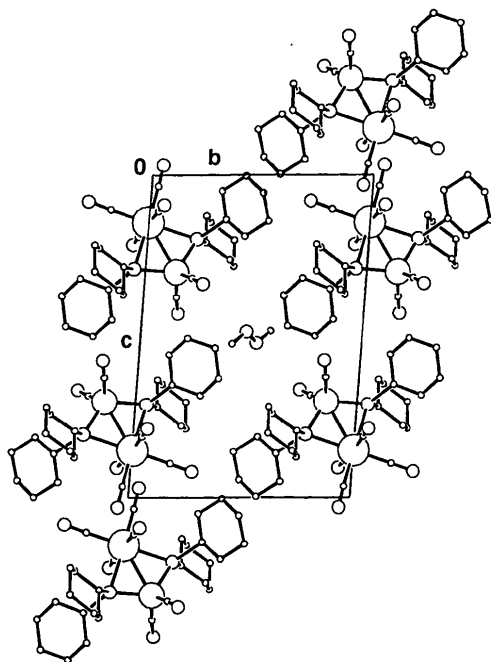Fig. 1. Molecular structure showing 50% probability displacement ellipsoids. H atoms are omitted for clarity.

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.

the distorted coordination polyhedron of each metal atom [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

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), ...].

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.

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

Crystal data

[CoRe(C$_{12}$H$_{22}$P)$_2$(CO)$_6$].- 0.5(CH$_3$OH)	$Z = 2$
$M_r = 823.7$	$D_x = 1.551$ Mg m^{-3}
Triclinic	Mo $K\alpha$ radiation
$P\bar{1}$	$\lambda = 0.71073$ Å
$a = 10.452$ (3) Å	Cell parameters from 40
$b = 11.664$ (4) Å	reflections
$c = 15.641$ (4) Å	$\theta = 7-16°$
$\alpha = 94.37$ (2)°	$\mu = 4.07$ mm^{-1}
$\beta = 89.75$ (2)°	$T = 293$ K
$\gamma = 111.87$ (2)°	Prism
$V = 1763.8$ (8) Å^3	0.50 × 0.34 × 0.28 mm
	Red

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

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}.

Data collection

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

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.

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, and ensure that the number of reflections used in the least-squares refinement is at least ten times the number of parameters refined.

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	Atomic scattering factors
379 parameters	from *SHELXTL-Plus*
H-atom parameters not refined	(Sheldrick, 1990)

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 (Å^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 (Å, °)*

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 Å^2). Structure solution and refinement used *SHELXTL-Plus* (Sheldrick, 1990). Other programs include *PARST* (Nardelli, 1983).

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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.