

## Notes for authors

*Acta Crystallographica Section C: Crystal Structure Communications* publishes full papers with details of crystal structures determined by diffraction methods. It specializes in the rapid dissemination of high-quality studies of novel and challenging crystal and molecular structures of interest in the fields of chemistry, biochemistry, mineralogy, pharmacology, physics and materials science. The unique checking, editing and publishing facilities of the journal ensure the highest standards of structural reliability and presentation, while providing for reports on studies involving special techniques or difficult crystalline materials.

### 1. Submission requirements

#### 1.1. Author checking of manuscripts

All papers must be submitted in Crystallographic Information File (CIF) ASCII format (MIME or other encoded formats should be avoided if possible). Details about CIFs are given in Hall, Allen & Brown [*Acta Cryst.* (1991), **A47**, 655–685]. Guidelines for the preparation and editing of a CIF, the data items required therein, standard data codes and keywords, CIF templates, example CIFs, and data-validation criteria and procedures are available *via* the online CIF help page (see §7). A free CIF editor (enCIFer) is under development by the Cambridge Crystallographic Data Centre (CCDC) and will be made available in due course. The Editor, Co-editors and Chester staff are also available to assist any author.

Authors are required to pre-check their submission by e-mailing their CIF to [checkcif@iucr.org](mailto:checkcif@iucr.org). A check report will be returned automatically to the sender's e-mail address. Any reported problems with the submitted data will need to be corrected before submission. If the report contains validation alerts about the consistency, adequacy or quality of the data, these will need to be addressed, or, if the authors consider there are specific valid or unavoidable reasons for these alerts, the validation response form (VRF) supplied by **checkcif** must be completed and included in the submitted CIF.

The text and tables of a paper, as distributed to the Co-editors and referees, may be previewed by sending the CIF (after completing the pre-check) to [printcif@iucr.org](mailto:printcif@iucr.org). A PostScript file of the paper will be returned for local printing. We strongly encourage authors to make use of this facility. Note that use of these automatic checking and printing facilities does not constitute a submission to *Section C*. The **checkcif** and **printcif** facilities are also directly accessible online (see §7).

#### 1.2. Categories of submission

*Section C* publishes two categories of papers. The requested category must be specified in the submitted CIF as `_publ_requested_category`, using one of the codes listed below.

(a) Full papers describe one or more structure determinations. These submissions are validated (see §3) and peer reviewed. The accepted paper is printed in the journal and is accessible electronically, together with the CIF and structure factors, from the **Crystallography Journals Online** service at the web address

<http://journals.iucr.org> (see §7). The category codes used to identify these papers are FI for inorganic, FM for metal–organic, and FO for organic structures.

(b) *Addenda and Errata* are short printed papers describing additions to, comments on, or errata to existing *Section C* publications and are *not* intended for interim reports of work in progress. The text should not exceed 1000 words. Addenda and Errata are peer reviewed. The category code for these papers is AD.

#### 1.3. Method of submission

CIFs must be submitted via the web at <http://journals.iucr.org/services/submit.html>. All submitted CIFs must have been pre-checked using the facilities described in §1.1.

Authors will be sent an e-mail that formally acknowledges receipt of the CIF and provides the Chester *refcode* (see §1.9). The Chester *refcode* has two letters and four digits (e.g. fg1795), with the two letters identifying the assigned Co-editor; the *refcode* should be used in all subsequent communications with the Chester office and Co-editor.

The acknowledgement e-mail also provides details of how to complete the submission process and the additional material required for submission. This includes the chemical scheme (see §2.10), crystallographic diagrams (see §2.11) and structure factors (see §2.14). This material should not be uploaded before the acknowledgement e-mail has been received. During the submission process, authors will also be asked to agree to transfer the copyright of their paper to the IUCr (see §1.6).

Contact details for the IUCr Editorial Office are as follows:

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

Telephone: +44 1244 342878  
Fax: +44 1244 314888

All e-mail communications concerning a particular paper should be sent to [refcode@iucr.org](mailto:refcode@iucr.org), where *refcode* is the Chester assigned code as described above.

#### 1.4. Languages of submission

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

#### 1.5. Author's warranty

The submission of a paper is taken as an implicit guarantee that the work is original, that it is the author(s) own work, that all authors concur with and are aware of the submission, that all workers involved in the study are listed as authors or given proper credit in the acknowledgements, that the results have not already been published (in any language or medium) or deposited in a public access database, and that the paper is not being considered and will not be offered elsewhere while under consideration for an IUCr journal.

#### 1.6. Copyright

Except as required otherwise by national laws, an author will be required to agree to the transfer of copyright before a manuscript can be accepted.

### 1.7. Handling of manuscripts

Each submitted CIF is checked in Chester for completeness and data integrity. If incomplete or inadequate it will be returned to the contact author for correction. Some of the specific data standards are summarized in §3, while full details of the required data items and the data-validation criteria are available *via* the online CIF help page (see §7). Papers failing to meet these criteria are handled differently according to whether a completed validation response form (VRF) giving reasons for the failure has been included in the CIF. If a VRF is present, the CIF and *Check Report* are e-mailed to the Data-Validation Editor who will assess the validity of the explanation. If a VRF is not present in a failed CIF, the submission will be returned to the contact author.

Papers will be forwarded, together with the *Check Report*, to a Co-editor, who is responsible for the review steps and future communications with the authors up to the acceptance stage. Failure to respond to a communication from either a Co-editor or the Chester editorial staff **within one month** will result in the automatic withdrawal of the paper. If major revisions are made to the submission the journal reserves the right to reset the date of receipt of the paper to the date of resubmission.

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. The Section Editor reviews all accepted papers and reserves the right to make appropriate changes to ensure conformity with *Section C* standards; in the unlikely event of a serious problem being detected at this stage, the authors will be contacted promptly.

### 1.8. Author grievance procedure

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

### 1.9. File naming and transfer

All files should be transferred via the web interface at <http://journals.iucr.org/services/submit.html>. Filenames should be constructed from the *refcode* supplied by Chester (§1.3). Files should not be encoded, compressed, in word processor native form or in any other program native form.

Files containing reflection data in CIF format should be identified by the filename extension **.hkl**. Where more than one structure is reported in the CIF, the names of the files containing the reflection data should be in the form *refcode.id.hkl* (e.g. fg1795.1.hkl) where *id* is the **data\_** block code for the corresponding structure in the CIF. Illustrations should be given the extensions **.hpg**, **.ps**, **.eps** or **.tif**. Multiple files for the same submission should be uniquely identified, e.g. fg1795fig1.ps and fg1795fig2.ps.

## 2. Publication requirements

The publication requirements for the text, tabular and graphical material are described in this section. The standards for numerical and codified data are summarized in §3, and a list of all items required for submission is available *via* the online CIF help page (see §7).

### 2.1. Title and authors

The *Title* should be short and informative; in many cases just the name(s) of the compound(s) studied will be perfectly adequate. Avoid complicated IUPAC names and redundant phrases such as '*Crystal structure of...*'. However, if the paper describes special techniques, such as powder, neutron or synchrotron diffraction studies, this could be alluded to in the title. The full first name of each author is preferred. The e-mail address of the correspondence author should be included in the CIF using the data item `_publ_contact_author_email`. This is the e-mail address which will be used to acknowledge receipt of the paper and for all subsequent communications with the authors, including despatch of electronic proofs. If the e-mail address of the submitting author is different from that of the correspondence author, only that of the correspondence author will appear in the published version of the paper. Note that the data items `_publ_section_title_footnote` and `_publ_author_footnote` are available, if required, for inserting footnotes to the title and to individual authors.

### 2.2. Synopsis (required for inorganic papers)

The synopsis should be one or two sentences (less than 40 words) in length, summarizing the main crystallographic results; it should be given in `_publ_section_synopsis`. There is no need to give formulae in the synopsis.

### 2.3. Abstract

The *Abstract* must be written in English, be informative, and should summarize only the most important aspects of the study. It should be capable of being understood on its own without access to the text or figures. 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*. The *Abstract* should include mention of any crystallographically imposed symmetry. Principal structural geometry results can be given here. Literature references should be avoided if possible; if required, they must be given in full, e.g. [Bürgi (1989). *Acta Cryst.* B45, 383–390].

### 2.4. Comment

The *Comment* is the descriptive section of a submission. It is expected to be an informative but concise discussion of the novel aspects of the study, and include the following key aspects:

- The reasons for the study.
- The origin of the material studied, including background material and references to related structural studies. [Note that details of the chemical extraction, synthesis and crystallization processes should be given in the *Experimental* section (see §2.5).]
- Information supporting the reported structure(s) based on other chemical or physical techniques.
- Novel or unusual aspects of the coordination, geometry, conformation, crystal packing, hydrogen bonding *etc.* A useful commentary on hydrogen bonds is available at the online CIF help page (see §7). A discussion of geometry values that agree with established values (see *International Tables for Crystallography*, Volume C, §§9.4–9.6) is **not** warranted. Note that if a study warrants little discussion (*i.e.* in the opinion of the referees and Co-editor the *Comment* section does not provide significant added value to the numerical data freely available in the CIF), the submission may be better suited to publication as an electronic paper in *Acta Crystal-*

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*lographica Section E*; if this is the case, authors will be advised of this during the review process.

## 2.5. Experimental data

Principal experimental data are extracted from the CIF and are tabulated under the sub-headings *Crystal data*, *Data collection* and *Refinement*. Some numerical items may be formatted with a revised number of decimal places to conform to a consistent style for the journal. The descriptive text item `_publ_section_exptl_prep` should give sufficient information on the chemical and crystal preparation, and identification (*e.g.* on melting points and densities), to reproduce the experiment. Additional details [*e.g.* lengthy synthesis descriptions and long lists of spectroscopic (NMR, IR *etc.*) data] supporting the crystallographic study should be placed in the `_exptl_special_details` section of the CIF. The item `_publ_section_exptl_refinement` should only be used to provide details of any unusual aspects of the data collection, space-group identification, data processing, structure determination, refinement and H-atom treatment; routine material should be placed in `_refine_special_details` and will be available from **Crystallography Journals Online** (see §7).

## 2.6. Acknowledgements

Acknowledgement should be given for any assistance provided to the study (see §1.5).

## 2.7. References

References to published work must be cited in the format detailed in §6. If reference is made to unpublished work, prior consent must be first obtained from the authors of that work. Identification of individual structures in the paper by use of database reference (identification) codes should be accompanied by a full citation of the original literature in the reference list. However, in tables containing more than ten such reference codes, citation in the reference list is not required.

## 2.8. Atomic sites

The `_atom_site_` coordinate and displacement parameters must be supplied with standard uncertainty values (see §5.1 and §2.16). The parameter constraints and restraints applied to the refinement process, and the anisotropic atomic displacement parameters (as  $U^{ij}$ ) must also be supplied. Note that only  $U$  or  $U^{ij}$  values are acceptable for atomic displacement parameters. The atom numbering should follow some recognised scheme (see §5.1) and the atom list should be in some sensible (not random) order.

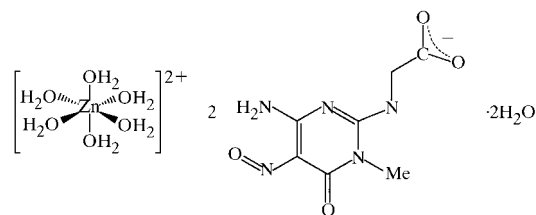
## 2.9. Selected geometrical data

Full details of molecular dimensions, including those involving H atoms, should be supplied, but only values that are of special interest should be flagged for printing by setting the `_geom_..._flag` value to `yes`. The data to be printed will be reviewed by the Co-editor and Section Editor. All submitted geometry data should be in some sensible order and are available to readers from **Crystallography Journals Online** (see §7).

## 2.10. Chemical scheme

A chemical structural diagram (a typical example is shown below) must be included for a molecular compound. Authors are required to submit such diagrams electronically in one of the formats listed in §4. The diagram should be complete, showing all species present in the

structure, including counter-ions and solvent molecules in their correct proportions.



## 2.11. Crystallographic diagram

Diagram requirements are given in §4. A labelled displacement ellipsoid diagram is required for each species either for publication or to be used in the review process. Authors are also encouraged to supply additional figures, *e.g.* packing diagrams. At the editor's discretion, figures printed in black and white may appear in colour in **Crystallography Journals Online** (see §7).

## 2.12. Contents

The Table of Contents of the journal will list the title and author(s) of all papers. Each entry will be accompanied by either a chemical structural scheme (see §2.10) for molecular compounds or a written synopsis for compounds that cannot be shown as a chemical structural scheme.

## 2.13. Powder diffraction data

Authors of powder diffraction papers should consult the notes provided at the online CIF help page (see §7). For papers that present the results of powder diffraction profile fitting or refinement (Rietveld) methods, the primary diffraction data, *i.e.* the numerical intensity of each measured point on the profile as a function of scattering angle, will be deposited. Papers reporting Rietveld refinements should include a figure showing the diffraction profile and the difference between the measured and calculated profiles.

## 2.14. Structure factors

The reflection data  $h, k, l, Y_{\text{meas}}, \sigma Y_{\text{meas}}, Y_{\text{calc}}$  (where  $Y$  is  $I, F^2$  or  $F$ ), must be supplied as an electronic file in CIF format.

## 2.15. Submission of related structures

Authors studying a series of closely related structures are encouraged to submit these for publication as a single paper. The CIF approach is well suited to multi-structure submissions. The journal reserves the right to require that two or more single structure papers on closely related materials be merged.

## 2.16. Standard uncertainties

The standard uncertainty (abbreviated *s.u.* and replacing the traditional term estimated standard deviation) should be expressed as a number in parentheses following the numerical result and should be on the scale of the least significant digits of the result. The *s.u.* value should be in the range 2–19. Note that *s.u.* values should not be

appended to parameters which are fixed by symmetry, geometry or other constraints.

### 3. Data requirements

A list of all data required for submission is available from the online CIF help page (see §7). If the submitted data are incomplete, inadequate or incorrect the author will be informed promptly. Authors are required to pre-check each CIF (see §1.1) prior to submission. A more complete description of the data-validation checks applied to submitted CIFs is available from the online CIF help page (see §7).

The most important data requirements are summarized below.

#### `_chemical_formula_moiety` `_chemical_formula_sum`

The chemical formula must be consistent with the atomic content specified by the `_atom_site_` information, and match the `_chemical_formula_weight`.

#### `_symmetry_space_group_name_H-M`

The space group must encompass the highest symmetry permitted by the diffraction intensities and be consistent with the `_cell_length_` and `_cell_angle_` values.

#### `_cell_formula_units_Z`

The number of formula units in the unit cell must comply with that expected from the chemical formula, the space group and the `_atom_site_` data.

#### `_exptl_crystal_colour`

The crystal colour should comply with the codes listed in the online CIF help page (see §7).

#### `_exptl_crystal_size_max`

Authors are encouraged to use crystals no larger than 0.5 mm in their X-ray diffraction experiments. For best results, the data crystal should be uniformly bathed in the X-ray beam. The size of the beam at the crystal is normally determined by *inter alia* the fine-focus X-ray tube and the monochromator. While use of a small collimator can reduce the size of the incident X-ray beam, use of a large collimator does not automatically increase the incident beam size.

#### `_exptl_absorpt_correction_type`

Permitted absorption-type codes are listed in the online CIF help page (see §7). A type code must be accompanied by a reference to the method or the software used; this should be given in the field `_exptl_absorpt_process_details`. The need for absorption corrections, and the appropriate type of correction, is dependent on the  $\mu$  value `_exptl_absorpt_coefficient_mu` and the crystal size values `_exptl_crystal_size_min`, `_mid` and `_max`. If  $x$  is the medial size `_mid`, the product  $\mu x$  provides an indication of the type of correction needed. Analytical or numerical corrections are strongly recommended if  $\mu x$  exceeds 1.0 and mandatory if  $\mu x$  is above 3.0. If

$\mu x$  is below 0.1 corrections are usually unnecessary, otherwise  $\psi$ -scan or empirical methods are acceptable. Refined absorption methods are discouraged except in special circumstances. The transmission-factor limits `_exptl_absorpt_correction_T_min` and `_max` should agree with those expected for the crystal shape and size, and  $\mu$ .

#### `_reflns_number_total`

The number of symmetry-independent reflections excludes the systematically extinct intensities. Authors are encouraged to use **all** symmetry-independent reflections in the refinement of the structure parameters.

#### `_reflns_threshold_expression`

This threshold, which is based on multiples of  $\sigma I$ ,  $\sigma F^2$  or  $\sigma F$ , serves to identify the significantly intense reflections, the number of which is given by `_reflns_number_gt`. These reflections are used in the calculation of `_refine_ls_R_factor_gt`. The multiplier in the threshold expression should be as small as possible, typically 2 or less.

#### `_diffrn_reflns_theta_max`

The  $\theta_{\max}$  of measured reflections should be such that  $\sin \theta_{\max}/\lambda$  exceeds  $0.6 \text{ \AA}^{-1}$  (*i.e.*  $\theta_{\max} > 25^\circ$  for Mo  $K\alpha$ ;  $\theta_{\max} > 67^\circ$  for Cu  $K\alpha$ ). It is assumed that all unique reflections out to the specified  $\theta_{\max}$  are measured. This provides the minimum number of reflections recommended for an average structural study. If intensities are consistently weak at the recommended  $\theta_{\max}$ , low-temperature measurements may be needed unless a study at a specific temperature (or pressure) is being reported.

#### `_diffrn_measured_fraction_theta_max`

This is intended for area-detector data, but is also useful as a general measure of data completeness. It is the fraction of unique (symmetry-independent) reflections measured out to `_diffrn_reflns_theta_max`. Ideally, this should be as close to 1.0 as possible.

#### `_diffrn_reflns_theta_full`

This is intended for area-detector data.  $\theta_{\text{full}}$  is the diffractometer angle at which the measured reflection count is close to complete. The fraction of unique reflections measured out to this angle is given by `_diffrn_measured_fraction_theta_full`. Alternatively, a breakdown of data completeness and merging statistics as a function of  $\theta$  may be requested if deemed necessary.

#### `_diffrn_reflns_av_R_equivalents`

Sufficient symmetry-equivalent reflections must be measured to provide a good estimate of the intensity repeatability. This is particularly important when absorption corrections are applied (this value is calculated *after* the corrections are applied to the intensities).

#### `_refine_ls_R_factor_gt`

Note that this value is **not** intended as a reliable gauge of structure precision which is better determined from the standard uncertainties of the parameters (these depend on the number and reliability of the measured structure factors used in the refinement process).

## **`_refine_ls_number_reflns`**

The number of reflections used in the refinement should be as large as possible, and should, if possible, be greater than the number of refined parameters `_refine_ls_number_parameters` by at least a factor of 10 if the structure is centrosymmetric, or by a factor of 8 if it is not.

## **`_refine_ls_number_parameters`**

This is the number of coordinate, atomic displacement, scale, occupancy, constraint, restraint, extinction and other parameters refined independently in the least-squares process. It is possible, and sometimes desirable, to reduce this number by the appropriate application of geometric constraints.

## **`_refine_ls_hydrogen_treatment`**

The codes which identify the treatment of H-atom parameters are listed in the online CIF help page (see §7). Detailed text about the treatment of H-atom sites should be placed in `_publ_section_exptl_refinement`. Authors should note the advice on H-atom treatment given in the *SHELXL97* manual, §4.6: '*For most purposes it is preferable to calculate the hydrogen positions according to well-established geometrical criteria and then adopt a refinement procedure which ensures that a sensible geometry is retained*'. Authors should note that H-atom sites which have been fixed or constrained by geometry will not have s.u. values associated with them.

## **`_refine_ls_weighting_scheme`**

Weighting schemes for refinements should be based on the standard uncertainties in the measured reflection data.

## **`_refine_ls_shift/su_max`**

This is the largest ratio of the refinement shift to standard uncertainty after the final round of refinement and is typically within  $\pm 0.01$  if sufficient least-squares refinement cycles have been employed. A value above  $\pm 0.05$  is considered unusual and values beyond  $\pm 0.1$  are a sign of incomplete refinement, unaccounted-for disorder or high correlation between parameters that should be constrained. Authors should explain the reasons for a high value in `_publ_section_exptl_refinement`.

## **`_refine_diff_density_min`**

## **`_refine_diff_density_max`**

These values are expected to be small, especially for light-atom structures. If their magnitudes exceed  $1 \text{ e } \text{Å}^{-3}$ , the label and the distance of the closest atom site should be reported in `_publ_section_exptl_refinement`.

## **`_geom_`**

All geometry values must originate from the submitted `_atom_site_fract_` values. Only geometry values of significance to the structure will be printed. These must be identified with a `_geom_..._flag` value of `yes` in the submitted CIF. Note that dimensions involving H-atom sites which have been fixed or constrained by geometry will not have s.u. values associated with them. Details of all bond lengths and angles involving H atoms should be included in the CIF.

## **`_atom_site_`**

Atomic coordinates for molecular structures should be supplied as connected sets. Whenever structure geometry permits, it is normally

expected that the set of connected coordinates which specify the asymmetric unit will lie within the basic unit cell. Values of `_atom_site_occupancy` should be 1.0 except for disordered or non-stoichiometric atom sites. Atom sites constrained to model disorder must be indicated by `_atom_site_disorder_group`. The overall packing in the structure will be checked for significant vacant regions (*i.e.* voids) indicating omitted solvent molecules. Note that s.u. values should not be appended to parameters which are fixed by symmetry, geometry or other constraints.

## **`_atom_site_aniso_U_`**

Checks will be made for non-positive-definite anisotropic atomic displacement parameters. The ratio of maximum to minimum eigenvalues should not, except in special circumstances (*e.g.* disorder), exceed 5.

## **`_refine_ls_abs_structure_details`**

This item should describe the method applied, and the number of Friedel-related reflections used, in the measurement of the absolute structure parameter (*e.g.* `_refine_ls_abs_structure_Flack` or `_refine_ls_abs_structure_Rogers`). If the structure is non-centrosymmetric, and atoms heavier than Si are present, an absolute structure parameter is expected. The reliability of this parameter increases with the number of Friedel-related intensities, and use of a complete set of Friedel pairs in the refinement is strongly recommended. With Mo radiation, if no atoms heavier than Si are present, the  $f''$  terms in the scattering factor expression are very small. In such cases, if no useful absolute structure parameter can be refined (*i.e.* the value of the absolute structure parameter is meaningless because of its large s.u. value), authors should consider merging Friedel-pair reflections before final refinement. They should then report in the `_publ_section_exptl_refinement` section of the CIF that they have merged Friedel pairs for the final refinement and quote the absolute structure parameter value (with its s.u. value) obtained from any refinement with Friedel pairs as justification for this merging. Authors are strongly advised to consult papers by Flack & Bernardinelli [*Acta Cryst.* (1999), **A55**, 908–915; *J. Appl. Cryst.* (2000), **33**, 1143–1148] which discuss the use and meaning of the Flack parameter and its s.u. value.

## **4. Diagram requirements**

Figures and chemical structure diagrams (see §2.10 for a typical example) should be prepared in HPGL, PostScript, encapsulated PostScript or TIFF format. The resolution of bitmap graphics should be a minimum of 600 d.p.i.

The use of ISIS/Draw, ChemDraw or ChemWindow for preparing chemical structure diagrams (schemes) is encouraged. Authors using the above programs are required to submit their schemes as HPGL, PostScript, encapsulated PostScript or TIFF format files; in addition, they may submit ISIS/Draw, ChemDraw or ChemWindow format files.

### **4.1. Publication**

For papers reporting molecular structures a labelled displacement ellipsoid molecular diagram is required; otherwise a packing or polyhedron diagram is required. All non-H unique atom sites should be identified with labels consistent with those for the supplied atomic coordinates. Distances and angles should not be shown in the crys-

tallographic diagram. A chemical structural diagram or scheme must be supplied for molecular compounds (see §2.10 for a typical example). Authors should consider having the orientation of crystallographic figures and chemical schemes correspond as closely as possible.

#### 4.2. Submission

Diagrams should be submitted electronically *via* the web submission interface (see §1.9 for details).

#### 4.3. Quality

Electronic files in the formats listed above are essential for high quality reproduction. For molecular compounds, a clear, well-presented ellipsoid plot will show the stereochemistry and any unusual atomic displacements or disorder.

#### 4.4. Size

Diagrams will normally be sized by the Chester staff so that the greatest width including lettering is less than the width of a column in the journal.

#### 4.5. Lettering and symbols

Fine-scale details and lettering must be large enough to be clearly legible (ideally 1.5–3 mm in height) after the whole diagram has been reduced to one column width. Atom site labels in crystallographic diagrams should not contain parentheses and should match labels used in the atom site lists and text. The labels should not overlap or touch ellipsoids or bonds. Descriptive matter should be placed in the legend. Packing diagrams must show the cell-axis directions (labelled *a*, *b*, *c*) and the cell origin (labelled *O*), but should normally exclude H-atom sites, unless these are involved in hydrogen bonding.

#### 4.6. Numbering and legends

Diagrams should be numbered in a single series in the order in which they are referred to in the text. A list of the legends ('figure captions') should be included in `_publ_section_figure_captions`. Legends of labelled displacement ellipsoid plots must state the probability limit used. If H atoms are shown by small spheres of an arbitrary size, this need not be stated in the caption.

### 5. Nomenclature

#### 5.1. Crystallographic nomenclature

Authors should follow the general recommendations produced by the IUCr Commission on Crystallographic Nomenclature (see reports at <http://www.iucr.org/iucr-top/comm/cnom/>).

Atom sites not related by space-group symmetry should be identified by unique labels composed of a number appended to the IUPAC chemical symbol (*e.g.* C5, C7 *etc.*). Label numbers should 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 diagrams and text with lower-case Roman numeral superscripts appended to the original atom labels and the symmetry operators defined [*e.g.* C5<sup>5</sup>; symmetry code: (i) 1–*x*, –*y*, 1–*z*].

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. A list of equivalent positions should also be

supplied. Hermann–Mauguin symbols should be used for designating point groups and molecular symmetry. If there is a choice of origin, this should be stated in `_publ_section_exptl_refinement`. The choice of axes should normally follow the recommendations of the Commission on Crystallographic Data [Kennard *et al.* (1967). *Acta Cryst.* **22**, 445–449].

#### 5.2. Nomenclature of chemical compounds

Names of chemical compounds and minerals should conform to the nomenclature rules of 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. Any accepted trivial or non-systematic name may be retained, but the corresponding systematic (IUPAC) name should also be given.

For crystal structures containing chiral molecules, authors should make it clear whether the crystal structure is a racemate or enantiopure, and if enantiopure whether or not the assignment of the absolute configuration is justified. Absolute configuration should be indicated using the CIF data item `_chemical_absolute_configuration`. The title, compound name, chemical diagrams, atomic coordinates and space group must correspond to the enantiocomposition and the selected configuration. It is also most helpful to indicate the crystallographic and non-crystallographic symmetry of each molecule in the asymmetric unit.

#### 5.3. Units

The International System of Units (SI) is used except that the ångström (symbol Å, defined as 10<sup>–10</sup> m) is generally preferred to the nanometre (nm) or picometre (pm) as the appropriate unit of length. Recommended prefixes of decimal multiples should be used rather than '×10<sup>n</sup>'.

### 6. References

References to published work must be indicated by giving the authors' names followed immediately by the year of publication, *e.g.* Neder & Schulz (1999) or (Neder & Schulz, 1999). Where there are three or more authors the reference in the text should be indicated in the form Smith *et al.* (1989) or (Smith *et al.*, 1989) *etc.* (all authors should be included in the full list).

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- Becker, T. M. & Krause Bauer, J. A. (1999). *Acta Cryst.* C55, IUC9900141.
- 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. (2001). In preparation.
- International Union of Crystallography (2001). (IUCr) Structure Reports Online, <http://journals.iucr.org/e/journalhomepage.html>
- 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.

Robinson, P. D. (2002). Acta Cryst. C58. In the press. [Paper reference fg1795.]

Sheldrick, G. M. (1997). SHELXL97. University of Göttingen, Germany.

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.

Yatsenko, A. V., Paseshnichenko, K. A. & Schenk, H. (2001). Acta Cryst. E57, o1156–o1157.

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