

## Notes for authors 2004

*Acta Crystallographica Section E: Structure Reports Online* is the IUCr's first electronic-only structural journal. It provides a fast, simple and easily accessible publication mechanism for the growing number of valuable inorganic, metal-organic and organic crystal structure determinations. The electronic submission, validation, refereeing and publication facilities of the journal ensure rapid and high-quality publication, whilst key indicator flags are used to provide measures of structural reliability. The journal encourages the publication of routine as well as interesting and difficult structures, and promotes the inclusion of colour illustrations and multimedia supplements.

### 1. Submission requirements

#### 1.1. Manuscript checking and preparation

All papers must be submitted in Crystallographic Information File (CIF) format. Details about CIFs are given in Hall *et al.* [*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 author help page (see §7). A free CIF editor (*enCIFer*) is available from <http://www.ccdc.cam.ac.uk/products/encifer/index.html>; a test version of *printCIF for Word* is available from <http://journals.iucr.org/e/services/cifinfo.html>. The Section Editors, Co-editors and Chester staff are also available to assist any author.

Authors are required to pre-check their submission using the *checkCIF* service at <http://journals.iucr.org/services/cif/checkcif.html>. Any reported problems with the submitted data should normally 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* should be completed and included in the submitted CIF, preferably with the addition of appropriate explanatory text in the published experimental section of the CIF.

The text and tables of a paper may be previewed by sending the CIF (after completing the pre-check) to the *printCIF* service at <http://journals.iucr.org/services/cif/printcif.html>. A PostScript or PDF file of the paper will be returned for local viewing or 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 E*.

#### 1.2. Categories of submission

*Section E* 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 the determination of a single structure. The submitted CIF is validated using *checkCIF* and database checks are applied by the Inorganic Crystal Structure Database (ICSD) or CCDC. The CIF, the checking results and associated files are then

passed to a Co-editor for peer review. Once accepted, the paper and associated graphics, together with the CIF and structure factors, will be accessible electronically from the **Crystallography Journals Online** service at <http://journals.iucr.org>. The category codes used to identify these papers are EI for inorganic, EM for metal-organic, and EO for organic structures.

(b) *Addenda and Errata* are short papers describing additions to, comments on, or errata to existing *Section E* 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*. The Chester *refcode* has two letters and four digits (*e.g.* cf6913), 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 §2.9), crystallographic diagrams (see §2.10) and structure factors (see §2.12). 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. Submissions in English may use either British or American spelling, but must do so consistently throughout.

#### 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 manuscript has not already been published (in any language or medium), and that it is not being considered and will not be offered elsewhere while under consideration for an IUCr journal. The inclusion of material in an informal publication, *e.g.* a preprint server or newsletter, does not preclude publication in an IUCr journal.

Important principles in relation to publication have been given in the ethical guidelines published in *Acc. Chem. Res.* (2002), **35**, 74–76.

## 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 for completeness and data integrity. If incomplete 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). For papers failing to meet these criteria, a completed validation response form (VRF) giving reasons for the failure should be included in the CIF. The Co-editor will assess the validity of the explanation as part of the review process.

The Co-editor is responsible for the review steps and future communications with the authors up to the acceptance stage. If nothing untoward is noted, the paper will be prepared for immediate electronic publication. If problems are perceived, the authors will be contacted directly and asked to rectify these before acceptance of the submission.

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. All communications to authors will normally be sent electronically to the e-mail address provided in the CIF. Authors who anticipate or become aware of difficulties with their e-mail service should alert their Co-editor as soon as they are aware that there is a problem. If major revisions (*i.e.* revisions involving a complete new CIF) 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 publication and to correspond with the authors and/or the Co-editor to resolve publication ambiguities or inadequacies. The Section Editors review all accepted papers and reserve the right to make minor changes to ensure conformity with *Section E* standards; in the unlikely event of a serious problem being detected at this stage, the authors will be contacted promptly. Occasionally the Section Editors may recommend the transfer of a manuscript to *Section C* at this stage; if the authors agree, the transfer will be handled rapidly by the editorial staff.

## 1.8. Author grievance procedure

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

## 1.9. File transfer

All files should be transferred *via* the web interface at <http://journals.iucr.org/services/submit.html>. Submission of files by email or ftp is not allowed.

## 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. A list of all items required for submission is available *via* the online CIF help page (see §7) where guidelines concerning the use of special characters (*e.g.* Greek letters and diacritical marks) and a set of Frequently Asked Questions are

also given. Note that a *Comment* section (§2.3) is optional, as are crystallographic diagrams (§2.10). A chemical structure diagram must be included for molecular compounds (§2.3).

### 2.1. Title and authors

The *Title* should be short and informative; in many cases just the name of the compound studied will be perfectly adequate. However, the use of titles consisting of only the chemical formula is discouraged. Avoid complicated IUPAC names and redundant phrases such as '*Crystal structure of...*'. For papers describing powder, neutron or synchrotron diffraction studies, the title should typically consist of the name of the compound followed by '(powder study)', '(neutron study)' or '(synchrotron study)', respectively. The full first name of each author is preferred. 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. 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].

### 2.3. Comment

Papers in *Section E* should normally include a short *Comment* section; however, this is not mandatory. When present, the *Comment* is expected to be an informative but concise discussion of the novel aspects of the study, and to cover the following key aspects:

(a) The reasons for the study.

(b) 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 §2.4).]

(c) Information supporting the reported structure based on other chemical or physical techniques.

(d) 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.

### 2.4. Experimental data

Principal experimental data are extracted automatically from the CIF and are tabulated under the sub-headings *Crystal data*, *Data collection* and *Refinement*. Some numerical items may be formatted so that a standard number of decimal places is published. The descriptive text item `_publ_section_expt1_prep` is the appropriate place to give information on the chemical and crystal preparation, and identification (*e.g.* on melting points and densities), the inclusion of which is encouraged. Additional details [*e.g.* lengthy synthetic descriptions and long lists of spectroscopic (NMR, IR *etc.*) data] supporting the crystallographic study should be placed in the `_expt1_special_details` section of the CIF, which is available

from **Crystallography Journals Online**. A reference should be given rather than full details of the preparation if these have already been published elsewhere. The text item `_publ_section_exptl_refinement` should be used to provide details of how H atoms were treated and report the ranges of  $X-H$  dimensions. Any unusual aspects of the data collection, space-group identification, data processing, structure determination and refinement (including any restraints used and the treatment of disorder) should also be given here. Routine material should be placed in `_refine_special_details` and will be available from **Crystallography Journals Online** (see §7).

## 2.5. Acknowledgements

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

## 2.6. 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.

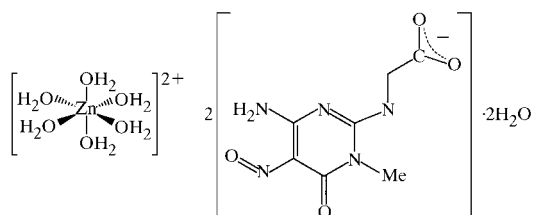
## 2.7. Atomic sites

The `_atom_site_` coordinate and displacement parameters must be supplied with standard uncertainty values (see §2.14). 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 recognized scheme (see §5.1) and the atom list should be in some sensible (not random) order.

## 2.8. Selected geometrical data

Full details of molecular dimensions, including those involving H atoms, should be supplied; only values that are of special interest should be flagged for publication by setting the `_geom_...flag` value to yes. The data to be published in the HTML/PDF versions of the paper will be reviewed by the Co-editor and a Section Editor. All submitted geometry data are available to readers from **Crystallography Journals Online**. Torsion angles, if provided in the CIF, should not normally include any involving H atoms; those in which three of the atoms are nearly collinear should be removed.

## 2.9. Chemical structural diagram



A chemical structural diagram (a typical example is shown above)

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.

## 2.10. Crystallographic diagram

Diagram requirements are given in §4. A labelled displacement ellipsoid diagram is strongly recommended for each structure either for publication or to be used in the review process. Authors are also encouraged to supply additional figures *e.g.* packing diagrams. The use of colour is encouraged, but poor contrast (*e.g.* pale colours with a white background) should be avoided.

## 2.11. 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.

## 2.12. 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 using the web submission interface at <http://journals.iucr.org/services/submit.html>. All unique reflections should be included.

## 2.13. Submission of related structures

To allow handling of papers to be automated, all submissions should report single structures only. Series of single structure papers on closely related materials should not be merged. It is possible for submissions reporting related structures to be handled together and published as adjacent papers. Authors should make this request in the `_publ_contact_letter` of each CIF. However, such studies may be more appropriately reported as a single paper in *Acta Crystallographica Section B* or *C*.

## 2.14. 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 preferably 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).

Data-precision indicators will be published for all papers. Details of these can be found at <http://journals.iucr.org/services/cif/dataprecision.html>.

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 author help page (see §7).

#### **`_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. 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 at least the above specified  $\theta$  limits 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_number_restraints`**

This gives the number of applied restraints. Concise details of what these restraints were should be included in the `_refine_special_details` section of the CIF.

## **`_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 published. 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.

## **`_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 merge 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. Authors are strongly advised to consult papers by Flack & Bernardinelli which discuss the use and meaning of the Flack parameter and its s.u. value [*Acta Cryst.* (1999), **A55**, 908–915; *J. Appl. Cryst.* (2000), **33**, 1143–1148].

## **4. Diagram requirements**

Figures and chemical structure diagrams (see §2.9 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 300 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 PostScript, encapsulated PostScript or TIFF format files; in addition, they may submit *ISIS/Draw*, *ChemDraw* or *ChemWindow* format files.

Authors are also encouraged to provide crystallographic and other diagrams (*e.g.* packing diagrams).

### **4.1. Publication**

For molecular compounds, a clear, well-presented ellipsoid plot is strongly recommended to show the stereochemistry and any unusual atomic displacements or disorder. For other structures, a packing or polyhedron diagram is strongly recommended. 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 crystallographic diagram. The orientation of crystallographic figures and chemical structural diagrams should correspond as closely as possible.

### **4.2. Submission**

Diagrams should be submitted electronically *via* the web submission interface. All diagrams must be submitted in this way.

### **4.3. Lettering and symbols**

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.

#### 4.4. 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>i</sup>; symmetry code: (i) 1-*x*, -*y*, 1-*z*]. If there are figures with packing plots in a paper, the atom labels in these plots should correspond with the asymmetric-unit coordinates. Symmetry-related atoms can be marked by suffixes to the atom labels; the symmetry operations to which these refer should be defined in the figure legend.

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`.

#### 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 by using the CIF data item `_chemical_absolute_configuration`. The title, compound name, chemical diagrams, atomic coordinates and space group must correspond to the enantio-composition and the selected configuration. It is also most helpful to indicate the crystallographic and non-crystallographic symmetry of each molecule in the asymmetric unit.

Authors may find nomenclature programs such as Autonom (<http://www.beilstein.com/products/autonom>) and ACD ([\[acdlabs.com/products/name\\\_lab\]\(http://www.acdlabs.com/products/name\_lab\)\) to be useful resources when naming compounds.](http://www.</a></p>
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#### 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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