Acta Crystallographica Section C
Crystal Structure Communications
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Notes for authors 2010

Acta Crystallographica Section C: Crystal Structure Communications publishes papers that provide a detailed discussion 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. Papers are expected to contain a discussion that goes beyond reporting just the principal numerical and geometrical data. Such value-added material might include: a meaningful discussion of multiple related structures reported in the same paper; non-routine structure determinations discussed in detail; placing the structure in an interesting scientific, physical or chemical context; or the discussion of interesting physical properties or modes of association. The journal accepts reports of difficult or challenging structures not meeting all validation criteria, provided the presented structures are correct and the difficulties and strategies used to treat them are scientifically discussed and properly documented. Such structures might display properties such as twinning, severe disorder, or diffuse solvent regions.

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), A**47**, 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 CIF editor for authors, *publCIF*, may be obtained from **http://journals.iucr.org/services/cif/publcif** and a general CIF editor (*enCIFer*) may be obtained from **http://www.ccdc.cam.ac.uk/products/encifer/index.html**; both editors are available free of charge. The Section Editor, Co-editors and Editorial Office staff are also available to assist any author with any technical CIF problems. Please note that this help does not include rewriting papers which do not reach the standards specified in §1.10.

Before submission, authors are required to check their CIF and associated structure factors using the **checkcif** service at **http://journals.iucr.org/services/cif/checking/checkfull.html**. All validation alerts returned by **checkcif** should be considered carefully and corrected as far as possible. Sometimes these alerts relate to simple omissions or errors in the CIF. If the report contains validation alerts about the consistency, adequacy or quality of the data or the refined model, 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, 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** or by using *publCIF*.

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 **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

Full details of the submission procedure can be found at **http://journals.iucr.org/c/services/helpsubmit.html**. CIFs must be submitted *via* the web at **http://journals.iucr.org/c/services/submitbdy.html**. All submitted CIFs must have been pre-checked using the facilities described in §1.1.

During the submission procedure, authors will be required to submit additional electronic files; these include the chemical scheme (see §2.10), crystallographic diagrams (see §2.11) and structure factors (see §2.14) or powder diffraction data (see §2.13). Authors will also be asked to agree to transfer the copyright of their paper to the IUCr (see §1.11).

On completion of the submission procedure, each paper will be assigned an Editorial Office refcode. The refcode has two letters and four digits (e.g. ln3127), with the two letters identifying the assigned Co-editor; the refcode should be used in all subsequent communications with the Editorial Office and Co-editor.

1.4. Handling of manuscripts

Each submitted CIF is automatically validated for completeness and data integrity, and checked for duplication. 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). For papers failing to meet these criteria, a completed validation response form (VRF) giving reasons for the failure must be included in the CIF. The Co-editor will assess the validity of the explanation as part of the review process. A copy of the final refinement instruction file should be inserted in the CIF as described in §2.5.

The Co-editor is responsible for the review steps and future communications with the authors up to the acceptance stage. 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 the Co-editor as soon as they are aware that there is a problem. If, after review, no revisions are necessary, the paper will be prepared for immediate electronic publication. If the review reveals that revision is required, the authors will be contacted directly and asked to revise the paper. Further revisions may be requested before acceptance of the submission if unresolved issues remain. Failure to respond to a communication from either a Co-editor or the Editorial Office 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. If a manuscript is not acceptable after two revisions it will not be considered further. A paper that has been rejected must not be resubmitted to any IUCr journal unless the reasons given for the rejection have been fully addressed in the revised version.

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 significant changes being required at this stage, the authors will be contacted promptly.

1.5. Revisions

After initial submission, any revised or new files should be uploaded *via* the web interface **only** after a specific request from a Co-editor; these files should be uploaded at the web address provided by the Co-editor.

1.6. 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 acknowledgments, 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 a newsletter, does not preclude publication in an IUCr journal.

The co-authors of a paper should be all those persons, and only those persons, who have made significant scientific contributions to the work reported, including the ideas and their execution, and who share responsibility and accountability for the results. Other contributions should be indicated in an *Acknowledgments* section. An administrative relationship to the investigation does not of itself qualify a person for co-authorship (but it may be appropriate to acknowledge major administrative assistance). Changes to the list of authors will normally require the agreement of the Editor and all authors.

Important considerations related to publication have been given in the ethical guidelines published in *Acc. Chem. Res.* (2002), **35**, 74–76 and Graf *et al.* [*Int. J. Clin. Pract.* (2007), **61**(Suppl. 152), 1–26].

1.7. Submission of related structures

Authors studying a series of closely related structures are strongly 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 papers on closely related materials be merged.

1.8. Previously published structures

If a structure has been redetermined correctly and the discussion adds significantly to the information already in the public domain then the paper can be considered for publication. Crystallographically interesting structures previously published elsewhere under circumstances that did not allow the crystallographic details to be described fully may be considered, provided such studies properly cite the original article and the manuscript primarily describes new information that was not presented in the original publication.

1.9. Languages of submission

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

1.10. Quality of writing

Papers should be clearly written and grammatically correct. If the Co-editor concludes that language problems would place an undue burden on the referee(s), the manuscript may be returned to the authors without review. Details of language-editing services can be found at **http://journals.iucr.org/services/languageservices.html**.

1.11. 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. Details of author rights can be found at **http://journals.iucr.org/services/authorrights.html**. See §7.3 for information on the licensing of open-access articles.

1.12. 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 for a new review and, finally, to the Editor-in-chief of IUCr journals if the author is still aggrieved by the decision. The initial appeal must be made within 3 months of rejection of the paper. The decision of the Editor-in-chief is final. Any resubmission after an appeal will be forwarded to the Section Editor.

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 data 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 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. If the paper describes the redetermination of a previously reported structure, this should be indicated in the *Title*.

2.2. Synopsis (required only 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 the most important aspects and results 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 or, usually, the space group. 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 or the presence of more than one molecule (or formula unit) in the asymmetric unit of the structure. 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.* [Bond, A. D., Davies, J. E. & Kirby, A. J. (2001). *Acta Cryst.* E**57**, o1242–o1244.].

2.4. Comment

The *Comment* is the descriptive section of a submission. For publication in *Acta Crystallographica Section C*, the study must warrant significant discussion (*i.e.* provide substantial added value to the numerical data freely available in the CIF). To this end, authors are encouraged to present and discuss multiple related structures in the same paper. The *Comment* is expected to be an informative but concise discussion of the novel aspects of the study, and include the following key aspects:

(*a*) The reasons for the study.

(*b*) The origin of the material studied, including background information. [Note that details of the chemical extraction, synthesis and crystallization processes should be given in the *Experimental* section (see §2.5).]

(*c*) Any information available supporting the reported structure(s) based on other chemical or physical techniques, or discussing the structure in an interesting scientific, physical or chemical context.

(*d*) Interesting or unusual aspects of the coordination, geometry, modes of association, extended connectivity, conformation, crystal packing, hydrogen bonding, *etc*. A discussion of geometry values that agree with established values (see *International Tables for Crystallography*, Volume C, §§9.4–9.6) is **not** warranted.

(*e*) A discussion of intermolecular interactions, if warranted, should describe the motifs and networks generated, but over-analysing weak interactions should be avoided. A useful commentary on hydrogen bonds is available at the online CIF help page (see §7).

(*f*) Where a difficult or challenging structure is reported, there should be a thorough discussion of the challenges together with full documentation, possibly in the `_publ_section_exptl_refinement` section, of the experimental and refinement strategies used to treat them, as well as details about the outcomes of these strategies.

The *Comment* should not be just a list of observations about the structure (for example, just stating, without description, that hydrogen-bonding or other weak interactions exist), but should include an analysis and discussion of how these observations help the understanding of the chemical, physical or structural properties of the compound and further the aims of the study stated in the opening paragraph, plus a detailed comparison with any closely related published structures, where such exist. Numerical values reported in Tables should generally not be repeated in the text.

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 compound isolation or synthesis, crystal preparation (method, solvents and their ratios), and identification (*e.g.* melting points and densities), to reproduce the experiment. Previously reported syntheses, isolation procedures or spectroscopic data need only be cited. 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, which is available from **Crystallography Journals Online**. Spectroscopic data should be reported in the `_publ_section_exptl_prep` section only when assignments are given. The item `_publ_section_exptl_refinement` should be used to provide details of how H atoms were treated, including the ranges of X—H dimensions and how the values of U_{iso}(H) were defined. Any non-routine or 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 be fully documented here. Routine material should be placed in the `_refine_special_details` section and will be available from **Crystallography Journals Online** (see §7). Authors are strongly encouraged to use *publCIF* to place a copy of their refinement instruction file(s) in the `_iucr_refine_instruction_details` section for each refinement. This will facilitate the review of the manuscript, particularly when special refinement strategies, such as the use of restraints, have been employed.

2.6. Acknowledgements

Acknowledgement should be given for any assistance provided to the study (see §1.6). If the diffraction data collection was not carried out by one of the authors, or in the laboratory of one of the authors,

details of who collected the data and where the data collection was carried out should be provided.

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.

2.8. Atomic sites

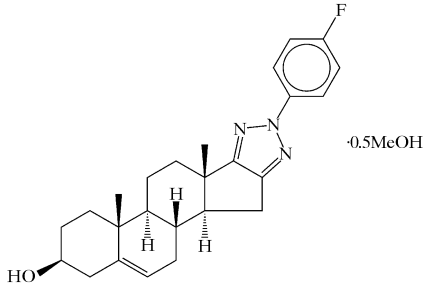
The `_atom_site_` coordinate and atomic displacement parameters (as U^{ij}) must be supplied with standard uncertainty values (see §5.1 and §2.15). The parameter constraints and restraints applied to the refinement process, and the anisotropic atomic displacement parameters must also be supplied. Note 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. H-atom labels should be directly related to the atom to which they are bonded.

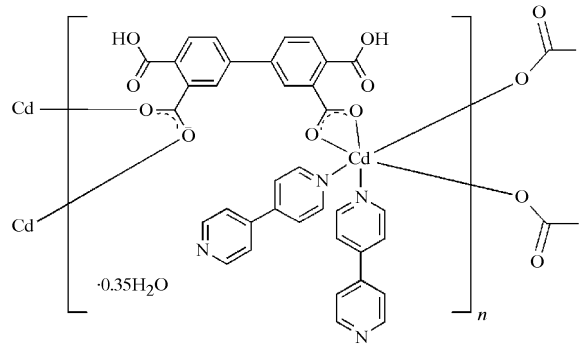
2.9. Selected geometrical data

All symmetry-unique bond lengths and angles, including those involving H atoms, should be provided in the CIF, but only values that are of special interest should be flagged for printing in a table by setting the `_geom_..._flag` value to `yes`. The inclusion of torsion angles in the CIF is encouraged, but should not normally include those involving H atoms; those in which three of the atoms are nearly collinear should be removed. 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 structure diagram (typical examples are shown below) must be included for all but inorganic materials. 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. Any relative or absolute stereochemistry must be shown and should be consistent with the crystallographic diagram (§2.11), the data reported in the *Abstract* (§2.3), *Comment* (§2.4) and *Title* (§2.1). Hydrogen bonding should not normally be indicated in the diagram.





2.11. Crystallographic diagrams

Diagram requirements are given in §4. A labelled displacement ellipsoid diagram is normally 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, provided that they display features of interest, are legible and contribute to the discussion in the *Comment* section. Figures submitted in colour will be printed in greyscale but will usually 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 structure diagram (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 **http://journals.iucr.org/services/cif/powder.html**. 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, should 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 $h, k, l, Y_{\rm meas}, \sigma Y_{\rm meas}, Y_{\rm calc}$ (where Y is I, F^2 or F), must be supplied as an electronic file in CIF format during the submission process. All unique reflections should be included.

2.15. 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 in the text and the tables. 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. If atoms are missing from the atomic model, the moiety and sum formulae should state the assumed overall formula.

_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 the incident X-ray beam diameter, particularly when heavy or strongly absorbing elements are present in the material. For best results, the 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 nature of the X-ray source and the beam optics. Note that with fine-focus sealed X-ray tubes, the use of a collimator larger than the filament diameter does not automatically increase the size of the uniform part of the incident beam.

_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 μ 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 μx provides an indication of the type of correction needed. Analytical or numerical corrections may be beneficial if μx exceeds 1.0 and are strongly recommended if μx is above 3.0. Empirical methods based on analyses of equivalent and redundant reflections (multi-scan methods) are acceptable. Corrections are usually unnecessary if μx is below 0.1. 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 μ.

_diffrn_reflns_av_R_equivalent
_diffrn_reflns_number
_diffrn_reflns_av_R_equivalent
_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

These items should refer to the complete set of measured data before any merging of symmetry-equivalent reflections, and not only to the unique set of data.

_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. Whenever a multi-scan type absorption correction is being employed (*e.g.* by using *SADABS*), authors are also encouraged to measure a multiplicity of observations (measurement of symmetry equivalents or the same reflection at different crystal orientations) of at least 4. The algorithms used in such programs work best and produce the highest quality data only when the multiplicity of observations is high.

_reflns_threshold_expression

This threshold, which is based on multiples of σI, σF^2 or σF, 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 θ_{max} of measured reflections should be such that $\sin\theta_{max}/\lambda$ exceeds 0.6 Å^{-1} (*i.e.* $\theta_{max} > 25^\circ$ for Mo $K\alpha$; $\theta_{max} > 67^\circ$ for Cu $K\alpha$). It is expected that all possible unique reflections out to at least the specified minimum θ limits are measured. This provides the minimum number of reflections recommended for an average structural study. If intensities are consistently weak at the recommended θ_{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 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

When _diffrn_measured_fraction_theta_max is less than 1.0 because of some missing high-angle reflections, θ_{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.

_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. Omission of outlier reflections should be avoided unless there is good reason and, in such cases, details of the omitted reflections and the reasons for doing so should be included in the `_publ_section_exptl_refinement section`.

_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 `_publ_section_exptl_refinement` 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 *SHELXL*97 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 (*e.g.* riding) 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 ± 0.01 if sufficient least-squares refinement cycles have been employed. A value above ± 0.05 is considered unusual and values beyond ± 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 are such that a validation alert is generated, 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 must be included in the CIF, even if they have been constrained.

_atom_site_

Atomic coordinates for molecular and nonmolecular species 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. In systems with hydrogen-bonded networks, it is expected that the asymmetric unit will be chosen so that the minimum number of symmetry operators is required to specify the hydrogen-bond network.

_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, with a literature citation if necessary, and the number of Friedel pairs used in the determination of the absolute structure parameter (*e.g.* `_refine_ls_abs_structure_Flack`). If the structure is noncentrosymmetric, an absolute structure parameter is expected. The reliability of this parameter increases with the number of Friedel-related intensities, and the use of a large fraction of the complete set of Friedel pairs in the refinement is strongly recommended. If the choice of X-ray wavelength means that the f'' terms of the atomic scattering factor expressions are very small and 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 the 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 [*Acta Cryst.* (1999), A**55**, 908–915; *J. Appl. Cryst.* (2000), **33**, 1143–1148] which discuss the use, meaning and significance of the Flack parameter and its s.u. value. For pertinent comments on the

determination of absolute structure, authors are also referred to the papers by Jones [*Acta Cryst.* (1986), A**42**, 57] and Hooft *et al.* [*J. Appl. Cryst.* (2008), **41**, 96–103].

4. Diagram requirements

A set of guidelines for preparing figures is available from **http://journals.iucr.org/c/services/help/artwork/guide.html**. 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.

4.1. Publication

For papers reporting molecular structures a labelled displacement ellipsoid molecular diagram is required for each independent species; for polymeric materials the displacement ellipsoid plot should show at least the chemically unique fragment; for other structures, 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 crystallographic diagram. A chemical structure 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.

Additional crystallographic diagrams, such as packing diagrams showing extended structures or intermolecular interactions, are welcome, but should be constructed carefully to show clearly the desired features and to maximise information content. Where features depicted in two diagrams could be combined, the authors may be asked to provide a single figure. Packing diagrams should normally exclude H-atom sites, unless these are involved in hydrogen bonding or other interactions.

Figures showing no significant features and not described in the text (*e.g.* packing diagrams without special intermolecular interactions), or which are illegible because of crowding will not be published.

4.2. Submission

Diagrams should be submitted electronically *via* the web submission interface (see §1.3).

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 Editorial Office staff so that the greatest width including lettering is less than the width of a column in the journal (8.8 cm).

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 caption. Packing diagrams must show the cell-axis directions (labelled *a*, *b*, *c*) and the cell origin (labelled *O*).

4.6. Numbering and figure captions

Diagrams should be numbered in a single series in the order in which they are referred to in the text. A list of the figure captions should be included in `_publ_section_figure_captions`. Captions 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. Symmetry-related atoms should be marked by additional symbols or letters and the figure caption should indicate to what symmetry operations these additional items in the atom labels refer (see also §5.1).

4.7. Enhanced figures

An online tool for authors to prepare standard and corresponding three-dimensional interactive structural diagrams is available from **http://submission.iucr.org/jtkt**.

5. Nomenclature

5.1. Crystallographic nomenclature

Authors should follow the general recommendations produced by the IUCr Commision on Crystallographic Nomenclature (see reports at **http://www.iucr.org/iucr/commissions/cnom.html**).

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 the text with lower-case Roman numeral superscripts appended to the original atom labels and the symmetry operators defined [*e.g.* C5^{i}; symmetry code: (i) $1-x$, $-y$, $1-z$]. In diagrams, Roman numeral superscripts are preferred, but symmetry-related atoms may be marked by additional symbols or letters, with these defined in the caption. Atom labels should be as concise as possible and not contain superfluous characters, *e.g.* leading zeroes are unnecessary so that C01, C02 should appear as C1, C2, *etc*. H-atom numbers should correspond with that of their parent atom label, *e.g.* a phenyl H on atom C1 should appear as H1, not H1A, and methylene H atoms on C1 should appear as H1A and H1B or H11 and H12, unless this leads to naming ambiguities. Chemically ambiguous labels such as HO1a (signifying an H atom attached to an O atom) should be avoided. If there are figures with packing plots in a paper, the atom labels with no symmetry code in these plots must correspond exactly with the asymmetric unit coordinates.

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 (IMA) 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. A corresponding CIF code should be entered into the 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.

Authors may find nomenclature programs such as AutoNom (http://www.mimas.ac.uk/crossfire/autonom.html) and ACDLABS (http://www.acdlabs.com/products/name_lab) to be useful resources when naming compounds.

5.3. Units

The International System of Units (SI) is used except that the ångström (symbol Å, defined as 10^{-10} 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 '$\times 10^n$'.

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).

In the reference list, entries for journals [abbreviated in the style of *Chemical Abstracts* (the abbreviations *Acta Cryst., J. Appl. Cryst.* and *J. Synchrotron Rad.* are exceptions)], books, multi-author books, computer programs and personal communications should be arranged alphabetically (note the order below for four references with the same first author) and conform with the following style:

Becker, T. M. & Krause Bauer, J. A. (1999). *Acta Cryst.* C**55**, IUC9900141.
Bond, A. D. (2003). *Acta Cryst.* E**59**, o1992–o1993.
Bond, A. D., Clayden, J. & Wheatley, A. E. H. (2001). *Acta Cryst.* E**57**, o292–o294.
Bond, A. D. & Davies, J. E. (2002). *Acta Cryst.* E**58**, o5–o7.
Bond, A. D., Davies, J. E. & Kirby, A. J. (2001). *Acta Cryst.* E**57**, o1242–o1244.
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. (2006). In preparation.
International Union of Crystallography (2008). *(IUCr) Structure Reports Online*, http://journals.iucr.org/e/journalhomepage.html
Jones, P. T. (1987). Personal communication.
Kiser, P. D., Lodowski, D. T. & Palczewski, K. (2007). *Acta Cryst.* F**63**, doi:10.1107/S1744309107020295.
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. (2007). PhD thesis, University of London, England.
Robinson, P. D. (2010). *Acta Cryst.* C**66**. In the press. [Paper reference ln3127.]
Sheldrick, G. M. (2008). *Acta Cryst*. A64, 112–122.
Smith, J. (2000). Private communication (refcode: PYMTLI01). CCDC, 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, except when the cited article has only one page, and that all computer programs given in the relevant `_computing_..._` entries must be referenced and included in the reference list. 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. The CIF editor, *publCIF* (see §1.1), allows the consistency of references and citations to be checked. Citations in supplementary material should also appear in the main body of the article.

7. Crystallography Journals Online

All IUCr journals are available on the web *via* **Crystallography Journals Online** at **http://journals.iucr.org/**. Full details of 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 can be found *via* the online CIF help page at **http://journals.iucr.org/c/services/cifinfo.html**.

7.1. Electronic status information

Authors may obtain information about the current status of their paper at **http://journals.iucr.org/services/status.html**.

7.2. Proofs

Proofs will be provided electronically in portable document format (pdf). The correspondence author will be notified by e-mail when the proofs are ready for downloading. Proofs will have been checked by the Section Editor, who reserves the right to make minor changes for consistency and conformity to *Section C* standards; any remaining problems will be referred back to the authors.

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