

Instructions to Contributors

General

It is understood that contributions which are submitted to **Zeitschrift für Kristallographie – New Crystal Structures** have not, nor will be simultaneously submitted or published elsewhere unless otherwise agreed. With the acceptance of the file for publication the publishers acquire full and exclusive copyright for all languages and for all countries.

The journal contains two kinds of New Crystal Structure publications (NCS):

- (i) results of determinations of hitherto unknown crystal structures with a short discussion of determination procedure, crystal structure, and/or structure-property relations (routine determinations and structures);
- (ii) refinements of previously published crystal structures which result in crystallographic data of higher quality in comparison with previously published ones.

Each publication should contain information about one structure only. For strongly related structures (*e.g.* isotopes) two (exceptionally more) data sets can be included in one publication. Both, single crystal and powder data are acceptable.

Paper charge

The correspondence author is asked to pay EUR 240 (+ 19 % VAT) for each published structure and should indicate his agreement clearly in the item `_publ_contact_letter` of the CIF-file.

Submission

Data files (CIF format), plot files shall be delivered via e-mail to: zkrist@oldenbourg.de

Samples of CIF-files can be downloaded from:
<ftp://ftp.oldenbourg.de/pub/download/frei/ncs>

For any question please contact the Technical Editor (e-mail: zkrist@oldenbourg.de) or the Managing Editor Prof. Yuri Grin (e-mail: grin@cpts.mpg.de).

Text part

The text part of the publication should be written in English and must be positioned in the following items:

`_publ_section_exptl_prep`
`_publ_section_experimental`
`_publ_section_comment`

It is expected, that item `_publ_section_exptl_prep` contains information about the source of the material and/or synthesis conditions, the item `_publ_section_experimental` contains information about non-routine details of the diffraction experiment and the item `_publ_section_comment` should include crystal structure description and discussion. Special details of the experiments (chemical analysis data, melting points, spectroscopic results) can be included in the text if they are absolutely necessary for the interpretation of the crystallographic data. These data will be available on-line in the CIF-file ([www.zkristallogr.de / Zeitschrift für Kristallographie – New Crystal Structures / news](http://www.zkristallogr.de/)).

Overall volume of the text part should not exceed 2800 characters (40 lines 70 characters each).

References

References in the text should read:
Arabic number in square brackets \Rightarrow [5].

References have to be ordered according to the mentioning in the text parts (see items order in the “Text part”).

The software used should also be referenced and the references should be added at the end of the reference list. The authors are required to complete data items in the `_computing` category of the CIF format containing details about the computer programs used in the crystal structure solution, refinement and analysis.

All references must be positioned in the item `_publ_section_references` and have to follow the standard rules of citation:

Journal publications:

Fitch, A. N.; Cockcroft, J. H. K.: The structure of solid carbon tetrafluoride. *Z. Kristallogr.* **203** (1993) 29–39.

Books:

Hausühl, S.: *Kristallphysik*. Physik-Verlag, Verlag Chemie, Weinheim 1983.

Articles in multi-author book publications:

Thompson, J. B.; Waldbaum, D. R.; Hovis, G. L.: Thermodynamic properties related to ordering in end member alkali feldspar. In: *The Feldspars* (Eds. W. S. MacKenzie, J. Zussman), p. 218–248. Manchester University Press 1974.

Figures

Figures can be accepted in the following format: PostScript (PS, EPS), BitMap (BMP), Windows Metafile (WMF), HPGL or TIF. The files containing figures should be submitted together with CIF-files per e-mail.

For reasons of quality the submitted figures should have the final size (85 mm wide). Letters and numbers may not be smaller than 2 mm.

Usually, only one figure is allowed for one structure. No figure caption will be printed.

International System of Units/IUPAC

The International System of Units (SI, *Système International d'Unités*) is to be used wherever possible (especially the temperature values should be given in K). Unit cell parameters and distances should be given in Å. The nomenclature should follow the IUPAC rules.

Please make sure, that you

- do not use word processors for editing CIF-files. At least the saving must be done in ASCII format.
- do not use LaTeX conventions for the text part.
- do not use non standard characters from the second half of the ASCII table (ã, Å, ç, Ć). In this case, the CIF convention should be applied (ã = \"a, α = \a); ask the editorial office for examples.
- do not write text lines longer than 80 characters.
- do not use tabs as separators in the CIF file.

- do not add or change information in the CIF items which contradicts their definition in CIF format.
- do not use word processors for preparing the plots and sending plots as WORD documents.
- do not send Bitmaps files without paying attention to the resolution of the lines and curves in the figure.
- do not forget atom labels in the figure(s) or use different labels in the figure(s) and the tables.
- do not forget to show the orientation of the unit cell (axes).

Proofs

Proofs will be sent only once to the author explicitly marked as correspondence author. Corrections are to be restricted to typographical errors. Substantial corrections exceeding the original typesetting costs by 5 % will be charged to the author(s).

Offprints

Thirty offprints of each article will be provided. Unless otherwise specified they will be sent to the correspondence author. Additional copies can be ordered upon return of the proofs. They will be charged according to the relevant price list.

The pdf-files of all publications are available from www.zkristallogr.de / Zeitschrift für Kristallographie – New Crystal Structures / news.

Depositing of Data

The authors are asked to keep structure factor lists for one year after publication in case they are requested.

After the publication is accepted, the submitted data will be deposited in the Fachinformationszentrum Karlsruhe (FIZ) and the Cambridge Crystallographic Data Centre (CCDC). Both databases provide the publisher with a deposition number which will be included in the contribution in Zeitschrift für Kristallographie – New Crystal Structures.