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. isotypes), 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 153 (+ 16 % VAT) for each publication 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:

e-mail: zkrist@verlag.oldenbourg.de

Samples of CIF-files can be downloaded from:

ftp://ftp.oldenbourg.de/pub/download/frei/ncs

For any question please ask the Technical Editor (e-mail: zkrist@verlag.oldenbourg.de) or the Managing Editor Prof. Yuri Grin (e-mail: grin@cpfs.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 the 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 (http://www.oldenbourg.de/verlag/zkristallogr/mn-ncsc.htm). 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 ⇒ [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 asked 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.; Cockroft, J. H. K.: The structure of solid carbon tetrafluoride. Z. Kristallogr. **203** (1993) 29–39.

Books:
Haussühl, 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.
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- do not write text lines longer than 80 characters.
- do not use tabs as separators in the CIF file.
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- 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. Any other changes involve time-consuming and expensive work, and the costs 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 are available from
http://www.oldenbourg.de/verlag/zkristallogr/mn-ncsc.htm.

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 has been accepted, the submitted data will be deposited with the Fachinformationszentrum Karlsruhe (FIZ) or 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.