Editorial **Open Access**

Twenty years of crystal structure publication and the road ahead

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Zeitschrift für Kristallographie – New Crystal Structures was founded as a *spin off* of *Zeitschrift für Kristallographie* in 1997 to provide a scientific journal which presents crystal structures in a compact format together with the most important crystallographic data. The circumstances of crystallographic research have changed dramatically in the last two decades in terms of quantity of results obtained and diffractometer access for researchers all over the world. In 2001, Frank H. Allen reported [1] the 200.000th crystal structure deposition with the CCDC since 1965. In 2015 the 800.000th deposited structure was announced [2], and we think that development will speed up. This development was and is driven by the simplification of structure determination and the purchase of hundreds of single-crystal diffraction systems each year, thus tens of thousands of datasets are collected each month. As already stated [3], the number of crystallographically experienced researchers does not increase with the rate of collected datasets. It is precisely this field of unresolved tension in which the *Editorial Board* of the *Zeitschrift für Kristallographie – New Crystal Structures* finds itself for some years.

In light of this development, we believe that there is a need to report strictly reviewed and validated new crystal structures in a compact format more than ever.

In the years 2012 to 2015 Mathias Wickleder filled the role as Editor-in-Chief of *Zeitschrift für Kristallographie – New Crystal Structures*. That period brought the transfer of the publishing house *Oldenbourg* to *De Gruyter* publishing. But, more importantly, the *Instructions to Contributors* have been revised to sharpen the profile of the journal. They have ensured a consistent level of quality. One major novelty was the more precise definition of a justification for a publication of so-called redeterminations. In the spring of 2016 Mathias Wickleder as well as the Assistant Managing Editor Katja Rieß left the Editorial Board. The *De Gruyter* publishing house and the members of the present Editorial board want to express their sincere gratitude for their work.

Since April 2016 the new Editor-in-Chief is Hubert Huppertz. He studied chemistry at the University of Bayreuth, Germany, performing his diploma thesis in the field of cyanamides. In 1997, he finished his doctorate with fundamental work on the structural extension of nitridosilicates. After changing to the Ludwig-Maximilians-University in Munich, he conducted his habilitation from 1998 to 2003 establishing a high-pressure laboratory with a chemical focus on the high-pressure/high-temperature syntheses of new oxoborates. From 2004 to 2008, he continued his investigations under extreme conditions in different areas of inorganic chemistry as an associate professor. In 2008 he was appointed as full professor for General and Inorganic Chemistry at the University of Innsbruck, Austria. His main research interests are dedicated to the explorative synthetic discovery of new compounds in the substance classes of borates, fluoride-borates, boro-germanates, boro-gallates, gallates, borate-nitrates, gallium-oxonitrides, rare earth molybdates, intermetallic compounds, and borides. Since 2013, he also fills the position of a Dean of the Faculty of Chemistry and Pharmacy at the University of Innsbruck.

Guido J. Reiss will continue his work in the Editorial Board as Co-Editor. He studied chemistry at the Saarland University, Germany and completed his studies with a diploma thesis on mercury and lead arene complexes. He earned his doctorate in 1996 from the University Kaiserslautern, Germany, working on complex hydrogen-bonded salts. Two postdoctoral short stays at the Institute of Physical and Theoretical Chemistry of Graz University of Technology, Austria were focussing on powder diffraction methods at non-ambient conditions. Since 1999 he is senior scientist at the Heinrich-Heine-University Düsseldorf working as service crystallographer. He is interested in the field of polyiodide synthesis and characterisation, as well as pseudosymmetry problems as a possible pitfall in crystal structure determination.

The Editorial office is occupied by the Managing Editor Holger Kleeßen, who is the administrative coordinator at the publishing house *De Gruyter*. The Assistant Managing Editor Michaela K. Meyer takes care of the technical preparation of the submitted data packages.

Beginning with Issue 3/2016 the paper's format and the *Instructions to Contributors* were slightly changed to take into account latest developments.

There are some important matters which were left unchanged:

- *Zeitschrift für Kristallographie – New Crystal Structures* provides a platform for the presentation of crystal structures in a compact format. Of particular importance for us is chemical and structural correctness which, e.g. includes the quality and quantity of solvate molecules and how they are modelled. If the structural information or the refinement strategy is unclear, one of the members of the Editorial Board will check the dataset. Therefore, it is required that the full data are uploaded at the very beginning of the review process.
- Each article is headlined by a title including the systematic name of the compound studied. The mere mentioning of educts/reactants, which reacted to the compound studied is definitely insufficient. At least one figure will be presented per article. It usually depicts the asymmetric unit and should ideally include ellipsoids of atomic displacements.
- Some details of the synthesis as well as analytical and spectroscopic results supporting the crystal structure determination are welcome, if presented in compact form. This information is located in the *Source of material* section of each article.
- Special features that are important to reflect the crystal structure determination (for example: twinning, disorder of some parts of the structure, decomposition) should be mentioned in the *Experimental details* section.
- The *Discussion* section comprises of two parts. The first 1–3 sentences should provide a short and focused introduction. Articles, books and programs cited, need to be concerned directly with the structure investigated or the methods used.
- The second part of the discussion should contain a brief structural description. Normally, this part begins with the enumeration of the asymmetric unit, which must be in accordance with the compound name. Unusual geometric features of the structure can be addressed and compared to the literature. For complexes we strongly recommend that the coordination modes are highlighted in the text and in the title. Finally, the intermolecular aspects of the structure can be described as far as they are of importance.

New items:

- Coloured figures will be printed, if there is a scientific reason and if an adequate justification can be provided. The same is true for a possible second figure, which will be presented as a split figure.
- The appearance of tables has been revised. Table 1 now contains more information: the R_{int} factor and the completeness of the data is now included. On the other hand the former Tables 2 and 3 were combined by eliminating the U_{ij} data. This decision is based on the fact that the complete cif file can be downloaded from the journals webpage as well as from the CCDC's webpage without any charge.

The team of *Zeitschrift für Kristallographie – New Crystal Structures* will maintain its fundamental philosophy that for each published crystal structure there is a strict need to verify the chemical and structural plausibility together with the interpretation of the findings by experienced reviewers. The additional use of an appropriate validation software is highly recommended, but it does not replace the reviewer's expertise.

Hubert Huppertz, Editor-in-Chief
Guido J. Reiss, Co-Editor

References

1. Allen, F. H.: The Cambridge Structural Database: a quarter of a million crystal structures and rising. Acta Crystallogr. **B58** (2002) 380–388.
2. http://www.ccdc.cam.ac.uk/Community/blog/post-58/
3. Spek, A. L.: Single-crystal structure validation with the program PLATON. J. Appl. Cryst. **36** (2003) 7–13.