Acta Crystallographica Section C Crystal Structure Communications

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# Broadening the scope of Acta Crystallographica Section C

## 30 years of Acta Crystallographica Section C

Acta Crystallographica Section C: Crystal Structure Communications celebrates its 30th anniversary in 2013. In 1983, Section C was created out of a merger of the Short Structural Papers, which had been included in Section B since 1972, with the successful journal Crystal Structure Communications, which had been published by the University of Parma, Italy, in the period 1972–1982. The new Section C adopted Crystal Structure Communications as its subtitle and published papers focusing on crystal structures of small molecules and continuous solids. The recognition of a continued demand to be able to publish very short reports of crystal structure determinations resulted in Section C including a Short Format Papers subsection in the period 1985–1993, CIF-access papers in the period 1997–1999 and Electronic Papers in 2000, and then the ultimate creation of Acta Crystallographica Section E in 2001.

Since then, *Acta Crystallographica Section C* has specialized in the rapid publication of articles that emphasize interesting scientific results and analyses based on the determination of high-quality or challenging crystal and molecular structures of interest in the fields of chemistry, biochemistry, mineralogy, pharmacology, physics and materials science. The journal has a reputation for publishing high-quality crystal structures, as well as articles describing difficult or challenging structures and the strategies used to address the difficulties. The depth of discussion has been an important aspect of articles presented in *Section C*.

### Making Section C fit for the next 30 years

The publishing business cannot stand still. New competition arises and the fields and interests of today's scientific community are constantly changing and expanding. As recently announced on the IUCr homepage, all of the IUCr journals are undergoing significant changes to keep them attractive to a wide range of scientists, to cater for new and exciting scientific fields and to remain competitive in the publishing marketplace. The changes are being implemented in conjunction with the activities planned for the International Year of Crystallography (IYCr2014) so as to gain the broadest exposure.

Some plans have already been developed through an extensive consultation process with the journal's editorial and co-editorial team, the relevant IUCr Commissions and some external scientists. I am very excited about the journal's future and would like to hear from current and potential authors on the concepts outlined below as well as any other suggestions for potential modifications to the journal so that we can fine-tune the proposed changes.

A sea change to the style and scope of *Section C* papers is envisaged with the aim of making the journal attractive to the broader scientific community, significantly increasing its size and more than doubling its impact factor within the next 2–3 years. Some of the proposed changes may initially appear to lessen the distinction between *Sections B* and *C*, but the relevant Section Editors will keep this matter under constant review as the two journals evolve and develop.

We are keen to publish science-facing papers, not just those focusing solely on a crystal structure determination. The idea is to engage the widest possible scientific community and to make them feel that *Section* C is the right choice for publishing work on any science to which structure contributes a role, whether that role be a major or minor one. Paper types might include lead articles, short reviews, research papers, letters to the editor or scientific community, while further fostering submission of manuscripts describing materials research and inorganic structures. To this end, we are currently

# editorial

discussing changing the journal subtitle from *Crystal Structure Communications* to *Structural Chemistry*. The aim of the change in subtitle is to cover a wide range of subject areas and broaden the scope of the journal to include and attract authors from across the chemical sciences.

In particular, we have identified a number of interest areas of structural chemistry from which the journal would welcome papers, although the list below should not be considered as exclusive: chemical reactions and mechanisms; computational chemistry; functional and porous materials; hydrogen bonding and weak interactions; inorganics, materials and minerals; metal–organic frameworks; mineralogy; molecular recognition; nanostructures; natural products; neutron and electron diffraction; pharmaceutical compounds; photocrystallography; polymers; polymorphs; powder diffraction; structure prediction; structures under extreme conditions; supramolecular chemistry; *etc.* 

#### **Special issues**

To relaunch the journal with this new scope, Section C will publish five special issues starting in September 2013. This is a new initiative for Section C as the journal has not published special issues before (the recent virtual issues notwithstanding). We have invited six eminent Guest Editors who are already hard at work inviting leading scientists to submit papers for their issue. There will be up to 12 invited papers in each special issue. The special issues are targeted at expanding the scope of the journal into the chosen focus areas, increasing the journal's impact and demonstrating to the scientific community the style of papers that the journal is now inviting. It is hoped that we can then continue to attract high-quality, high-impact papers from a broad range of scientists and so sustain the future of Section C for the community.

The Guest Editors who have agreed to prepare special issues, along with the issue title and release date, are given below.

Dr Glenn Yap (University of Delaware) – *Scorpionates* (chemical reactions and mechanisms), September 2013

Professor Chris Frampton (Pharmorphix) – Pharmaceutical compounds and natural products, October 2013

Professor Artem Oganov (SUNY, Stony Brook) – Computational materials discovery, November 2013

Professor Larry Falvello (University of Zaragoza) and Professor Alberto Albinati (University of Milan) – Interplay of crystallography, spectroscopy and theoretical methods for solving chemical problems, December 2013 Professor Andrei Khlobystov (University of Nottingham) – Nanostructures, April 2014

In addition, we are also planning this year's virtual issue to be on metal-organic frameworks and its publication is planned for late 2013. Authors interested in contributing papers for this virtual issue should submit their articles to *Section C* in the usual way. Articles that are published before October 2013 will be considered for inclusion in the issue. The virtual issue dedicated to the subject of absolute structure was released in December 2012 and includes papers relating to this topic published in *Section C* between January 2011 and November 2012. The issue is available at http://journals.iucr. org/special\_issues/2012/absolutestructure/.

Of course, we will continue to accept the traditional short structure communication papers we have been publishing up to now and indeed the above-mentioned special issues will still contain such papers as part of the issue. We encourage authors of the shorter papers to include some discussion of the science behind their crystal structure determinations, thereby ensuring that the importance of their structures is not lost on the wider community.

#### Changes to manuscript submission procedures

The Section C Notes for Authors are currently being redrafted to take the planned changes into account and will be published soon. A lot of very prescriptive instructions that have been inserted over the years have been removed in order to make the instructions more author-friendly. We will be more flexible about what needs to be in a paper and how the material should be presented, as long as the structures are correct and any unusual features or difficulties are properly documented. One of the strengths of Section C is that its team of knowledgeable Co-editors and reviewers ensure that the validation reports on structural results are assessed in a fair and realistic fashion without unreasonable requests being returned to authors.

Submission of full papers with everything in CIF format will still be welcome. However, we recognize that some authors are not keen to write the text of their papers in this format, despite the ease of pasting pre-prepared text into a CIF using *publCIF*. For longer papers, or those that do not actually report a crystal structure determination, it is now possible to submit the text parts of a paper as a Word document, rather than incorporating the text within the CIF file. Word document templates are available. The structural data will still need to be submitted in the usual CIF format along with separate files for the figures.