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On the scope of *Acta Crystallographica Section C*

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At the end of the IUCr Congress in Osaka last August, I took over from George Ferguson as Section Editor of *Acta Crystallographica Section C*. It is my great pleasure to express my warm appreciation to George for his exceptional stewardship of the journal over the last nine years, as well as his undying dedication to, and keen eye for, ensuring the continuing very high quality of the publications appearing therein.

The preamble in the 2009 *Section C Notes for Authors* states: '*Acta Crystallographica Section C: Crystal Structure Communications* publishes full papers with 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 particular quality of *Section C* that distinguishes it from *Acta Crystallographica Section E* is that each *Section C* paper contains an extended discussion that goes beyond reporting just the principal numerical and geometrical data of one or more crystal structures. The core of the discussion in a paper usually describes the significant, non-trivial and interesting or unusual features of each reported structure, plus a detailed comparison with any closely related structures and the presentation of the scientific background of the study. The discussion of results from other physical or chemical experiments is encouraged, as well as how the new knowledge of the reported structures helps the understanding of the chemical, physical or structural properties of the compound and promotes the aims of the study. Furthermore, to provide additional value-added material, a paper might include the presentation and meaningful discussion of multiple related structures, discuss in detail non-routine structure determinations or place the structure in an interesting scientific, physical or chemical context.

Many chemical journals nowadays limit the reporting of supporting crystal structures to very brief details or even just deposition of the data in the supplementary material or a database. As a result, some structures with interesting features remain obscure. Where the previous publication did not allow a crystallographically interesting structure to be described fully, a detailed report may be considered by *Section C*, provided such reports cite the original article and the manuscript primarily describes new information that was not presented in the original publication.

Section C also welcomes reports on studies involving special techniques and difficult or challenging structures, which are sometimes difficult exactly because the material has interesting properties or structural features, such as severe disorder, diffuse solvent regions or twinning. It is not the case that difficult, disordered or low-quality, yet interesting structures do not qualify for publication in *Section C* whenever severe checkCIF validation alerts are present. It is true that the unique checking, editing and publishing facilities of the journal are designed to ensure the highest standards of structural reliability, correctness and presentation. However, reports of structures that do not pass the validation criteria because of special properties of the material, special experimental techniques and/or difficulty in modelling the structure will be accepted, provided that (*a*) the structure is correct, (*b*) the experiment has been performed under the best possible conditions for the material concerned, including optimized crystal growth, use of low-temperature if weakly diffracting, appropriate data collection speeds and suitable modelling and refinement strategies, and (*c*) the root of the difficulties and the experimental procedures used to address them, together with the outcomes of the tried strategies, have been fully and properly documented in the *Experimental* section or discussed in the *Comment* section. In fact, a paper whose focus is on a detailed description of the reasoning and proper strategies for treating one or more non-routine structure determinations may be an interesting contribution to the journal even when the underlying

substance itself is not particularly novel. It should be emphasized that full documentation of non-routine experimental procedures (*e.g.* restraints used, disorder treatment, H-atom treatment, twinning details) is a normal part of any paper, not just those reporting difficult structures.

The mandatory use of the *checkCIF* facility prior to submission was introduced just over ten years ago. In his 1999 *Section C* Editorial, Syd Hall wrote: 'Coeditors and referees play a pivotal role in the review, with data validation filtering out problem submissions.... Automatic validation is not meant to be a precise arbiter of data quality or correctness, only an efficient tool for measuring compliance with a set of data rules.... While these criteria provide an explicit and consistent benchmark by which to gauge structural studies, they are not considered universal. Charge density analyses, for example, will probably require higher precision, whereas the data quality of some difficult studies may be lower.' [Hall, S. R. (1999). *Acta Cryst.* C**55**, 1]. The intent of the above statements still applies today. Co-editors and referees are still the final arbiters. *checkCIF* is not a firewall preventing the publication of difficult structures. If authors clearly document their difficult or challenging experiment in the paper and can show that they have done the very best that they can for the material at hand and clearly understand the problems, then the paper should pass technical scrutiny from the referees. The validation response form (VRF) required whenever severe *checkCIF* alerts are present should not be seen as a chore to be filled out in endless detail; it can simply point to explanations already given in the paper.

A new feature of IUCr journals is the ability to generate additional enhanced crystallographic diagrams online either before or at the time of submission. Such diagrams are dynamic in the online version of the journal, thereby allowing readers to rotate and view the image from various directions, zoom in and out, and view additional animations prepared by the authors. A static view will appear in the print version of the journal. Details of this facility are at http://submission.iucr.org/jtkt.

Sadly, a few cases of deliberately manipulated CIF data have recently been detected in submissions to this journal. Fraudulently misrepresenting a structure is taken very seriously. The validation procedures are able to detect many manipulations of the data. Authors should not attempt to hide features in a structure determination that lead to validation alerts, because those very features may be an indication of something interesting about the structure that is worth highlighting, such as disorder or twinning, or that there is an error in the model, such as an incorrect element assignment. Authors who do not understand the meaning of a validation alert, should not hesitate to enquire about it, and those who do not yet have enough experience to interpret and treat certain unusual features or non-routine aspects of a structure determination should seek assistance from a colleague.

It is a pleasure to welcome Len Barbour (University of Stellenbosch), Ulli Englert (RWTH Aachen), Phil Fanwick (Purdue University), Andreas Goeta (University of Durham), Maciej Kubicki (Adam Mickiewicz University), Vratislav Langer (Chalmers University of Technology), Peter Müller (MIT) and Hidehiro Uekusa (Tokyo Institute of Technology) as new members of the *Section C* editorial board. In addition, Alexander Blake has been appointed as Deputy Section Editor to assist with reading of the proofs and to act as a sounding board for new ideas.

I wish to warmly thank those Co-editors who have recently retired from the *Section C* editorial board for their excellent services to the journal and the crystallographic community: Leonid Aslanov, Nobuo Ishizawa, Shigeru Ohba, Maryjane Tremayne and Madeleine Helliwell. I would also like to take this opportunity to thank all the current *Section C* Co-editors and the Chester Editorial Office staff for their outstanding contributions to *Section C* and for the support they have given me as a newly appointed Section Editor.