Chemical Communications

Notice to Authors

Publication of *X*-Ray Crystallographic Work in the Journal

Preamble

At a meeting of the Primary Journals Committee held in October, 1975 a sub-committee was set up to consider policy with regard to publication in the *Journal* of both preliminary communications and substantive papers concerned with *X*-ray crystallographic work. This step was taken in the light of correspondence received by the Society which indicated concern by many referees on the problems created by the large number of routine *X*-ray crystallographic studies submitted to the Society as a result of the increasing ease of carrying out such work.

Since the sub-committee's terms of reference were wide it was able to consider both this problem and others relating to publication of *X*-ray crystallographic work in all sections of the *Journal*. Its recommendations which are outlined below fall into two groups: those concerned with preliminary communications and those with full papers. These recommendations have been endorsed by the Primary Journals Committee and now represent the Society's policy with regard to crystallographic work submitted for publication in its primary journals.

Preliminary Communications

(1) Evidence was presented to the sub-committee that a major problem associated with the publication of preliminary reports of crystallographic work in *J.C.S. Chem. Comm.* arose as a result of the non-availability to interested readers of the atomic co-ordinates associated with the work. Although in the normal course of events such data would be expected to appear in the follow-up paper, many cases were cited where the period between publication of the preliminary report and the substantive paper was many years or the full papers never appeared in print. The evidence presented suggested that there was considerable disquiet among crystallographers at this state of affairs. In an attempt to improve this situation and after consultation with the Cambridge Crystallographic Data Centre (C.C.D.C.) the Society has resolved to press authors of preliminary reports of *X*-ray crystallographic work to submit together with their communication certain material for deposition with the Centre.* This material will be checked at the Centre for internal consistency and, afterwards, will be available on request to interested readers. The procedure to be adopted will be as follows:

(i) In addition to the communication and the customary covering letter of justification the authors will be expected to provide a complete list of refined co-ordinates (in the form of computer print-out and NOT a retyped version) and a table of bond distances unless these are given in full in the manuscript. If the complete 'crystal data' (i.e. cell dimensions and standard deviations, space group, number Z of formula units per cell) are not listed in the manuscript these must also be submitted.
It should be emphasised that the co-ordinates submitted for deposition, whilst not necessarily being 'fully' refined, should correspond to the stage of refinement described in the preliminary communication and should be the set for which the R factor is quoted. It follows that all bond distances given in the preliminary communication should correspond, apart from any rounding-off errors, with bond distances which can be calculated from the deposited co-ordinates.

(ii) The communication will be assessed in the customary fashion, the material for deposition also being made available to the referees concerned. If the communication is accepted the Society will forward the material for deposition to the C.C.D.C. A statement will be made in the communication that particular material is available from the Centre on request.

(iii) The C.C.D.C. will acknowledge receipt of the material. When a communication is published the deposited material will be evaluated and included in their files as part of their normal abstracting cycle. The evaluation consists of recalculation of the bond lengths from the author's co-ordinates and comparison of these with the author's values. All data on the Centre's files have to pass this internal consistency test. It will not, however, be possible for the evaluation to be made before the appearance of the preliminary communication in print.

(iv) Finally, where an author plans not to follow-up his preliminary communication with a full paper he will be required to submit, in addition to the material outlined above, a copy of the structure factor table for the work presented for deposition with the British Library, Lending Division. In this way it too will be available to interested readers.

(2) In order to aid the readability of communications it is recommended that each should contain a line drawing of the compound under discussion where appropriate.

* Applies only to compounds containing organic carbon atoms.

Papers in Dalton and Perkin Transactions

The sub-committee considered evidence which indicated that *X*-ray crystallographic papers submitted to the *Journal* were assessed in a less rigorous fashion than those reporting other areas of work. Although the sub-committee felt that this claim was largely unsubstantiated it was agreed that improvement of both assessment procedure and presentation of work was possible. The following recommendations have, therefore, been adopted.

(1) Crystallographic papers will be assessed for their chemical as well as their crystallographic interest.

(2) Unless both specifically requested by the author and recommended by the referees for publication, vibrational parameters will be routinely deposited with the structure factors as a Supplementary Publication. Where vibrational parameters are to be published they should be in the form of U_{ij} with units of Å^2.
Referees are reminded that they may, at their discretion, recommend other material for deposition where in their view its inclusion in the parent paper is not justifed by its interest.

(3) Each paper should contain a line drawing of the compound under discussion where appropriate in addition to the usual crystallographic figures.