

reflections, source of the material, and such other information (especially structural) as can be conveyed in approximately 50 further words.

The *Introduction* will briefly state the reason for undertaking the structure determination and its chemical, physical, biological or other interest. If organic, or containing complicated organic ligands, a display of the structural formula of the material studied should be given, in accordance with IUPAC convention.

The *Experimental* section will give the source of the material, the method of measuring D_m , the crystal shape and size, the diffractometer used, the reflections used for measuring the lattice parameters, the systematic absences, the absorption correction applied (with maximum and minimum values), the maximum value of 2θ reached in the intensity measurements, the range of hkl measured, the standard reflections and their intensity variation throughout the experiment with their overall e.s.d.'s, the number of reflections measured, the number of unique reflections, the value of R_{int} (from merging equivalent reflections), the number of unobserved reflections, the criterion for recognizing unobserved reflections, the method used to solve the structure, the use of F or F^2 magnitudes in least-squares refinement, the methods of locating and refining hydrogen-atom coordinates (if applicable and if by methods other than least squares), the parameters refined, the final R [$= \sum (|F_o| - |F_c|) / \sum F_o$] given only in the *Abstract*, wR [$= \sum w(|F_o| - |F_c|)^2 / \sum wF_o^2$]^{1/2}, S [$= \sum w(|F_o| - |F_c|)^2 / (m - n)$]^{1/2} [where w is the weight, m is the number of observations, n is the number of variables, F_o is the observed and F_c is the calculated value of $F(hkl)$], the method used to evaluate w , the ratio of maximum least-squares shift to error in the final refinement cycle, the average ratio of shift to error, the maximum and minimum height in the final difference Fourier synthesis, the secondary-extinction value (if used), $F(000)$, the source of atomic scattering factors and (if used) anomalous-dispersion corrections, and all computer programs used.

The *Discussion* will generally include two tables [as in (1) and (2) above] and two figures [as in (3) and (4) above]. Additional tables and figures may be deposited. If the table of bond distances and angles is very long, this will be deposited and unusual values only given for publication. Comment should be made on any unusual features of coordination, bonding, bond lengths, bond angles, thermal vibrations, etc.

Any nonroutine measurement of physical properties (magnetic susceptibility, dielectric permittivity, elastic moduli, etc.) should be mentioned in the *Abstract* and the numerical values quoted there if possible. If the numerical values are too lengthy to be given in the *Abstract*, they should be given in a suitably headed paragraph in the paper, normally preceding the *Discussion*.

Tables of structure factors, anisotropic thermal parameters, least-squares planes and hydrogen-atom coordinates if not refined must be submitted in duplicate with the paper, but will not normally be published. After acceptance of the paper they will be deposited along with any other extensive tables or figures, in accordance with the Union's procedures.

The requirements regarding figures and references remain unchanged. Acknowledgements may be included at the end of the text.

Acta Cryst. (1982). B38, 700

Commission on Journals Chemical Formulae and Nomenclature

Authors are reminded that chemical formulae and nomenclature in papers submitted to *Acta Crystallographica* and *Journal of Applied Crystallography* should conform to the rules of nomenclature established by the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry (IUB) and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name. A structural formula should generally be given for all organic and organometallic compounds.

All papers in *Acta Crystallographica*, Section B, reporting crystal structure determinations and all Crystal Data in *Journal of Applied Crystallography* should include the approved name(s) of the compound(s) in the title of the paper or in a footnote to the title. Any paper in *Acta Crystallographica*, Section A, or in *Journal of Applied Crystallography* dealing with the crystal physics or the properties of a particular material should also include the approved name of the compound concerned. It is desirable that any accepted trivial name, trade mark, recommended International Non-proprietary Name (INN), United States Adopted Name (USAN) or British Pharmacopoeia Approved Name be retained, but the corresponding systematic (IUPAC) name should be provided. For a list of available nomenclature sources see *Acta Cryst.* (1979). B35, 2827. [Approved Names 1977 – a list of approved names for pharmaceutical compounds with their corresponding systematic (IUPAC) names, published for the British Pharmacopoeia Commission – is available from Her Majesty's Stationery Office.]

Assistance in the naming of compounds in accordance with IUPAC and IUPAC-IUB rules may be obtained from Dr K. L. Loening, Director of Nomenclature, Chemical Abstracts Service, PO Box 3012, Columbus, Ohio 43210, USA; from Mr E. W. Godly, Chemical Nomenclature Advisory Service (CNAS), Laboratory of the Government Chemist, Department of Industry, Room A-510, Cornwall House, Stamford Street, London SE1 9NQ, England; and in the particular naming of inorganic compounds from Professor Y. Jeannin, Laboratoire de Chimie des Métaux de Transition, Université Pierre et Marie Curie, 4 place Jussieu, 75230 Paris CEDEX 05, France. Enquiries may also be addressed to Dr J. E. Derry, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. If advice on chemical nomenclature is sought from any of the above advisory sources authors are requested, when submitting a manuscript to the Union's journals, to indicate the source consulted.

The attention of authors is also drawn to other notices concerning the submission of papers to this journal. The last such notice and cross-references to earlier ones appear in *Acta Cryst.* (1981), B37, 1162.