Suggested guidelines for the publication of Rietveld analyses and pattern decomposition studies

A letter from R. A. Young, E. Prince and R. A. Sparks to the Editor of Journal of Applied Crystallography has been published [J. Appl. Cryst. (1982), 15, 357-359] with the above title. The first paragraphs read as follows:

At the request of the Commission on Journals, we drew up some draft guidelines for the publication of Rietveld analyses and of pattern decomposition studies with powder diffraction patterns. The draft was sent for comment to some 25 persons in Europe, Australia, Japan, and the USA. We are grateful for their responses, which both were generally supportive of the idea that there be guidelines and were most helpful in illuminating oversights and other deficiencies. Not all suggestions were incorporated in the revised draft, of course (in fact, a number were mutually contradictory), but all were carefully considered and many were incorporated in the version which follows.

In presenting these suggested guidelines, we emphasize that we offer them as guidelines, not rigid rules. They are intended primarily to be helpful to the co-editors; they are not intended to infringe on a co-editor’s judgement of scientific worth of a submitted manuscript, nor should they be allowed to do so. For the most part, these suggested guidelines address matters of format and presentation of details, and not the fundamental question of scientific interest and worth of the submission. It is primarily for the making of such fundamental judgements that the co-editor system exists; for the health of our science it cannot and should not be replaced with a system of blind rules on a check-off sheet. It is against this background of more overreaching considerations that we offer the following suggestions for guidelines to assist, but not to control or coerce, the co-editors in their acceptance decisions.

Notes and News


Suggested guidelines for the publication of Rietveld analyses and pattern decomposition studies


This is the first of a series intended for science teachers in secondary schools in order to keep them informed of current developments in science. After a short discussion of atomic structure and chemical bonds, the author classifies matter in two states: the disordered (the perfect gas) and the ordered (the perfect crystal). A major part of the book is concerned with the field between these two extremes from liquids via colloids, liquid crystals, polymers, crystalline aggregates with their preferred orientations, to real crystals with their defects.

While the work covers the whole field of crystallography, there is little use of mathematics. The author’s aim is not to give rigorous proofs of physical laws but to demonstrate the consequences of these laws in everyday life.

Many university teachers would do well to incorporate in