Letters to the Editor

To: Deane K. Smith, Editor   November 26, 1990

A significant error was included in an article published in the September issue of *Powder Diffraction*. The article in question dealt with structural properties of various barium sodium niobates (pp. 125-30).

On p.129 we are informed that "... nearly all reflections of BNN-S appear with hkls of h + k = 2n and l = 2n, equivalent to h + k + l = 2n. This condition suggests that BNN-S has a body-centered pseudocell. However, the BNN-S sample showed an obvious SHG effect and consequently it must be non-centrosymmetric, and cannot be body-centered."

The authors' optical measurements indicated that their material is acentric. That seems to be correct. What is confusing is their conclusion that the material therefore cannot be body-centered. That is incorrect. The acentric nature of the specimen does not rule out the possibility that their material is also body-centered. One of the best known of the materials which display a Second Harmonic effect is potassium dihydrogen phosphate, an acentric body-centered crystal. Also there are at least 12 acentric body-centered space groups in the tetragonal system as well as several in other crystal systems. Clearly, correction or clarification of the authors' statement is needed.

Ben Post
1111 Beacon St.,
Brookline, Massachusetts
02146 U.S.A.

Erratum

The entry for the number of reflections given in Table 1, p. 28, Volume 6, Number 1, 1991 (Determination of Crystal Structure of $Cd_3(BO_3)_2$ by Powder X-Ray Diffraction, Laureiro *et al.*) should read: 198, not 5.

To: Deane K. Smith, Editor   January 14, 1991

The latest issue of *Powder Diffraction* (Vol. 5, Number 4 of December 1990) contains a rather large amount of disinformation, for which the journal should apologize to its readers. The second column of Computer Comments (right hand part of page 234) is nearly entirely wrong. The contents of this part are announced as an abstract of a paper by John Bradberry in DR DOBBS JOURNAL (1990) **15** (9) 26-32 entitled: 'Porting FORTRAN Programs from Mini's to PC's.', a method to prevent software madness. If anything, this paper contributes to software madness, especially its DOs and DONOTs, since most of these are wrong.

There is only one way of making programs portable, and that is to adhere to the ANSI FORTRAN 77 standard. As far as I know, all manufacturers of compilers adhere to the requirement that their compilers will at least compile an ANSI Fortran 77 program correctly. Their compilers may be able to handle a number of useful enhancements, but correctly compiling ANSI Fortran 77 is the minimum requirement.

The Fortran Standard can be learned from the ANSI publication 'ANSI X3.9 – 1978 FORTRAN 77', obtainable from your bookstore or from the American National Standards Institute, 1430 Broadway, New York NY 10018. This publication should be on the desk of every serious FORTRAN programmer.

In short, there are only three, easily memorisable, rules for writing FORTRAN programs that will survive your next change of computer:

Write only ANSI FORTRAN 77
Write only ANSI FORTRAN 77
Write only ANSI FORTRAN 77

Yours sincerely

J.W. Visser
Henry Dunantlaan 81
2614 GL Delft
The Netherlands