

from SUP 43571) and 104 parameters. The $P1$ model of Fornasini involves 197 parameters.

Despite the change in space group, the $P\bar{1}$ structure reported here (Table 1)* differs little from the $P1$ structure of Fornasini (1987); indeed, all coordinates agree (after translation of the origin) within 0.04 Å. Thus, the coordination polyhedra described by Fornasini are little changed and the structure remains complex. However, 'the low symmetry, very unusual for an intermetallic phase' is not quite so low. In addition, the $P\bar{1}$ structure shows coordinate e.s.d.'s that are smaller by factors of about $\frac{1}{4}$ – due, of course,

* A list of anisotropic U_{ij} values has been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44474 (1 p.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

to the removal of the near-singularities inherent in refining an approximately centrosymmetric model in a non-centrosymmetric space group.

The $P\bar{1}$ model considered by Fornasini (1987), which was derived by 'direct methods', apparently differs from our model in that the two atoms In(1) and In(6), rather than In(3) and In(5), were located on centers of symmetry (0,0,0 and $0, \frac{1}{2}, \frac{1}{2}$). In that model, the In atoms map fairly closely – within 0.3 Å – onto the In atoms in our model; however, many of the Ca atoms do not. It seems likely that further pursuit of the $P\bar{1}$ model of Fornasini, perhaps using difference maps, might have led to the correct structure.

Reference

FORNASINI, M. L. (1987). *Acta Cryst.* **C43**, 613–616.

Notes and News

Acta Cryst. (1988). **C44**, 396

Publish your Crystallographic Computer Programs

A large number of new crystallographic computer programs (or modifications to existing programs) presented at international and national conferences, summer schools, private demonstrations, or referred to only passingly in other publications remain unpublished. Consequently, potential users are deprived of valuable information and access to state-of-the-art computer code. The IUCr Commission on Crystallographic Computing is well aware of this problem and is particularly anxious to encourage authors of computer programs to publish their software. The journal of choice for crystallographic computer programs is:

Journal of Applied Crystallography – a publication of the IUCr – which provides two categories of publication concerned with crystallographic computer programs: *Computer Programs* is intended for complete articles giving in-depth information on the program and algorithm whereas *Computer Program Abstracts* provides a condensed format that contains only essential details.

In *Computer Programs*, a brief description of the purpose, strategy, computer language, machine requirement, input requirements and the type of results obtained should be included. Ordinarily, it is required also that the adequacy of

the documentation shall have been proven by the successful use of the program by someone outside the authors' institution. Examples of *Computer Programs* are: *TREOR*, a semi-exhaustive trial-and-error powder-indexing program for all symmetries [Werner, P.-E., Eriksson, L. & Westdahl, M. (1985). *J. Appl. Cryst.* **18**, 367–370]; *STRUPLO84*, a Fortran plot program for crystal structure illustrations in polyhedral representation [Fischer, R. X. (1985). *J. Appl. Cryst.* **18**, 258–262]. *Notes for Authors* may be found in *Acta Cryst.* (1983), **A39**, 174–186 and a checklist in *J. Appl. Cryst.* (1985). **18**, 1–2.

Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing programs. Following normal submission, a *Computer Program Abstract* will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given in *J. Appl. Cryst.* (1985). **18**, 189–190. Examples of publications in this category are: *PATMET* – program for determination of orientation and position of a known fragment in the unit cell [Wilson, C. C. & Tollin, P. (1986). *J. Appl. Cryst.* **18**, 411–412], *DREAM* – data reduction and error analysis routines for accurate single-crystal diffraction intensity measurements [Blessing, R. H. (1986). *J. Appl. Cryst.* **19**, 412].