benzene transform and incorrect signs to those in the negative region. For each of the two new problems the *MULTAN* solution with the highest figure of merit was chosen as a starting point. For reflections lying in the positive region of the benzene transform the phase was taken as found; for reflections lying in the negative region of the benzene transform the phase was changed by 180°. The first 50 reflections on the *E* list were given fixed phases assigned in this way and another cycle of *MULTAN* was run. The resulting *E* maps are shown in Figs. 1(*b*) and 2(*b*). In both cases the solutions are essentially correct (15 out of 17 correct peaks in the first case, 26 out of 28 in the second). In both cases this trial structure led to successful refinement.

These two examples suggest that the triangular pattern in the false *E* map must coincide with the hexagonal pattern in the correct structure in order for this method to work. If the peaks in the false solution were displaced from the correct peaks by something other than a bond vector, as sometimes happens in normal structures even when the figure of merit is large, our procedure would not be expected to lead to the correct solution.

References

BRITTON, D. & DUNITZ, J. D. (1981). *Acta Cryst.* A**37**, 131–132; erratum: *Acta Cryst.* A**38**, 172.

MAIN, P., WOOLFSON, M. M., LESSINGER, L., GERMAIN, G. & DECLERCQ, J. P. (1974). *MULTAN. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

THEISSEN, W. E. & BUSING, W. R. (1974). *Acta Cryst.* A**30**, 814–821.

Acta Cryst. (1982). A**38**, 172

Recognition and use of systematically aberrant phase relationships. I: Erratum.

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Abstract

In the paper by Britton & Dunitz [*Acta Cryst.* (1981), A**37**, 131–132] three errors have been printed. On p. 131, 2nd column, line 5: '−2' should be changed to '−3'; on p. 132, 1st column, line 6: 'one-third' should be changed to 'half'; p. 132, 2nd column, lines 2–3: 'relatively even deeper' should be changed to 'only slightly less deep'.

All the information is given in the *Abstract*.

Notes and News

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ICSD – Inorganic Crystal Structure Data Base

Complementary to the well known Cambridge Crystallographic Data File, a similar file for inorganic substances has been established at the University of Bonn (G. Bergerhoff and I. D. Brown). The current file contains information on 9000 structures: chemical name, chemical formula, mineral name, unit cell, space group, coordinates, temperature factors, references, remarks. More detailed information will be given in a paper to be published in *Acta Crystallographica*. The data base will be made available by Fachinformationszentrum Energie Physik Mathematik GmbH (Dr H. Behrens), D-7514 Eggenstein-Leopoldshafen, Federal Republic of Germany, from 1982 on, in three versions:

1. On-line access *via* telecommunications systems (Euronet, Datex-P, *etc.*).

2. Leasing the up-to-date data base and retrieval programs (IBM-Fortran) at an annual rate.

3. Leasing only the up-to-date data base at an annual rate.

Detailed conditions are available on request from Dr Behrens at the address given above.

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