

Table 1. *Matrices found for a cubic primitive cell*

|    |        |        |        |    |       |        |        |
|----|--------|--------|--------|----|-------|--------|--------|
| 1  | -1 0 0 | 0 -1 0 | 0 0 1  | 13 | 0 0 1 | -1 0 0 | 0 -1 0 |
| 2  | -1 0 0 | 0 0 -1 | 0 -1 0 | 14 | 0 0 1 | 0 -1 0 | 1 0 0  |
| 3  | -1 0 0 | 0 0 1  | 0 1 0  | 15 | 0 0 1 | 0 1 0  | -1 0 0 |
| 4  | -1 0 0 | 0 1 0  | 0 0 -1 | 16 | 0 0 1 | 1 0 0  | 0 1 0  |
| 5  | 0 -1 0 | -1 0 0 | 0 0 -1 | 17 | 0 1 0 | -1 0 0 | 0 0 1  |
| 6  | 0 -1 0 | 0 0 -1 | 1 0 0  | 18 | 0 1 0 | 0 0 -1 | -1 0 0 |
| 7  | 0 -1 0 | 0 0 1  | -1 0 0 | 19 | 0 1 0 | 0 0 1  | 1 0 0  |
| 8  | 0 -1 0 | 1 0 0  | 0 0 1  | 20 | 0 1 0 | 1 0 0  | 0 0 -1 |
| 9  | 0 0 -1 | -1 0 0 | 0 1 0  | 21 | 1 0 0 | 0 -1 0 | 0 0 -1 |
| 10 | 0 0 -1 | 0 -1 0 | -1 0 0 | 22 | 1 0 0 | 0 0 -1 | 0 1 0  |
| 11 | 0 0 -1 | 0 1 0  | 1 0 0  | 23 | 1 0 0 | 0 0 1  | 0 -1 0 |
| 12 | 0 0 -1 | 1 0 0  | 0 -1 0 | 24 | 1 0 0 | 0 1 0  | 0 0 1  |

allow the computer program to seek matrices with integer elements as high as  $\pm 10$  (typical computer run time of less than 5 s on an UNIVAC 1108). In contrast, when using reduced cells, matrix elements of 0 and  $\pm 1$  may be used (typical run time of about 0.03 s). The 24 matrices listed in Table 1 for a primitive cubic cell were output from the computer program used to calculate B matrices. Multiplication of the matrices in Table 1 by  $-1$  generates a set of 48 matrices which are identical to those listed for the 48 symmetry operations compatible with a cubic lattice (Rigault, 1980).

Computer analysis of approximately 30 000 lattices from the National Bureau of Standards Crystal Data File has proved that the matrix procedure for metric symmetry determination is fast, efficient and reliable. The method predicts a metric lattice symmetry which, in most cases, is consistent with the reported crystal symmetry. In a relatively low percentage of cases, the matrix procedure predicts a higher symmetry. Our analysis has revealed that many rhombohedral crystals have been incorrectly reported in centered monoclinic or in triclinic space groups. The computer analysis has also shown that many metrically centered orthorhombic crystals have been reported in primitive monoclinic or in triclinic space groups. Further discussions are planned concerning the cases for which the metric symmetry exceeds the reported crystal symmetry.

It has become apparent that metric symmetry, and possibly crystal symmetry, is often missed by techniques

employed on modern automated diffractometers. Ideally, the check for metric symmetry should be carried out as soon as a refined unit cell has been determined. Our experience shows that the matrix procedure offers a direct and convenient way to determine the metric lattice symmetry.

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#### References

- CLEGG, W. (1981). *Acta Cryst.* **A37**, 913–915.  
*International Tables for X-ray Crystallography* (1969). Vol. I, 3rd ed., p. 8. Birmingham: Kynoch Press.  
MIGHELL, A. D. & RODGERS, J. R. (1980). *Acta Cryst.* **A36**, 321–326.  
RIGAULT, G. (1980). *Metric Tensor and Symmetry Operations in Crystallography*. Published for the International Union of Crystallography Commission on Crystallographic Teaching by Univ. College Cardiff Press, Cardiff, Wales.  
SANTORO, A., MIGHELL, A. D. & RODGERS, J. R. (1980). *Acta Cryst.* **A36**, 796–800.

#### Notes and News

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#### Formation of the British Crystallographic Association

The following note by Professor D. M. Blow, Chairman of the UK National Committee for Crystallography, has been reprinted from the *Royal Society News*, by kind permission of the Royal Society:

For many years the organisation of crystallography at a national level in the UK has been split between a number of scientific societies. The two largest are the Crystallography Group of the Institute of Physics and the Chemical Crystallography Group of the Royal Society of Chemistry,

but a number of other societies cover crystallographic aspects of metallurgy, materials science, geology and biophysics. The UK Crystallographic Council provided a loose link between groups of crystallographers but it could not provide a speedy, collective response of UK crystallographers on, for instance, draft Health and Safety Executive legislation or EEC directives. Nor did its structure allow it to undertake activities with financial responsibilities, such as the organisation of a European Crystallographic Meeting in the UK.

The British National Committee for Crystallography, in addition to its duties as corresponding body to the International Union of Crystallography, provided a forum where matters concerning crystallography in the UK could be discussed. But it was not appropriate for it to deal with

internal national matters. On the initiative of the National Committee, a working party was set up with the aim of establishing a new independent body covering all areas of crystallographic interest, to present the views of crystallographers collectively, to organise meetings of a crystallographic nature and to act as a centre for the dissemination of information on crystallography both within the profession and to a wider audience.

This initiative gained strong support. Particular help was given by the committees of the two largest groups in devising a system for incorporating their activities into the new Association. The British Crystallographic Association was inaugurated on 5 April 1982 at a meeting in Durham. The elected Officers of the new body are: President: Sir David Phillips, Professor of Molecular Biophysics in the University of Oxford and Biological Secretary, Royal Society; Vice-President: Professor Dorothy M. Hodgkin, Emeritus Professor in the University of Oxford; Treasurer: Professor C. A. Taylor, Professor of Physics at University College, Cardiff, in the University of Wales; Secretary: Dr A. C. Skapski, lecturer in physical chemistry at the Imperial College of Science and Technology, London.

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### **International Summer School on Crystallographic Computing, Kyoto, Japan**

The International Summer School on Crystallographic Computing will be held in Kyoto, Japan, from August 18th to 27th, 1983. The school is organized by the IUCr Computing Commission under the auspices of the International Union of Crystallography and the Crystallographic Society of Japan.

For further information on the school write to Professor T. Ashida, Faculty of Engineering, Nagoya University, Chikusa-ku, Nagoya 464, Japan.

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### **European Crystallographic Committee Co-operation Schemes**

The European crystallographers, through the European Crystallographic Committee, invite colleagues in developing countries to join in co-operation schemes.

The purpose of these schemes is to exchange information and to assist in data collection by automatic diffractometers and micro-densitometers.

Active crystallographers, who are interested, are invited to contact any one of the following persons, who will try to organize contacts with appropriate partners.

France—Professor A. Authier

Laboratoire de Minéralogie Crystallographie,  
Tour 16,  
Université Pierre et Marie Curie (Paris 6),  
4 Place Jussieu,  
75230 Paris CEDEX 05,  
France.

Germany, Federal Republic—Professor H. Burzlaff

Lehrstuhl für Kristallographie der Universität,  
Loewnichstrasse 22,  
D8520 Erlangen  
Federal Republic of Germany.

Italy—Professor M. Nardelli

Istituto di Chimica Generale e Inorganica,  
Università di Parma,  
Via M. D'Azeglio 85,  
43100 Parma,  
Italy.

Netherlands—Professor D. Feil

Twente University of Technology,  
Chemical Physics Laboratory,  
PO Box 217,  
7500 AE Enschede,  
The Netherlands.

Spain—Professor S. Garcia Blanco

Departamento de Rayos X  
Instituto de Quimica-Fisica Rocasolano,  
Serrano 119,  
Madrid 6,  
Spain.

Sweden—Professor I. Olovsson

Institute of Chemistry,  
University of Uppsala,  
Box 531,  
S-75121 Uppsala 1,  
Sweden.

USSR—Professor D. Kheiker

Institute of Crystallography,  
Academy of Sciences of the USSR,  
Leninsky prospekt 59,  
Moscow 117333,  
USSR.

UK—Dr O. Kennard

University Chemical Laboratory,  
Lensfield Road,  
Cambridge CB2 1EW,  
England.