

limited. There are basic differences between the two methods which could account for the discord and these will be discussed.

The perfect* crystal does not exist. Just as the bilateral symmetry of the human body does not stand up to close scrutiny neither does the normal crystal. For instance in a crystal of AgNO_3 , 4.9% of the unit cells will contain an ^{18}O atom, 3.0% an ^{15}N atom, while the isotopes of ^{107}Ag and ^{109}Ag are 51.8 and 48.2% abundant. If added to this are packing faults, defects, strains and anharmonic factors the crystal is far from perfect and the concept of symmetry becomes less precise. It does appear that infrared and Raman spectroscopy can occasionally differentiate between the ordered and the disordered parts of the lattice. Typically vibrational spectroscopy detects the normal modes near the zone centre ($k \approx 0$) which are the in-phase motions of coupled unit cells. Both substitutional and anharmonic shallow-well defect centres may be incorporated into the ordered spectrum for certain modes but deep-well defects will be decoupled from the ordered lattice and appear as local modes (Belousov, Pogarev & Shultin, 1977; Brooker, 1979). Usually the local modes are not included in the vibrational analysis and symmetry arguments are based only on the ordered part of the spectrum. In a diffraction analysis all atoms are included and small discrepancies probably appear in the thermal parameters. Some of the problems associated with treating thermal motions of atoms have been discussed by Willis & Pryor (1975). They point out that anharmonic effects can cause mean-square displacements to be anisotropic as well as giving rise to the appearance of theoretically forbidden reflections. Since the root-mean-square rotation of the plane of the NO_3^- groups in AgNO_3 may be as great as 8° at room temperature (TG) it is difficult to envisage the atomic positions being placed with a high degree of certainty. MRC employed only isotropic thermal factors for the N and O atoms and it is possible that these do not adequately account for the large thermal motions. Careful low-

temperature diffraction data would provide useful information on the anharmonic motions in AgNO_3 and could perhaps help resolve the AgNO_3 structure problem.

References

- ASAWA, C. K. & BARNOSKI, M. K. (1970). *Phys. Rev. B*, **2**, 205–213.
- BATES, J. B. & BROOKER, M. H. (1973). *Chem. Phys. Lett.* **21**, 349–353.
- BELOUSOV, M. V., POGAREV, D. E. & SHULTIN, A. A. (1977). *Phys. Status Solidi B*, **80**, 417–424.
- BIRNSTOCK, R. (1967). *Z. Kristallogr.* **124**, 310–334.
- BROOKER, M. H. (1973). *J. Chem. Phys.* **59**, 5828–5829.
- BROOKER, M. H. (1979). *J. Solid State Chem.* In the press.
- BROOKER, M. H. & BATES, J. B. (1973). *Spectrochim. Acta Part A*, **29**, 439–452.
- BROOKER, M. H. & HUANG, C.-H. (1975). Paper presented at the 22nd Spectroscopy Society of Canada Symposium, Montreal, Canada.
- HARTWIG, C. M., ROUSSEAU, D. L. & PORTO, S. P. S. (1969). *Phys. Rev.* **188**, 1328–1335.
- HUANG, C.-H. & BROOKER, M. H. (1976). *Spectrochim. Acta Part A*, **32**, 1715–1724.
- LINDLEY, P. F. & WOODWARD, P. (1966). *J. Chem. Soc. A*, pp. 123–126.
- MEYER, P., RIMSKY, A. & CHEVALIER, R. (1978). *Acta Cryst.* **B34**, 1457–1462.
- NIGGLI, A. (1959). *Z. Kristallogr.* **111**, 269–282.
- POGAREV, D. E. & SHULTIN, A. A. (1973). *Kristallografiya*, **18**, 311–314.
- TROTTER, J. & GIBBONS, C. S. (1971). *J. Chem. Soc. A*, pp. 2058–2062.
- WEBER, H.-J. & HAUSSÜHL, S. (1977). *Z. Kristallogr.* **146**, 303–307.
- WILLIS, B. T. M. & PRYOR, A. W. (1975). *Thermal Vibrations in Crystallography*, pp. 142–174. Cambridge Univ. Press.
- ZACHARIASEN, W. (1928). *Untersuchung über die Kristallstrukturen von Sesquioxiden und Verbindungen ABO_3 . Partie 4.* Oslo: Skrifter.

* The use of the word perfect employed here does not appear to be the same as that used by MCR.

International Union of Crystallography

Acta Cryst. (1979). **B35**, 1539

Structure Reports

Volumes 43A and 42B of *Structure Reports* have recently been published. Volume 43A, covering the literature for metals and inorganic compounds for 1977 (vi + 393 pages), costs 97.75 Netherlands guilders for subscribers with standing orders. The full price for individual copies is 115 guilders but personal subscribers may buy a copy for their own use at 57.50 guilders.

Volume 42B, covering the literature for organic compounds for 1976, is bound in two parts (vi + 506 pages and iv + 625 pages) and costs 272 Netherlands guilders for subscribers with standing orders. The full price for individual copies is 320 guilders but personal subscribers may buy a copy for their own use at 160 guilders.

Orders for these publications may be placed direct with the publisher, Bohn, Scheltema & Holkema, PO Box 23, 7400 GA Deventer, The Netherlands, with Polycrystal Book Service, PO Box 11567, Pittsburgh, PA 15238, USA, or with any bookseller.