JOUBERT-BETTAN, C. A., LACHENAL, R., BERTAUT, E. F. & PARTHÉ, E. (1969). *J. Solid State Chem.* **1**, 1.
MARUMO, F. & NOWACKI, W. (1967). *Z. Kristallogr.* **124**, 1.
NITSCHE, R. & WILD, P. (1970). *Mat. Res. Bull.* **5**, 419.
PARTHÉ, E. (1967). In *Intermetallic Compounds*, Chapter 11. Edited by J. H. WESTBROOK. New York: John Wiley.
PARTHÉ, E. (1971). *Allg. prakt. Chem.* **22**, 317.
PARTHÉ, E. (1972). *Cristallochimie des Structures Tetraédriques*. Paris: Gordon & Breach.
PARTHÉ, E. & GARIN, J. (1971). *Mh. Chem.* **102**, 1197.
PARTHÉ, E., YVON, K. & DEITCH, R. (1969). *Acta Cryst.* B**25**, 1164.
WEST, A. R. & GLASSER, F. P. (1972). *J. Solid State Chem.* **4**, 20.

Acta Cryst. (1972) B**28**, 3674

A rapid method of assessing the number of molecules in the unit cell of an organic crystal.

By C. J. E. KEMPSTER and H. LIPSON, *Physics Department, University of Manchester Institute of Science and Technology, Manchester M60 1QD, England.*

(*Received* 12 *July* 1972)

A rough relationship is empirically derived between the volume of the unit cell of an organic crystal and the number of atoms it contains.

When the unit cell of a crystal has been derived, one needs to know the number of atoms that it contains before deciding whether the determination of its structure is practicable. The determination of the density can be time-consuming, and it is the purpose of the present note to point out that for organic crystals the result can be derived accurately enough from the volume of the unit cell alone.

Organic molecules normally crystallize in a space group which permits fairly close packing with a minimum of empty space between molecules (see, for example, Kitaigorodsky, 1957). This behaviour presumably arises from the non-directional nature of van der Waals forces, and is not seriously affected by a small proportion of hydrogen bonds between molecules or by a few 'foreign' atoms. Since carbon, oxygen and nitrogen atoms are about the same size, there should be a roughly linear relation between the volume and the number of atoms (excluding hydrogen). We have made the calculations for forty crystals, arbitrarily chosen, and the result is shown in Fig. 1. It will be seen that for most crystals $N \simeq V/18$. The individual points are shown in order to indicate the spread of the relationship.

The graph can be used to estimate the number of C, N and O atoms in a given unit cell to an accuracy of about 10%. This should be adequate for determining the number of molecules. We must emphasize that it should be used only for a first estimate; the final figure should always be checked by an accurate determination of the density.

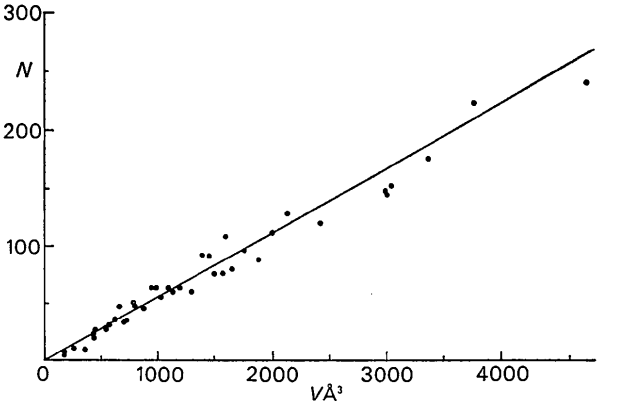

Fig. 1. Relation between the number of C, N, O atoms in the unit cell and the volume of the unit cell for 40 arbitrarily chosen crystals. A few crystals contain other atoms, which are also included.

References

KITAIGORODSKY, A. I. (1957). *Organic Chemical Crystallography*. New York: Consultants Bureau.

Acta Cryst. (1972). B**28**, 3674

Structural relationships in compounds with $R\bar{3}c$ symmetry: erratum.

By C. MICHEL, J. M. MOREAU and W. J. JAMES, *Department of Chemistry and Physics and the Graduate Center for Materials Research, University of Missouri-Rolla, Rolla, Missouri, U.S.A.*

(*Received* 7 *August* 1972)

The values of c/a and α_r for $LaAlO_3$ in Table 1 of Michel, Moreau & James [*Acta Cryst.* (1971), B**27**, 501] should be 2·443 and 60·10.

Dr Helen Megaw has pointed out to us an error in Table 1 of our paper (Michel, Moreau & James, 1971). The values of c/a and α_r for $LaAlO_3$ should read 2·443 and 60·10 rather than 2·462 and 59·90 respectively. The corrected values are taken from Geller & Bala (1956).

References

GELLER, S. & BALA, V. B. (1956). *Acta Cryst.* **9**, 1019.
MICHEL, C., MOREAU, J. M. & JAMES, W. J. (1971). *Acta Cryst.* B**27**, 501.