and/or an asymmetric peak, as is often encountered in a $\theta/\omega$ scan. Data collection by the ordinate analysis method is, however, normally carried out by means of an $\omega$ scan, which usually gives a symmetric peak profile, since experience indicates that intensities measured in this way are less sensitive to crystal motion.

**References**

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# On the method of assessing the number of atoms in the unit cell of an organic crystal.* By R. SRINIVASAN and S. S. RAJAN, *Centre of Advanced Study in Physics, University of Madras, Guindy Campus, Madras-600025, India*

It is shown that the rough method of arriving at the number of non-hydrogen atoms from the volume of the unit cell of an organic crystal [Kempster & Lipson (1972). *Acta Cryst.* B**28**, 3674] can be improved by including hydrogen atoms. The empirical relation $V = 8\cdot9N$, where $V$ = volume of the unit cell and $N$ = number of atoms including hydrogen, is arrived at by a least-squares fit of data from 114 compounds.

Kempster & Lipson (1972), hereinafter referred to as KL, obtained empirically a relationship between the volume ($V$) of the unit cell of an organic crystal and the number ($N$) of atoms it contains, and gave the relation $N \simeq V/18$. They, however, excluded hydrogen atoms. Although the above is a rough relation and gives the number of non-hydrogen atoms with reasonable accuracy we felt that the hydrogen atoms cannot be excluded. The van der Waals radius for hydrogen is about 1·2 Å whereas carbon, nitrogen and oxygen have a value around 1·6 Å. We therefore carried out the following calculations on a total of 114 organic compounds (aliphatic). In the first case the calculations of KL were repeated and a least-squares fit was obtained for the parameter $A'$ in the relation, $V = N_1 A'$ where $N_1$ now is the total number of atoms excluding hydrogen. In the second case the value of $A$ in the relation $V = NA$ was obtained by a least-squares calculation where $N$ denotes the total number of atoms including hydrogen. In the third case a two-parameter fit was attempted by least-squares calculation for the relation $V = B_1 N_1 + B_2 N_2$ where $B_1$ and $B_2$ are the parameters to be determined and $N_1$ and $N_2$ are the number of non-hydrogen atoms (C,N,O) and hydrogen atoms respectively. The values obtained are given in Table 1. For comparison the r.m.s. value of the fractional error $\langle[(V - V_c)/V]^2\rangle^{1/2}$ where $V_c$ is the calculated value of the volume using the appropriate parameters was also obtained for each of the cases and is given in Table 1.

It may be seen that the value of $A'$ (18·5) is close to that reported by KL. The use of a single parameter (including hydrogen atoms) may be seen to yield an appreciable improvement in the fit since the r.m.s. error is much lower (0·098) than for the earlier case (0·158). The two-parameter case seems to give a slightly better result with a standard error of 0·093 but the improvement is perhaps not as

pronounced as might be expected from the use of two parameters.

Fig. 1. gives $\langle(V - V_c)/V\rangle$ as a function of $\langle N_1/N_2\rangle$ where the average is over selected groups of compounds with approximately equal number in the different ranges of $N_1/N_2$. The agreement may be seen to be poor for the case
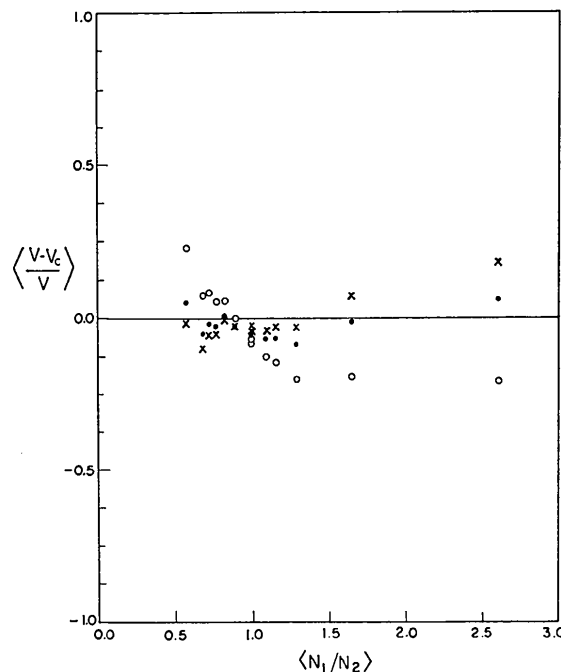


Fig. 1. Average fractional error in the calculated volume as a function of $\langle N_1/N_2\rangle$ for the cases with $A'$ (O), $A$ (×) and $B_1$ and $B_2$ (●).

with $A'$ whereas with $A$ and with $B_1$ and $B_2$ the agreement is reasonably good over a much larger range of $N_1/N_2$. The

Table 1. *Parameters obtained by least-squares fit*

Standard deviations are given in parentheses.

| Parameter | Value | $\langle[(V-V_c)/V]^2\rangle^{1/2}$ |
|---|---|---|
| $A'$ | 18·5* (0·256) | 0·158 |
| $A$ | 8·9 (0·086) | 0·098 |
| $B_1$ | 11·8 (0·161) | |
| $B_2$ | 6·3 (0·075) | 0·093 |

\* The value obtained by KL is 18·0.

use of a single parameter $A=8\cdot9$, which gives the total number of atoms inclusive of hydrogen, seems to be therefore preferable. As Kempster & Lipson emphasise this is only for a first estimate and the final figure should be checked by an accurate determination of the density.

**Reference**

KEMPSTER, C. J. E. & LIPSON, H. (1972). *Acta Cryst.* B28, 3674.

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# The crystal structure of the δ-form of 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (δ-HMX): erratum.

By R. E. COBBLEDICK and R. W. H. SMALL, *Chemistry Department, The University, Lancaster, England*

The observed and calculated densities in Table 1 of Cobbledick & Small [*Acta Cryst.* (1974). B30, 1918–1922] should read $D_{obs}=1\cdot76$, $D_{calc}=1\cdot760$ g cm$^{-3}$.

In the paper by Cobbledick & Small (1974) the observed and calculated densities given in Table 1 are erroneous. They should be $D_{obs}=1\cdot76$, $D_{calc}=1\cdot760$ g cm$^{-3}$.

**Reference**

COBBLEDICK, R. E. & SMALL, R. W. H. (1974). B30, 1918–1922.