SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1991). C**47**, 2514

Iminodiacetonitrile – space group correction.

By F. H. HERBSTEIN, *Department of Chemistry, Technion – Israel Institute of Technology, Haifa, Israel* 32000

(*Received* 20 *January* 1991; *accepted* 2 *May* 1991)

Abstract

The crystals of iminodiacetonitrile are not monoclinic, as reported by Kaida, Minemoto, Shimizu, Sonoda, Miki & Kasai [*Acta Cryst.* (1990), C**46**, 2269–2270] but orthorhombic. The revised crystal data are $a = 11{\cdot}836\ (3)$, $b = 5{\cdot}345\ (2)$, $c = 7{\cdot}821\ (2)$ Å, space group $Cmc2_1$ (No. 36), $Z = 4$, molecular symmetry C_s–m.

The crystal structure of iminodiacetonitrile was reported in space group $P2_1$, $Z = 2$ (Kaida, Minemoto, Shimizu, Sonoda, Miki & Kasai, 1990); approximate C_s symmetry of the molecule was noted. Application of *TRACER* (Lawton, 1969) to the monoclinic cell parameters showed that the true symmetry was *C*-centred orthorhombic (interaxial angles were equal to 90° well within experimental error). Transformation of atomic coordinates showed that the space group was $Cmc2_1$, the C_s symmetry of the molecule now being exact. The relation between monoclinic and orthorhombic cells is shown in Fig. 1. The *c*-glide plane of $Cmc2_1$ requires the systematic extinction of reflections $hk0$ with k odd in the monoclinic indexing; this is confirmed for 21 reflections of this type by reference to SUP 53031. The symmetry-averaged atomic coordinates in the orthorhombic cell in standard orientation are given in Table 1. Further refinement is not necessary as both revised and original cells are non-centrosymmetric (Schomaker & Marsh, 1979).

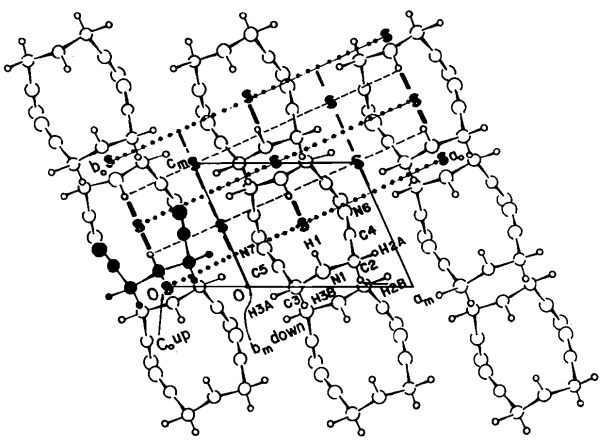

Fig. 1. Projection of molecular packing viewed along [001] in the orthorhombic cell (adapted from Fig. 2 of Kaida *et al.*). The monoclinic cell (with only some of the 2_1 axes inserted) is denoted by $\mathbf{a}_m$, $\mathbf{c}_m$. The orthorhombic cell, with symmetry elements of space group $Cmc2_1$ inserted, is denoted by $\mathbf{a}_o$, $\mathbf{b}_o$. The labels are for the atoms of Table 1 of Kaida *et al.*, while our reference molecule (coordinates in Table 1) is darkened.

Table 1. *Atomic coordinates (numbering of Kaida et al.) in the orthorhombic cell shown in Fig.* 1

Atoms N(1) and H(1) lie on the mirror plane at $x = 0$. The z_o coordinate of N(1) has been fixed at 0·75 (it seems that this coordinate was refined, unjustifiably, in the original study). Round brackets indicate e.s.d.'s taken from Kaida *et al.*, who report e.s.d.'s of 4–6 $\times 10^{-4}$ for C, N and 5–8 $\times 10^{-3}$ for H; square brackets show one half of the range of symmetry-related coordinates.

The transformation equations between the coordinates below and those given by Kaida *et al.* (x_K *etc.*) are: $x_o = \frac{1}{2}(x_K - \frac{1}{2})$; $y_o = z_K - \frac{1}{2}(x_K - \frac{1}{2})$; $z_o = 1 - y_K$.

	x_o	y_o	z_o
N(1)	0	0·1276 (4)	0·75 (–)
C(2)	0·1037 [0]	0·0952 [7]	0·6554 [3]
C(4)	0·1290 [0]	0·2937 [1]	0·5283 [3]
N(6)	0·1468 [5]	0·4533 [2]	0·4356 [2]
H(1)	0	0·266 (8)	0·799 (5)
H(2*A*)	0·181 [4]	0·096 [12]	0·735 [9]
H(3*A*)	0·100 [3]	–0·046 [0]	0·595 [1]

References

KAIDA, S., MINEMOTO, H., SHIMIZU, T., SONODA, N., MIKI, K. & KASAI, N. (1990). *Acta Cryst.* C**46**, 2269–2270.

LAWTON, S. L. (1969). *TRACER*. Northwestern University, Evanston, Illinois, USA.

SCHOMAKER, V. & MARSH, R. E. (1979). *Acta Cryst.* B**35**, 1933–1934.

0108-2701/91/112514-01$03.00