SHORT COMMUNICATIONS

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N-Methylacetamide hemihydrochloride: corrigendum.*

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Abstract

The crystal structure of $C_3H_7NO.\frac{1}{2}HCl$ should be described in the orthorhombic space group *Fdd*2 rather than the monoclinic *C*2 reported by Jaber, Guilhem & Loiseleur [*Acta Cryst.* (1983), C**39**, 485–487].

The crystal structure derived for *N*-methylacetamide hemihydrochloride was based on the monoclinic space group *C*2 with $a = 8.454$ (4), $b = 10.597$ (5), $c = 11.754$ (5) Å, $\beta = 111.09$ (8)°, $Z = 8$ (Jaber, Guilhem & Loiseleur, 1983; JGL). The vectors $|102|$, $|100|$, $|010|$ define an effectively orthorhombic unit cell with $a' = 21.933$, $b'\ (= a) = 8.454$, $c'\ (= b) = 10.597$ Å, $\alpha' = \beta' = 90$, $\gamma' = 90.01°$, $Z = 16$. The corresponding transformations $x' = \frac{1}{2}z$, $y' = x - \frac{1}{2}z$, $z' = y$ lead to atomic coordinates that are consistent with space group *Fdd*2 within their reported uncertainties. The *Fdd*2 coordinates are given in Table 1.

Since the increase in symmetry from *C*2 to *Fdd*2 does not involve the addition of a center of symmetry, the coordinate shifts necessary to achieve the higher symmetry are no larger

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than the formal e.s.d.'s (Schomaker & Marsh, 1979) and the molecular dimensions as found in *C*2 (JGL) remain essentially unchanged; all molecular units become equivalent by symmetry.

Table 1. *Atom coordinates* ($\times 10^4$) (*space group Fdd*2)

The *C*2 coordinates (JGL, Table 1) have been averaged according to the symmetry of *Fdd*2; numbers in square brackets are shifts necessary to achieve this symmetry, and numbers in parentheses are averaged e.s.d.'s in the original values.

	x'	y'	z'
Cl (1,2)	0	0	5012 |0| (1)
C(1,4)	788 |2| (1)	3730 |4| (3)	3143 |3| (3)
N(1,2)	988 |0| (1)	2342 |0| (2)	3836 |2| (2)
C(2,5)	1560 |1| (1)	1995 |4| (2)	4029 |0| (2)
O(1,2)	1970 |1| (1)	2916 |3| (2)	3614 |2| (2)
C(3,6)	1714 |0| (1)	533 |1| (3)	4745 |0| (2)

References

JABER, M., GUILHEM, J. & LOISELEUR, H. (1983). *Acta Cryst.* C**39**, 485–487.
SCHOMAKER, V. & MARSH, R. E. (1979). *Acta Cryst.* B**35**, 1933–1934.

Half-normal probability plot of 3,3'-dithiodipropionic acid.

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Abstract

A half-normal probability plot comparing the reported structural parameters of 3,3'-dithiodipropionic acid, $(SCH_2CH_2COOH)_2$, published by two different authors is presented.

Results of the crystal structure analysis of the title compound published by two different authors (Prout, 1982; Appa Rao, Seshasayee, Aravamudan, Nageswara Rao & Venkatasubramanian, 1982) have been compared by a half-normal probability plot (Abrahams & Keve, 1971) (Fig. 1):