SHORT COMMUNICATIONS

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. (1983). C**39**, 1473

N-Methylacetamide hemihydrochloride: corrigendum.*

By RICHARD E. MARSH, *Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California* 91125, *USA*

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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 $a = 8{\cdot}454$ (4), $b = 10{\cdot}597$ (5), $c = 11{\cdot}754$ (5) Å, $\beta = 111{\cdot}09$ (8)°, $Z = 8$ (Jaber, Guilhem & Loiseleur, 1983; JGL). The vectors |102|, |100|, |010| define an effectively orthorhombic unit cell with $a' = 21{\cdot}933$, b' $(= a) = 8{\cdot}454$, c' $(= b) = 10{\cdot}597$ Å, $\alpha' = \beta' = 90$, $\gamma' = 90{\cdot}01°$, $Z = 16$. 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 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)

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JABER, M., GUILHEM, J. & LOISELEUR, H. (1983). *Acta Cryst.* C**39**, 485–487.

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

By M. SESHASAYEE, *Department of Physics, Indian Institute of Technology, Madras* 600 036, *India*

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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):

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$\delta p_i = |\,|p(1)_i| - |p(2)_i|\,| / |\sigma^2 p(1)_i + \sigma^2 p(2)_i|^{\frac{1}{2}}$, where $p(1)_i$ and $p(2)_i$ are the two sets of parameters refined in the structure analysis and the σ's are the corresponding standard deviations.

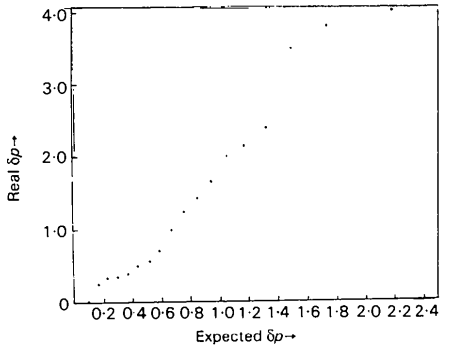

Fig. 1. Half-normal probability plot with real δp and expected δp as ordinate and abscissa.

A least-squares straight-line fit of the plot ignoring two points (16th and 17th in the figure) gave a slope of 1·83 (4) and an intercept of −0·16 (3). The non-zero intercept indicates systematic errors in the data. The slope of the straight line deviates from the ideal value of 1 by 0·85 indicating that either the $\Delta p_i = p(1)_i - p(2)_i$ are large or the corresponding standard deviations $\sigma(p_i)$ are small. The near linearity of the plot excludes the first possibility since for Δp_i to be large $p(1)_i$ and $p(2)_i$ must differ from the true value in opposite directions. The second possibility is more likely, which could arise if both sets of data are refined by least squares to a greater degree than warranted by the accuracy of the data.

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International Union of Crystallography

Chemical nomenclature

The attention of authors is drawn to the following recommendations of the IUPAC Commission on Nomenclature of Organic Chemistry: *The Designation of Non-Standard Classical Valence Bonding in Organic Nomenclature* [*Pure Appl. Chem.* (1982), **54**, 217–227], *Revision of the Extended Hantzsch–Widman System of Nomenclature for Heteromonocycles* [*Pure Appl. Chem.* (1983), **55**, 409–416]; and to the following recent recommendations of the IUPAC–IUB Joint Commission on Biochemical Nomenclature: *Symbols for Specifying the Conformation of Polysaccharide Chains* [*Eur. J. Biochem.* (1983), **131**, 5–7], *Abbreviations and Symbols for the Description of Conformations of Polynucleotide Chains* [*Eur. J. Biochem.* (1983), **131**, 9–15].

Authors are reminded that, wherever possible, chemical nomenclature in the Union's journals should conform to IUPAC rules. Basic rules for the nomenclature of inorganic chemistry are given in *Nomenclature of Inorganic Chemistry* (1970) ('The Red Book'), London: Butterworths and, for organic chemistry, in the two volumes *Nomenclature of Organic Chemistry, Sections A,B,C,D,E,F, & H* (1979) ('The Blue Book'), Oxford: Pergamon Press and *Biochemical Nomenclature and Related Documents* (1978), London: Biochemical Society. For additional details on nomenclature requirements see p. 179 of *Notes for Authors* [*Acta Cryst.* (1983), A**39**, 174–186].

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