

had also been done by Sato & Nakada (1989) using single-crystal X-ray diffraction, and by Hunter *et al.* (1990) using powder neutron diffraction. We found that our refined atomic coordinates agreed within e.s.d.'s with those by Sato & Nakada (1989) although our refined temperature factors were somewhat smaller.

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Structure of 3-amino-4H-1,2,4-benzothiadiazine 1,1-dioxide (1). Corrigendum. By G. BOMBIERI and F. DEMARTIN, *Istituto Chimico Farmaceutico, Università di Milano, Viale Abruzzi 42, 20131 Milano, Italy* and D. BRAGHIROLI, S. TODESCHI and M. DI BELLA, *Dipartimento di Scienze Farmaceutiche, Università di Modena, Via S. Eufemia 19, 41100 Modena, Italy*

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Abstract

The crystal structure of (1) was described as monoclinic, space group *Cc* with $a = 14.259$ (2), $b = 22.539$ (3), $c = 8.741$ (3) Å, $\beta = 114.10$ (2)°, $Z = 12$. [Bombieri, Demartin, Braghiroli, Todeschi & Di Bella (1989). *Acta Cryst.* **C45**, 1905–1908]. The application of the *MISSYM* program [Le Page (1987). *J. Appl. Cryst.* **20**, 264–269] has shown that it should rather have been described as rhombohedral, space group *R3c* with $a = 22.539$ (3), $c = 8.741$ (3) Å, $Z = 18$. The refinement carried out in the correct space group

converged to $R = 0.025$ and $wR = 0.030$ [686 independent reflections with $I > 2\sigma(I)$], without significant differences in the molecular parameters.

The vectors defining the new cell edges are [0.0, 1.0, 0.0], [1.5, -0.5, 1.0] and [0.0, 0.0, -1.0]. The asymmetric unit in the space group *R3c* is a single molecule with the refined coordinates reported in Table 1.*

The molecular parameters in the revised structure are not significantly different from those reported for the structure refined in the space group *Cc*; all the bond lengths and angles agree within three e.s.d.'s with the averaged values given in the previous determination (Bombieri *et al.*, 1989).

Table 1. Table of positional parameters with e.s.d.'s in parentheses

	<i>x</i>	<i>y</i>	<i>z</i>	$B(\text{Å}^2)$
S	0.26563 (3)	0.05361 (2)	0.412	3.06 (1)
O(1)	0.31674 (9)	0.09133 (8)	0.2963 (2)	4.36 (4)
O(2)	0.25317 (9)	0.09749 (8)	0.5107 (2)	4.48 (4)
N(2)	0.2886 (1)	0.00952 (9)	0.5076 (3)	3.98 (5)
N(3)	0.2791 (1)	-0.08904 (9)	0.5982 (3)	4.05 (5)
N(4)	0.19365 (8)	-0.09722 (8)	0.4429 (2)	3.05 (4)
C(3)	0.2536 (1)	-0.05799 (9)	0.5148 (3)	2.79 (4)
C(5)	0.0971 (1)	-0.1185 (1)	0.2855 (3)	3.75 (6)
C(6)	0.0646 (1)	-0.0942 (1)	0.1938 (4)	4.81 (7)
C(7)	0.0940 (2)	-0.0252 (1)	0.1619 (4)	5.88 (8)
C(8)	0.1566 (1)	0.0205 (1)	0.2266 (4)	5.31 (7)
C(9)	0.1605 (1)	-0.07321 (9)	0.3507 (2)	2.81 (4)
C(10)	0.1888 (1)	-0.0033 (1)	0.3220 (3)	3.28 (5)

Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as: $(4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

* Lists of crystallographic data, selected bond lengths and angles, H-atom coordinates, anisotropic temperature factors and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53000 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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