Acta Cryst. (1984). C**40**, 902

Structure of 2-amino-3,5-dibromo-*N*-cyclohexyl-*N*-methylbenzenemethanamine–salicylic acid (1:1) (ABCMBMA–SALA), $C_{14}H_{20}Br_2N_2.C_7H_6O_3$: errata.

By NOBUYUKI SHIMIZU and SADAO NISHIGAKI, *Pharmaceutical Institute, School of Medicine, Keio University, Shinjuku-ku, Tokyo* 160, *Japan*, YOSHINOBU NAKAI, *Faculty of Pharmaceutical Sciences, Chiba University, Chiba* 260, *Japan* and KENJI OSAKI, *Faculty of Pharmaceutical Sciences, Kyoto University, Kyoto* 606, *Japan*

(*Received* 18 *October* 1983; *accepted* 16 *January* 1984)

Abstract

The space group of the title compound [Shimizu, Nishigaki, Nakai & Osaki (1983). *Acta Cryst.* C**39**, 891–893] is not $P\bar{1}$ but $C2/c$ with *a*, *b*, *c* taken along $[0\bar{1}1]$, $[011]$, $[\bar{1}0\bar{2}]$, giving cell edges $a = 15{\cdot}466\ (45)$, $b = 11{\cdot}799\ (13)$, $c = 24{\cdot}335\ (27)$ Å, $\beta = 99{\cdot}33\ (18)°$, $Z = 8$. The final discrepancy index for the correct space group is 5·8% for 2274 symmetry-independent reflections.

Final atomic parameters are listed in Table 1 and bonding geometry is shown in Table 2,* the latter being within 1σ of the average of the corresponding two sets of values reported previously.

The atomic coordinates (x,y,z) and the Miller indices (h,k,l) of the $C2/c$ structure are given by the following equations.

(i) *Atomic coordinates*

$$x = -x' + (-y' + z')/2 + 1,$$
$$y = -x' + (y' + z')/2,$$
$$z = -x' + 1,$$

where x', y', z' are the coordinates of the *A* and *C* molecules reported previously.

(ii) *Index transformation*

$$h = l' - k', \qquad k = l' + k', \qquad l = -h' - 2l',$$

where h', k', l' relate to the previous $P\bar{1}$ structure.

There are essentially no changes involving the intermolecular H-bond contacts.

Table 1. *Positional parameters and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

	x	*y*	*z*	B_{eq}(Å²)*
ABCMBMA				
Br(1)	0·93879 (6)	0·51399 (7)	0·56482 (3)	6·19
Br(2)	0·95684 (6)	0·06942 (6)	0·64870 (4)	6·47
C(1)	0·8922 (4)	0·3766 (5)	0·7139 (2)	3·32
C(2)	0·9004 (4)	0·4558 (5)	0·6724 (2)	3·58
C(3)	0·9239 (4)	0·4134 (5)	0·6232 (2)	3·90
C(4)	0·9398 (4)	0·3003 (6)	0·6144 (3)	4·47
C(5)	0·9325 (4)	0·2265 (5)	0·6575 (3)	4·22
C(6)	0·9091 (4)	0·2623 (5)	0·7065 (3)	3·83
N(1)	0·8836 (4)	0·5690 (4)	0·6780 (2)	4·71
C(7)	0·8700 (4)	0·4100 (5)	0·7693 (2)	3·78
N(2)	0·7775 (3)	0·3766 (4)	0·7748 (2)	3·45
C(8)	0·7123 (4)	0·4587 (5)	0·7458 (3)	4·27
C(9)	0·7635 (4)	0·3543 (5)	0·8343 (2)	3·85
C(10)	0·7925 (4)	0·4541 (6)	0·8724 (3)	4·68
C(11)	0·7765 (5)	0·4272 (8)	0·9313 (3)	6·37
C(12)	0·8246 (6)	0·3197 (8)	0·9531 (3)	6·54
C(13)	0·7943 (5)	0·2215 (7)	0·9145 (3)	6·48
C(14)	0·8083 (5)	0·2450 (5)	0·8545 (3)	4·58
SALA				
C(15)	0·6153 (4)	0·2706 (5)	0·6315 (3)	4·02
C(16)	0·5279 (5)	0·3022 (5)	0·6117 (3)	4·82
C(17)	0·5062 (6)	0·3469 (7)	0·5589 (4)	6·72
C(18)	0·5703 (9)	0·3621 (7)	0·5263 (3)	7·94
C(19)	0·6574 (8)	0·3331 (8)	0·5450 (4)	8·47
C(20)	0·6794 (5)	0·2867 (6)	0·5978 (3)	6·23
C(21)	0·6391 (5)	0·2233 (5)	0·6886 (3)	3·94
O(1)	0·7175 (3)	0·2040 (3)	0·7069 (2)	4·78
O(2)	0·5778 (3)	0·2059 (4)	0·7154 (2)	6·18
O(3)	0·4653 (3)	0·2897 (4)	0·6442 (2)	6·02

* B_{eq} defined according to Hamilton (1959).

We would like to thank Dr Y. Le Page of the National Research Council, Ottawa, for pointing out this error. The atomic coordinates in Table 1, after suitable transformation, agree within 3×10^{-4} with those given by Marsh (1984), whose results were made known to us by Professor D. H. Templeton.

* Lists of structure factors, H-atom parameters, anisotropic thermal parameters and bonding geometry (Table 2) have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39136 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/84/050902-01$01.50

References

HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.
MARSH, R. E. (1984). *Acta Cryst.* C**40**, 901.
SHIMIZU, N., NISHIGAKI, S., NAKAI, Y. & OSAKI, K. (1983). *Acta Cryst.* C**39**, 891–893.