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SHORT COMMUNICATIONS

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Structure of 2-amino-3,5-dibromo-N-cyclohexyl-N-methylbenzenemethanamine–salicylic acid (1:1): 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 $C_{14}H_{20}Br_2N_2 \cdot C_7H_6O_3$ should be described in the monoclinic space group $C2/c$ rather than the triclinic $P\bar{1}$ reported by Shimizu, Nishigaki, Nakai & Osaki [*Acta Cryst.* (1983), **C39**, 891–893].

The crystal structure of this compound was described as triclinic, space group $P\bar{1}$, with $a = 29.146$ (34), $b = 9.710$ (3), $c = 9.719$ (9) Å, $\alpha = 105.18$ (5), $\beta = 124.18$ (6), $\gamma = 85.99$ (6)°, $Z = 4$ (Shimizu, Nishigaki, Nakai & Osaki, 1983). The vectors $[01\bar{1}]$, $[011]$, $[102]$ define a C -centered cell with $a' = 15.433$, $b' = 11.803$, $c' = 24.306$, $\alpha' = 89.97$, $\beta' = 99.11$, $\gamma' = 90.06$ °, $Z = 8$.† The corresponding transformations $x' = x + \frac{1}{2}(y - z)$, $y' = -x + \frac{1}{2}(y + z)$, $z' = x$ lead to atomic coordinates that are consistent with the symmetry of the monoclinic space group $C2/c$ within the reported uncertainties. (No translation of origin is necessary since, by even chance, the center of symmetry chosen as origin in the triclinic description corresponds to a conventional origin in $C2/c$.) The $C2/c$ parameters are given in Table 1.

The c -glide plane of $C2/c$ requires the systematic extinction of reflections hkk with h odd in the triclinic indexing.

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† The relative e.s.d.'s in the triclinic cell translations are highly disparate, and since covariances are not given it is impossible even to estimate appropriate e.s.d.'s for the monoclinic cell dimensions.

Table 1. Coordinates ($\times 10^4$) for space group $C2/c$

The $P\bar{1}$ coordinates (Shimizu *et al.*, 1983) have been averaged according to the symmetry of $C2/c$; numbers in square brackets are shifts necessary to achieve this symmetry.

	x'	y'	z'
Br(1)	612 [1]	5140 [0]	4352 [0]
Br(2)	432 [0]	695 [1]	3513 [1]
C(1)	1077 [2]	3766 [12]	2860 [0]
C(2)	996 [8]	4556 [6]	3276 [2]
C(3)	760 [10]	4137 [3]	3768 [2]
C(4)	604 [2]	3002 [2]	3856 [4]
C(5)	673 [6]	2265 [9]	3425 [8]
C(6)	908 [4]	2623 [3]	2935 [4]
N(1)	1164 [1]	5692 [3]	3220 [2]
C(7)	1299 [4]	4099 [2]	2306 [0]
N(2)	2225 [1]	3768 [1]	2252 [0]
C(8)	2878 [4]	4586 [1]	2543 [2]
C(9)	2363 [6]	3544 [4]	1658 [4]
C(10)	2074 [4]	4540 [0]	1276 [2]
C(11)	2233 [2]	4270 [0]	686 [0]
C(12)	1755 [2]	3196 [6]	469 [2]
C(13)	2055 [2]	2215 [2]	856 [6]
C(14)	1917 [2]	2448 [2]	1454 [0]
C(15)	3847 [1]	2707 [5]	3684 [2]
C(16)	4724 [2]	3022 [4]	3882 [2]
C(17)	4938 [10]	3469 [3]	4411 [1]
C(18)	4294 [5]	3621 [5]	4736 [2]
C(19)	3423 [4]	3333 [5]	4549 [0]
C(20)	3207 [2]	2865 [5]	4021 [0]
C(21)	3609 [1]	2233 [3]	3114 [2]
O(1)	2826 [2]	2039 [4]	2930 [2]
O(2)	4222 [0]	2059 [3]	2846 [2]
O(3)	5348 [2]	2897 [1]	3558 [0]

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