SHORT COMMUNICATIONS

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Acta Cryst. (1989). C**45**, 347

Structure of ammonium oxalohydroxamate: corrigendum.

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

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Abstract

The structure of this compound, $NH_4^+.C_2H_3N_2O_4^-$, was described [Sameena Begum, Jain, Ramakumar & Khetrapal (1988). *Acta Cryst.* C**44**, 1047–1049] as triclinic, space group $P\bar{1}$, with $a = 3{\cdot}952$ (1), $b = 6{\cdot}772$ (1), $c = 9{\cdot}993$ (1) Å, $\alpha = 98{\cdot}06$ (1), $\beta = 89{\cdot}96$ (1), $\gamma = 106{\cdot}96$ (1)°, $Z = 2$. It should be described as monoclinic, space group $C2/c$, with $a' = 12{\cdot}955$ (2), $b' = 3{\cdot}952$ (1), $c' = 9{\cdot}993$ (1) Å, $\beta' = 98{\cdot}42$ (2)°, $Z = 4$. The $C2/c$ coordinates are given. All anions are structurally equivalent and lie on centers of inversion; the ammonium cation lies on a twofold axis.

The vectors describing the new cell are [120], [$\bar{1}$00] and [001]. The corresponding coordinate transformations are: $x' = y/2 + 0{\cdot}25$, $y' = -x + y/2 + 0{\cdot}25$, $z' = z$; the translations are needed to place the origin at a conventional center of symmetry in $C2/c$. After averaging the transformed coordinates over corresponding atoms in the two (independent) molecules in $P\bar{1}$, the coordinates in Table 1 result. For the averaging, no atom needed to be shifted as much as its reported e.s.d.

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

The e.s.d.'s, in parentheses, are estimated from the values in Table 2 of Sameena Begum *et al.* (1988).

		x	y	z
O(1)	8(*f*)	4287 (2)	6932 (6)	−435 (2)
C	8(*f*)	2981 (2)	3538 (7)	260 (3)
N	8(*f*)	3400 (2)	4963 (6)	−715 (3)
O(2)	8(*f*)	3324 (2)	3776 (6)	1490 (2)
N*W*	4(*e*)	0	3877 (8)	2500

The anions lie on equivalent centers of symmetry and the ammonium ion lies on a twofold axis. Otherwise, the structure is effectively unchanged from that described by Sameena Begum *et al.* (1988).

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Reference

SAMEENA BEGUM, A., JAIN, V. K., RAMAKUMAR, S. & KHETRAPAL, C. L. (1988). *Acta Cryst.* C**44**, 1047–1049.

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Structure of high-T_c superconducting tetragonal $Ba_2YCu_{2.856}Al_{0.04}O_{6.76}$ at 298 and 120 K.

By S. SATO, *The Institute for Solid State Physics, The University of Tokyo, Roppongi* 7-22-1, *Minato-ku, Tokyo* 106, *Japan*, I. NAKADA, *Institute of Research and Development, Tokai University, Tomigaya* 2-28-4, *Shibuya-ku, Tokyo* 151, *Japan*, T. KOHARA, *Basic Research Laboratory, Himeji Institute of Technology, Shosha* 2167, *Himeji, Hyogo* 671-22, *Japan*, Y. ODA, *Faculty of Engineering Science, Osaka University, Machikaneyama-machi, Toyonaka, Osaka* 560, *Japan* and H. DAIDOJI, *Rigaku Industrial Co. Ltd, Matsubara-cho* 3-9-12, *Akishima, Tokyo* 196, *Japan*

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Abstract

It was found by chemical analysis that a slight amount of aluminium existed as an impurity in the crystals of the Y–Ba–Cu–O system whose structure was determined by Sato, Nakada, Kohara & Oda [*Acta Cryst.* (1988), C**44**, 11–14]. Occupancies of atoms in 1(*a*) [the Cu(1) site] were 0·856 (5) Cu, 0·04 Al and 0·104 vacancy.

We have prepared superconducting tetragonal crystals of the Y–Ba–Cu–O system, and determined their structure (Sato,

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