SHORT COMMUNICATIONS

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

Structure of ammonium oxalohydroxamate: corrigendum.

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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).

* Contribution No. 7827 from the Noyes Laboratory of Chemical Physics.

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.

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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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Table 1. *Revised parameters*

	Occupancy	x	y	z	U_{eq}(Å^2)
Cu(1)	0·856 (5)	0	0	0	
Al	0·04	0	0	0	0·025 (298 K)
					0·012 (120 K)

Nakada, Kohara & Oda, 1988). Recently it was reported that crystals were contaminated by aluminium when they were prepared in an alumina crucible (Siegrist, Schneemeyer, Waszczak, Singh, Opila, Batlogg, Rupp & Murphy, 1987; Haneda, Isobe, Hishita, Ishizawa, Shirasaki, Yamamoto & Yanagitani, 1987). Our crystals were also grown in an alumina crucible near the melting temperature; the material slightly wetted the crucible due to partial melting. Therefore, we exmained the crystals for the presence of aluminium by means of atomic absorption spectrometry. The analysis showed a small amount of aluminium and a trace of magnesium: the aluminium and magnesium contents were 1·75 and 0·091 mg g^{-1}, respectively. A specimen prepared at a slightly lower temperature indicated no melting. The impurity level lowered to 17·7 μg g^{-1} of aluminium and 4·7 μg g^{-1} of magnesium. The Al atom was assumed to occupy the Cu(1) site statistically, because the atomic deficiency of cations was observed only at this site (the magnesium was ignored). From the result of the chemical analysis, the occupancy of the Al atom was estimated as 0·04.

Structure refinements with the inclusion of the Al atom at both temperatures converged to the same R values as the previous work (Sato *et al.*, 1988) and showed no changes in the parameters except the occupancy of the Cu(1) atom as listed in Table 1. The value of D_x changed to 6·20 g cm^{-3}.

References

HANEDA, H., ISOBE, M., HISHITA, S., ISHIZAWA, Y., SHIRASAKI, S., YAMAMOTO, T. & YANAGITANI, T. (1987). *Appl. Phys. Lett.* **51**, 1848–1850.

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SIEGRIST, T., SCHNEEMEYER, L. F., WASZCZAK, J. V., SINGH, N. P., OPILA, R. L., BATLOGG, B., RUPP, L. W. & MURPHY, D. W. (1987). *Phys. Rev. B*, **36**, 8365–8368.

International Union of Crystallography

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Nominations for the Ewald Prize

The International Union of Crystallography is pleased to invite nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Professor Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography. Professor Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first Editor of the Union's publication *Acta Crystallographica* from 1948 to 1959 and the President of the Union from 1960 to 1963.

The Prize consists of a medal, a certificate and a financial award. It is presented once every three years during the triennial International Congresses of Crystallography. The first Prize was presented at the XIV Congress at Perth, Australia, in 1987. The second Prize, for which nominations are now being invited, will be presented at the XV Congress in Bordeaux, France, in July 1990.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible for the Ewald Prize, irrespective of nationality, age or experience. The only exceptions are the current members of the Prize Selection Committee and the President of the Union, none of whom are eligible. No restrictions are placed on the time or the means of publication of the nominee's contributions. The Prize may be shared by more than one contributor to the same scientific achievement.

Nominations for the Ewald Prize should be submitted in writing, preferably using the Ewald Prize Nomination Form and accompanied by supporting documentation, to The Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England, from whom copies of the Nomination Form, the names of the Selection Committee and advice on the submission of nominations may be obtained. **The closing date for nominations is 31 August 1989.**

M. Nardelli, President — A. I. Hordvik, General Secretary

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