

Table 1. Revised parameters

	Occupancy	x	y	z	$U_{eq}(\text{\AA}^2)$
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 examined 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<sup>-1</sup>, respectively. A specimen prepared at a slightly lower temperature indicated no melting. The impurity level lowered to 17.7 µg g<sup>-1</sup> of aluminium and

4.7 µg g<sup>-1</sup> 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<sup>-3</sup>.

#### References

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## International Union of Crystallography

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M. Nardelli  
President

A. I. Hordvik  
General Secretary

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