

## ERRATA

Volume **107**, Number 1 (1993), in the article, "Synthesis and Characterization of  $\text{Cu}_3\text{NbSe}_4$  and  $\text{KCu}_2\text{TaSe}_4$ ," by Ying-Jie Lu and James A. Ibers, pages 58–62: We reported the structure of  $\text{KCu}_2\text{TaSe}_4$  in space group  $C_s^4-Cc$  of the monoclinic system in a cell of dimensions  $a = 5.660(1)$ ,  $b = 18.829(4)$ ,  $c = 7.662(2)$  Å,  $\beta = 90.04(3)^\circ$ . This assignment to the monoclinic system was based on two observations: (1) Weissenberg photographs taken at room temperature displayed monoclinic symmetry, and (2) rapid scans of the data crystal at  $-167^\circ\text{C}$  on a diffractometer showed apparent monoclinic and not orthorhombic symmetry for a dozen or so low-angle  $\{hkl\}$ . The data crystal had been cut from the larger crystal used for the photography. Data collection, structure solution, and refinement were detailed. As we noted, the resultant structure of  $\text{KCu}_2\text{TaSe}_4$  is closely related to that of  $\text{KCu}_2\text{NbSe}_4$  (Y.-J. Liu and J. A. Ibers, *J. Solid State Chem.* **94**, 381, 1991). Indeed it is! Reexamination of the data indicates that the compounds are isostructural.  $\text{KCu}_2\text{TaSe}_4$  crystallizes in space group  $C_{2v}^{16}-C2cm$  of the orthorhombic system in a cell of dimensions  $a = 5.660(1)$ ,  $b = 18.829(4)$ ,  $c = 7.662(2)$  Å,  $\beta = 90^\circ$ . The absorption-corrected data average nearly as well in the orthorhombic system ( $R_{\text{int}} = 0.101$  for 7017 observations averaged to 1890 unique reflections) as they do in the monoclinic system ( $R_{\text{int}} = 0.098$  for 7017 observations averaged to 3554 unique reflections). Refinement of the structure in space group  $C_{2v}^{16}-C2cm$  of the orthorhombic system leads to values of  $R(F)$  of 0.025 and  $R_w(F^2)$  of 0.066, significantly lower than the values of 0.030 and 0.084 found for refinement in space group  $C_s^4-Cc$  of the monoclinic system. This improvement in agreement indices arises from better data (owing to additional averaging) rather than to a better model, as the resultant parameters (Table 1) lead to no significant changes in the structural details.

We have no explanation for the apparent monoclinic symmetry of the photographs taken at room temperature. Possibilities are that the photographs are deceiving owing to misalignment of the crystal or absorption effects, or that there is a second-order phase change between  $-167^\circ\text{C}$  and room temperature.

We are indebted to Dr. Richard E. Marsh for suggesting that we reexamine the assignment of the space group.

TABLE 1  
Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic  
Displacement Parameters ( $\text{Å}^2 \times 10^3$ ) for  $\text{KCu}_2\text{TaSe}_4$

Atom	x	y	z	U(eq)
Ta	-5006(1)	-1105(1)	$-\frac{1}{4}$	6(1)
Cu(1)	-5208(2)	0	0	10(1)
Cu(2)	-11(3)	-1081(1)	$-\frac{1}{4}$	10(1)
Se(1)	-2536(1)	-37(1)	$-\frac{1}{4}$	7(1)
Se(2)	-2527(2)	-2133(1)	$-\frac{1}{4}$	15(1)
Se(3)	-7467(1)	-1095(1)	$\frac{7}{2}(1)$	10(1)
K	-7574(4)	-3175(1)	$-\frac{1}{4}$	21(1)

Volume **109**, Number 1 (1994), in the article "Synthesis of Cuprates of Perovskite Structure in the Ba-Pb-Cu-O, Ba-Bi-Cu-O, and Ba-Pb-Tl-Cu-O Systems: Possible High  $T_c$  Superconductivity in a Perovskite-like Phase in the Ba-Pb-Tl-Cu-O System," by V. Manivannan, J. Gopalakrishnan, and C. N. R. Rao, pages 205-209: On page 205, right column, the sentence starting on line 12 should read as follows: "We believe that the formation of perovskite-like phases in the Ba-Pb-Cu-O, Ba-Bi-Cu-O, and Ba-Pb-Tl-Cu-O systems incorporating copper along with lead/bismuth/thallium at the *B*-site is of considerable interest." On page 208, left column, the sentence starting on line 12 should read as follows: "While we could not prepare a perovskite-like phase in the Ba-Tl-Cu-O system by this procedure, we did obtain a perovskite-like phase of nominal composition  $\text{BaPb}_{0.25}\text{Tl}_{0.25}\text{Cu}_{0.5}\text{O}_{3-y}$ ."