# SHORT COMMUNICATIONS

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## Electron-density distribution in crystals of $KCuF_3$ with Jahn–Teller distortion: errata.

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**Abstract**

The previously published results [Tanaka, Konishi & Marumo (1979). *Acta Cryst.* B**35**, 1303–1308] for the electron-density distribution in $KCuF_3$ crystals contain errors. The coefficient $\cos(\varphi/2)$ of the wave function of $3d_y$ orbitals should be 0·908 (19), which is in precise agreement with the theoretically estimated value. The $K^+$ ions at positions $(\frac{1}{2},\frac{1}{2},\frac{1}{4})$ and $(\frac{1}{2},\frac{1}{2},\frac{3}{4})$ were omitted from Fig. 1. Amendments to Table 3 are given. $R_1$, $R_2$ values for refinements (*c*) and (*d*) should be 0·0129, 0·0130 and 0·0127, 0·0128 respectively.

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The following corrections should be made in the paper by Tanaka, Konishi & Marumo (1979). In Fig. 1 on p. 1303, two $K^+$ ions at the positions $(\frac{1}{2},\frac{1}{2},\frac{1}{4})$ and $(\frac{1}{2},\frac{1}{2},\frac{3}{4})$ were omitted. The values in columns (*c*) and (*d*) in Table 3 should be replaced by those in Table 3 (amendments). $R_1$ and $R_2$ values of refinement (*c*) on p. 1305 should be 0·0129 and 0·0130, respectively, and those of refinement (*d*) on p. 1306 should be 0·0127 and 0·0128, respectively.

Unfortunately, an error in the computer program resulted in the omission of the term $\sin(\varphi)f_{z^2,x^2-y^2}$ of the $\Psi_e$ orbital. The value 0·964 (18) for $\cos(\varphi/2)$ in refinement (*c*) should be replaced by 0·908 (19), obtained with the corrected program. The new value is in precise agreement with the theoretically estimated value of 0·908 by Kadota, Yamada, Yoneyama & Hirakawa (1967). Since the dropped term has little effect on the structure factors compared to the other terms in $\Psi_g$ and $\Psi_e$, the difference Fourier maps calculated with the new parameter sets have essentially the same features as those in Figs. 4 and 5 on pp. 1306 and 1307, respectively, and only slight peak-height changes are observed. The corrected deformation density map of Fig. 4 will be presented later (Tanaka & Marumo, 1980).

*Note added in proof:* The third term of $f_{3d}$ on p. 1305 should be $B(\sin^2\beta\cos 2\gamma)\langle j_2\rangle$, with $B = -15/14$ and $15/14$ for $d_{xz}$ and $d_{yz}$ orbitals respectively in Table 4. None of the results are, however, affected by this correction, since the effects of these terms are cancelled out in the calculation of the scattering factor of the $Cu^{2+}$ ion. We are grateful to Professor B. Rees for drawing our attention to this error.

### References

KADOTA, S., YAMADA, I., YONEYAMA, S. & HIRAKAWA, K. (1967). *J. Phys. Soc. Jpn*, **23**, 751–756.

TANAKA, K., KONISHI, M. & MARUMO, F. (1979). *Acta Cryst.* B**35**, 1303–1308.

TANAKA, K. & MARUMO, F. (1980). To be published.

Table 3. (*amendments*)

Figures in parentheses are e.s.d.'s of the values.

| | Cu | | | K | | F(1) | | F(2) | | | | 3*d* | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Refinement | $U_{11}$ | $U_{33}$ | $U_{12}$ | $U_{11}$ | $U_{33}$ | $U_{11}$ | $U_{33}$ | $x$ | $U_{11}$ | $U_{33}$ | $U_{12}$ | $U_{11}$ | $U_{33}$ | $U_{12}$ | $\cos(\varphi/2)$ | $G_{11}$ | $G_{22}$ | $G_{33}$ | $G_{12}$ | $G_{13}$ | $G_{23}$ |
| (*c*) | 759 | 574 | −105 | 1541 | 1444 | 2228 | 718 | 22764 | 1358 | 1954 | −639 | | | | 908 | 92 | 147 | 326 | 79 | −59 | −0 |
| | (4) | (4) | (4) | (6) | (8) | (21) | (18) | (7) | (13) | (23) | (17) | | | | (19) | (4) | (5) | (37) | (2) | (9) | (17) |
| (*d*) | 759* | 575* | −102* | 1542 | 1445 | 2230 | 717 | 22765 | 1357 | 1951 | −640 | 683† | 801† | −208† | 941 | 92 | 147 | 322 | 79 | −59 | +1 |
| | (2) | (3) | (4) | (5) | (7) | (21) | (18) | (7) | (12) | (22) | (16) | (38) | (64) | (57) | (8) | (3) | (5) | (36) | (2) | (9) | (16) |

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