The fluorine ion F(5) is shared only by U^{4+} ions across the K^+ layers but is too distant, 4Å, to be considered shared by K^+ ions.

The interatomic distances F(1)–F(1), 2·49(3)Å and F(1)–F(3), 2·55(3)Å are considerably shorter than twice 1·36Å, the usual ionic radius for F^- (Pauling, 1960). Recent structure determinations show that F^-–F^- interatomic distances may be as short as 2·241(11)Å in $Na_7Zr_6F_{31}$ (Burns, Ellison & Levy, 1968) and 2·40(3)Å in $RbPaF_6$ (Burns, Levy & Keller, 1968). These two compounds are similar to KU_2F_9 in that they are complex fluorides with similar sizes and kinds of ions. The Zr–8F antiprism in $Na_7Zr_6F_{31}$ has F^-–F^- distances as short as 2·504(3)Å and the 2·40(3)Å distances observed for $RbPaF_6$ occur in the Pa–8F dodecahedron. In KU_2F_9 the six K–F distances and the nine U–F distances are equal to the sum of the ionic radii so that the bonding is primarily ionic. The application of Hannay & Smyth's (1946) formula for the calculation of percentage of ionic character indicates that the K–F bond is 88% ionic while the U–F bond should have 55% ionic character. It is evident that most of the F^-–F^- distances in these complex fluorides reflect the ionic nature of the bonding but that some covalent bonding occurs in the same compound.

References

BROWN, G. M. & LEVY, H. A. (1964). *J. Phys.* **25**, 497.

BURNS, J. H., ELLISON, R. D. & LEVY, H. A. (1968). *Acta Cryst.* B**24**, 230.

BURNS, J. H., LEVY, H. A. & KELLER, O. L. JR (1968). *Acta Cryst.* B**24**, 1675.

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). USAEC Report ORNL-TM-305, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

CROMER, D. T. & WABER J. T. (1965). *Acta Cryst.* **18**, 104.

DAUBEN, C. H. & TEMPLETON, D. H. (1955). *Acta Cryst.* **8**, 841.

HANNY, N. B. & SMYTH, C. P. (1946). *J. Amer. Chem. Soc.* **68**, 171.

PAULING, L. (1960). *Nature of the Chemical Bond,* 3rd Ed. p. 514. Ithaca: Cornell Univ. Press.

THOMA, R. E., INSLEY, H., LANDAU, B. S., FRIEDMAN, H. A. & GRIMES, W. R. (1958). *J. Amer. Ceram. Soc.* **41**, 538.

ZACHARIASEN, W. H. (1948). *J. Amer. Chem. Soc.* **70**, 2147.

ZACHARIASEN, W. H. (1967). *Acta Cryst.* **23**, 558.

Acta Cryst. (1969). B**25**, 1669.

The crystal structure of calcium 1,3-diphosphorylimidazole hexahydrate (revised title).

By L. NEEL BEARD and P. GALEN LENHERT, *Department of Physics, Vanderbilt University, Nashville, Tennessee* 37203, *U.S.A.*

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A correction of the title of *Acta Cryst.* (1968), B**24**, 1529.

A paper on the structure of the title compound was published (Beard & Lenhert, 1968) under thetitle *The Crystal Structure of* 1,3-*Diphosphorylimidazole*. This title should be replaced by *The Crystal Structure of Calcium* 1,3-*Diphosphorylimidazole Hexahydrate* in order to reflect the actual composition of the substance studied.

Reference

BEARD, L. N. & LENHERT, P. G. (1968). *Acta Cryst.* B**24**, 1529.