Crystal Structure of $K_2Cu(ZrF_6)_2,6H_2O$

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To complete our study of the stereochemistry of zirconium in the hydrated fluorozirconate complexes,[1-2] we have determined the crystal structure of $K_2Cu(ZrF_6)_2,6H_2O$.

The *X*-ray analysis of this complex in the solid state shows that it is built up from dinuclear $[Zr_2F_{12}]^{4-}$ anions, $[Cu(H_2O)_6]^{2+}$, and K^+ cations. The centrosymmetrical $[Zr_2F_{12}]^{4-}$ units result from the association, by a common edge, of two distorted pentagonal-bipyramidal ZrF_7 groups as shown in the Figure. The existence and the structure of such units has not previously been reported. The octahedral $[Cu(H_2O)_6]^{2+}$ cations are very similar to those found in a number of crystal structures containing this complex ion.[2-4]

Approximate standard deviations are: $\sigma_{Zr-Zr} = 0{\cdot}001$ Å, $\sigma_{F-F} = 0{\cdot}010$ Å. Crystal data: $K_2Cu(ZrF_6)_2$, $6H_2O$, $M = 660{\cdot}18$, monoclinic, $a = 6{\cdot}631$ (06), $b = 9{\cdot}981(10)$, $c = 12{\cdot}921(12)$ Å, $\beta = 114°12'$ (10'), $U = 780$ Å^3, $D_m = 2{\cdot}89$, $Z = 2$, $D_c = 2{\cdot}83$, space group, $P2_1/c$, $\lambda = 0{\cdot}71069$ Å.

The intensities of 1750 independent non-zero reflexions were recorded on a Pailred diffractometer using Mo-K_α radiation. A spherical crystal, of mean radius 0·3 mm., was used and absorption corrections were applied ($\mu = 33{\cdot}4$ cm.$^{-1}$).

The structure was derived by Patterson and Fourier techniques. The refinement to an *R*-value of 0·063 was carried out by isotropic full-matrix least-squares analysis and difference function techniques. Allowance was made for anomalous dispersion of zirconium, copper, and potassium atoms.

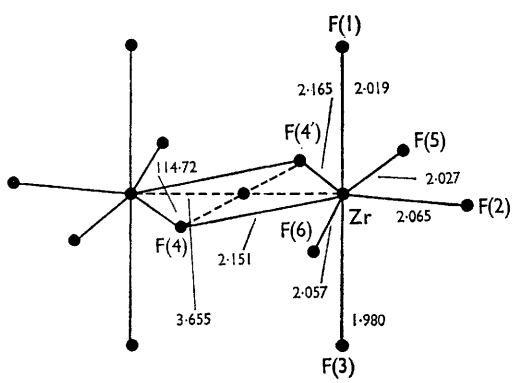

FIGURE.

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