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ON THE KNOWLEDGE OF $KCuAlF_6$

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$KCuAlF_6$ has been prepared for the first time as colourless single crystals. It crystallizes as a new orthorhombic variant of the pyrochlore type similar to that of $CsAgFeF_6$.

Four -circle diffractometer scans with graphite-monochromatized Mo K_a radiation

($3° < \Theta < 30°$, ω - Scan) gave the following data

a= 6.731 (1) Å, b= 7.040 (1) Å, c= 9.793 (1) Å

Pnma - D_{2h}^{16}

R= 5.65%, R_w= 4.36% for 727 from 727 I_o (hkl).

Strikingly we observe compressed octahedra $[CuF_6]$ with copper-fluorine distances of d [Cu-F]: 1.88 Å (2 x), 2.12 Å (4 x);

D(Al-F): 1.82 Å (2 x), 1.79 Å (4 x).

The madelungpart of the lattice energy, MAPLE, of $KCuAlF_6$ (2647.5 kcal/mol) compares very well with the sum of those of the corresponding binary fluorides (2657.6 kcal/mol).