

Syntheses and structures of two new
Cu/Nb/pyrazine complexes:
three dimensional $\text{CuNb}(\text{pyz})_2\text{OF}_5 \cdot (\text{pyz})(\text{H}_2\text{O})$
and two dimensional $[\text{Cu}(\text{pyz})_{2.5}]^+[\text{NbF}_6]^- \cdot (\text{pyz})$

Paramasivan Halasyamani, Kevin R. Heier, Michael J. Willis,
Charlotte L. Stern, Kenneth R. Poeppelmeier

Abstract

Crystals of $\text{CuNb}(\text{pyz})_2\text{OF}_5 \cdot (\text{pyz})(\text{H}_2\text{O})$ (1) and $[\text{Cu}(\text{pyz})_{2.5}]^+[\text{NbF}_6]^- \cdot (\text{pyz})$ (2) were grown (150 bar and autogeneous pressures) from CuO , $1/2(\text{Nb}_2\text{O}_5)$, $(\text{HF})_x$ pyridine, and H_2O in excess pyrazine. Light blue single crystals of (1) are orthorhombic, crystg. in space group Cccm , with a 14.547(1), b 16.135(2), c 13.803(2) Å, and $Z = 8$. The structure of (1) contains corner shared $[\text{Cu}(\text{pyz})_{4/2}\text{F}_2/2]^+$, $[\text{Cu}(\text{pyz})_{4/2}\text{O}_2/2]$, and $[\text{NbF}_4\text{O}_{1/2}\text{F}_{1/2}]^{-0.5}$ octahedra. Orange crystals of (2) are monoclinic, crystg. in space group $\text{C}2/c$, with a 11.792(8), b 17.123(3), c 17.051(5) Å, β 90.04(4)° and $Z = 8$. The structure of (2) contains puckered rings of corner shared $[\text{Cu}(\text{pyz})(\text{pyz})_{3/2}]^+$ tetrahedra and isolated $[\text{NbF}_6]^-$ anions within the rings.