Green-yellow Thermochromism of (N-methyl-2,6-lutidinium)$_2$ CuCl$_4$

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The previously reported, green, room temperature phase of N-methyl-2,6-lutidinium)$_2$ $CuCl_4$ consists of layers of square-planar $CuCl_4^{2-}$ anions interspersed with coplanar organic cations.

The temperature behavior of the compound was studied, and a thermochromic phase transition from green to yellow found at 67 °C. The crystal structure of the high temperature yellow phase of $(C_8H_{12}N)_2CuCl_4$ was determined at 77(1) °C with unit cell parameters triclinic, P1-bar, a = 7.9350(5) Å, b = 9.1550(7) Å, c = 16.144(2) Å, α= 75.467(4)°, β= 86.975(4)°, γ= 64.505(5)°, V = 1022.64(15) Å^3, Z = 2.

The structure of the high temperature phase consists of flattened $CuCl_4^{2-}$ tetrahedra with the two unique organic cations now canted relative to one another rather than coplanar. The canting of the organic cations lengthens the short aromatic C-H--Cl contacts in the low temperature phase which appear to stabilize the square planar over the flattened tetrahedral anion geometry.

Previous examples of green-yellow thermochromism in the A_2CuCl_4 family have occurred only in the presence of strong N-H--Cl hydrogen bonding, which stabilizes the square planar anion geometry in the low-temperature phase. The title compound is the first known to exhibit this behavior in the absence of strong N-H--Cl hydrogen bonding.

Keywords: copper complexes, phase transitions, hydrogen bonding