Synthesis and Structural Study of the Thermochromic Compounds Bis(2-amino-4-oxo-6-methylpyrimidinium) Tetrachlorocuprate(II) and Bis(2-amino-4-chloro-6-methylpyrimidinium) Hexachlorodicuprate(II)

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Thermochromic Compounds, Copper, Chloride

The compound bis(2-amino-4-oxo-6-methylpyrimidinium) tetrachlorocuprate(II) **1** contains $CuCl_4^{2-}$ square-planar anions, and bis(2-amino-4-chloro-6-methylpyrimidinium) hexachlorodicuprate(II) **2** quasi-planar $Cu_2Cl_6^{2-}$ anions. Both compounds show thermochromic behaviour. This phenomenon has been studied by X-ray crystallography at variable temperature, with the result that no major change is observed in the geometry of the copper atom. Thus it is possible to assume some influence of the hydrogen bonds and of the different geometries of intermediate states on the color of the compounds due to the modifications provoked in the L→M charge transfer and in the energy of the metal d-d transitions. Magnetic measurements of the compounds give information on magneto-structural correlations. Compound **1** is ferromagnetic ($T_c \cong 20$ K) due to the perpendicular arrangement of the square anions that allows exchange pathways only *via* Cu-Cl···Cu , H-bonding or cationic π electron interactions. Compound **2** shows a very complicated behavior at low temperature with local antiferromagnetic fluctuations. Crystal data: **1** $C_{10}H_{16}N_6O_2Cl_4Cu$, triclinic, P1; 393(2) K: a = 11.053(2), b = 11.334(2), c =14.038(3) (Å), α = 95.76(3), β = 101.35(3), γ = 90.15(3)(°); 293(2) K: a = 11.022(2), b = 11.289(2), c = 14.001(3) (Å), α = 95.86(2), β = 101.34(2), γ = 90.09(3)(°); 155(2) K: a = 11.008(2), b = 11.231(2), c = 13.967(3) (Å), α = 95.86(2), β = 101.37(2), γ = 89.99(2)(°); Z = 4. **2** $(C_5H_7N_3Cl_3Cu)_2$, monoclinic, $P2_1/c$; 293(2) K: a = 5.998(1), b =18.669(4), c = 9.466(2) (Å), β = 100.93(3)(°); 150(2) K: a = 5.971(1), b = 18.655(4), c = 9.383(2) (Å), β = 101.64(1)(°); Z = 4.