Synthesis, Crystal Structure and Properties of CuBr(2,3-dimethylpyrazine) Coordination Polymers

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Reaction of CuBr with an excess of 2,3-dimethylpyrazine in acetonitrile leads to the formation of the literature known ligand-rich 1:1 compound poly[\(\mu_2\)-bromo-\(\mu_2\)-2,3-dimethylpyrazine-\(N,N'\)-copper(I)] (1). On heating this compound in a thermobalance a transformation into the new ligand-deficient 2:1 compound poly[di-\(\mu_3\)-bromo-\(\mu_2\)-2,3-dimethylpyrazine-\(N,N'\)-dicopper(I)] (3) is observed, which later was also prepared in solution. This compound crystallizes in the monoclinic space group \(P2_1/n\) with all atoms in general positions. In the crystal structure the Cu atoms are surrounded by three Br atoms and one 2,3-dimethylpyrazine ligand within a distorted tetrahedron. The tetrahedra are connected via common Br edges into CuBr double chains, which are connected by the ligands into layers located in the \(ab\) plane. The formation of compounds 1 and 3 was also investigated in solution. The results have shown that compound 1 can only be prepared if an excess of the ligand is used. If CuBr and the ligand are reacted in a ratio of 1:1, in the beginning the literature known ligand-deficient 3:2 intermediate catena[tribromo-\(\mu_2\)-bis(\(\mu_2\)-2,3-dimethylpyrazine-\(N,N'\)-tricopper(I))] (2) is obtained, which transforms within minutes into compound 3. If a crystalline suspension of compound 1 is stirred in acetonitrile a transformation into the most stable compound 3 is also observed. The luminescence properties of compounds 1 and 3 were investigated. The complexes show differences mainly in the emission spectra.

\textit{Key words}: Coordination Polymers, CuBr(2,3-dimethylpyrazine), Crystal Structures, Thermal Properties, Luminescence Properties