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

Inke Jeß[a], Petr Taborsky[b], and Christian Näther[a]

[a] Institut für Anorganische Chemie der Christian-Albrechts-Universität zu Kiel, Olshausenstraße 40, D-24098 Kiel, Germany
[b] Department of Analytical Chemistry, Faculty of Science, Masaryk University in Brno, Kotlarska 2, 611 37 Brno, Czech Republic

Reprint requests to Dr. Christian Näther. E-mail: cnaether@ac.uni-kiel.de

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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[μ_2-bromo-μ_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-μ_3-bromo-μ_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-μ_2-bis(μ_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.

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