Halocuprate(I) Zigzag Chain Structures with N-Methylated DABCO Cations – Bright Metal-Centered Luminescence and Thermally Activated Color Shifts

Sebastian Maderlehner a‡, Markus J. Leitl b‡, Hartmut Yersin *b, Arno Pfitzner *a

a Institute for Inorganic Chemistry, University of Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany. Fax: +49 941 943814551; Tel: +49 941 943 4551; E-mail: arno.pfitzner@chemie.uni-regensburg.de

b Institute for Physical Chemistry, University of Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany. Fax: +49 941 9434488; Tel: +49 941 943 4464; E-mail: hartmut.yersin@chemie.uni-regensburg.de

‡These authors contributed equally to this work

Electronic Supporting Information

Figure S1. Experimental and calculated powder diffraction pattern of I showing the excellent match of experimental and simulated data.
Figure S2. Experimental and calculated powder diffraction pattern of 2 showing a very good match of experimental and simulated data.
Figure S3. IR-spectra of DABCO(HBr)$_2$ and 1.
Figure S4. IR-spectra of DABCO(HI)$_2$H$_2$O and 2.

The IR-spectra clearly show the quantitative twofold $N$-methylation of the DABCO molecules. The N-H-stretching modes present in the spectra of the starting materials in the range from 2000 to 2800 cm$^{-1}$ are absent in 1 and 2. Only one large peak at approximately 3000 cm$^{-1}$ which is caused by the C-H-stretching modes of the methyl and methylene groups of the DABCOMe$_2^{2+}$ cations can be observed in 1 and 2.