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

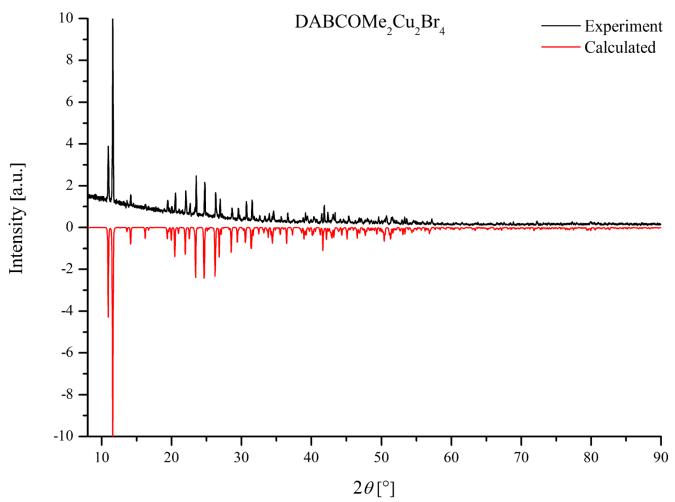


Figure S1. Experimental and calculated powder diffraction pattern of 1 showing the excellent match of experimental and simulated data.

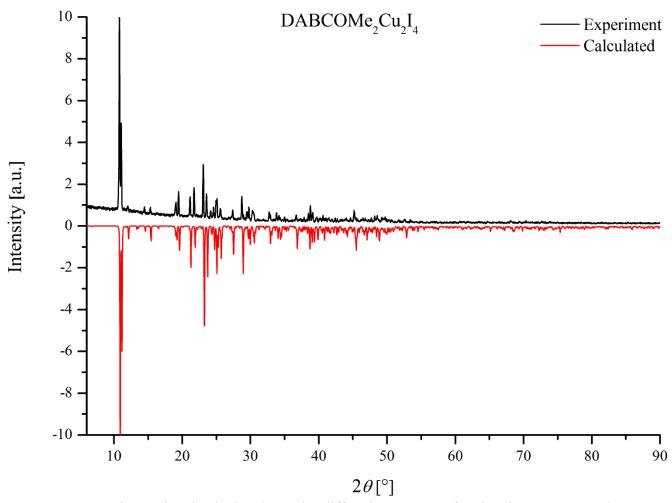


Figure S2. Experimental and calculated powder diffraction pattern of 2 showing a very good match of experimental and simulated data.

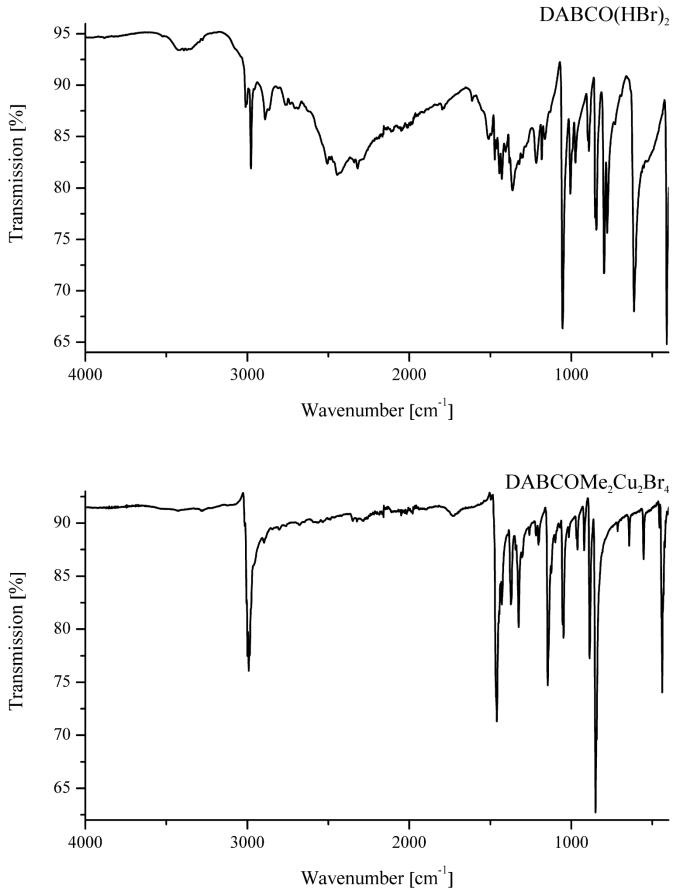


Figure S3. IR-spectra of DABCO(HBr)₂ and 1.

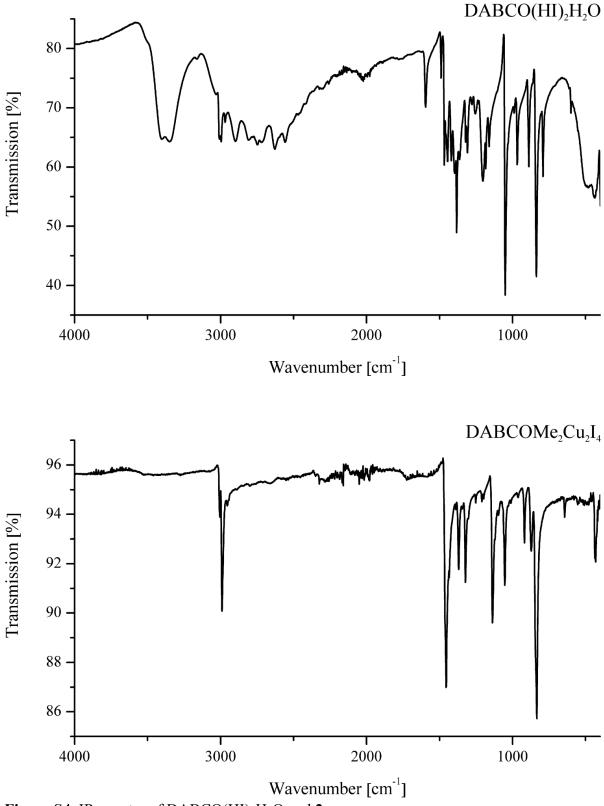


Figure S4. IR-spectra of DABCO(HI)₂H₂O and 2.

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 DABCOMe₂²⁺ cations can be observed in **1** and **2**.