MnBr₂/(18-crown-6) Coordination Complexes Showing High Room Temperature Luminescence and Quantum Yield

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SUPPORTING INFORMATION
A comparison of diffractograms that were calculated based on data from single crystal structure analysis and X-ray powder diffraction data of powder samples validates the structure of the compounds MnBr$_2$(18-crown-6) (1), Mn$_3$Br$_6$(18-crown-6)$_2$ (2) and Mn$_3$Br$_6$(18-crown-6) (3) (Figure S1). Certain shifts of the Bragg peaks result from the different temperatures of measurement (single crystal diffraction analysis at -75 °C; powder diffraction analysis at 20 °C).

**Figure S1.** Comparison of measured (X-ray powder diffraction) and calculated (based on the data from single-crystal structure analysis) powder diffraction patterns of (a) MnBr$_2$(18-crown-6) (1), (b) Mn$_3$Br$_6$(18-crown-6)$_2$ (2), and (c) Mn$_3$Br$_6$(18-crown-6)$_2$ (3).
Figures S2 to S4 show the packing of the building units in the crystalline lattice, which is illustrated by (2×2) unit cells for MnBr$_2$(18-crown-6) (1) (Figure S2), Mn$_3$Br$_6$(18-crown-6)$_2$ (2) (Figure S3) and Mn$_3$Br$_6$(18-crown-6) (3) (Figure S4).

**Figure S2.** (2×2) unit cells of MnBr$_2$(18-crown-6) (1) (hydrogen atoms not shown).

**Figure S3.** (2×2) unit cells of Mn$_3$Br$_6$(18-crown-6)$_2$ (2) (hydrogen atoms not shown).
Figure S4. (2×2) unit cells of Mn₃Br₆(18-crown-6) (3) (hydrogen atoms not shown).