

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 $\text{MnBr}_2(18\text{-crown-6})$ (**1**), $\text{Mn}_3\text{Br}_6(18\text{-crown-6})_2$ (**2**) and $\text{Mn}_3\text{Br}_6(18\text{-crown-6})$ (**3**) (Figure S1). Certain shifts of the Bragg peaks result from the different temperatures of measurement (single crystal diffraction analysis at $-75\text{ }^\circ\text{C}$; powder diffraction analysis at $20\text{ }^\circ\text{C}$).

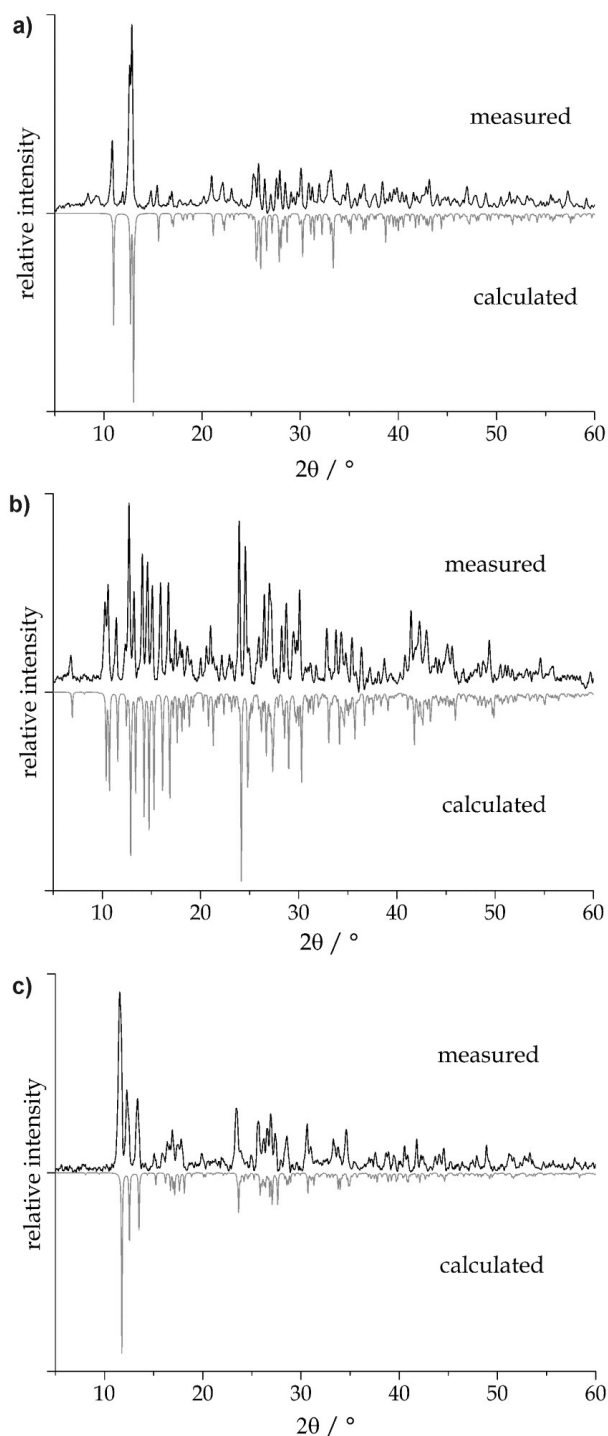


Figure S1. Comparison of measured (X-ray powder diffraction) and calculated (based on the data from single-crystal structure analysis) powder diffraction patterns of (a) $\text{MnBr}_2(18\text{-crown-6})$ (**1**), (b) $\text{Mn}_3\text{Br}_6(18\text{-crown-6})_2$ (**2**), and (c) $\text{Mn}_3\text{Br}_6(18\text{-crown-6})$ (**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 $\text{MnBr}_2(18\text{-crown-6})$ (**1**) (Figure S2), $\text{Mn}_3\text{Br}_6(18\text{-crown-6})_2$ (**2**) (Figure S3) and $\text{Mn}_3\text{Br}_6(18\text{-crown-6})$ (**3**) (Figure S4).

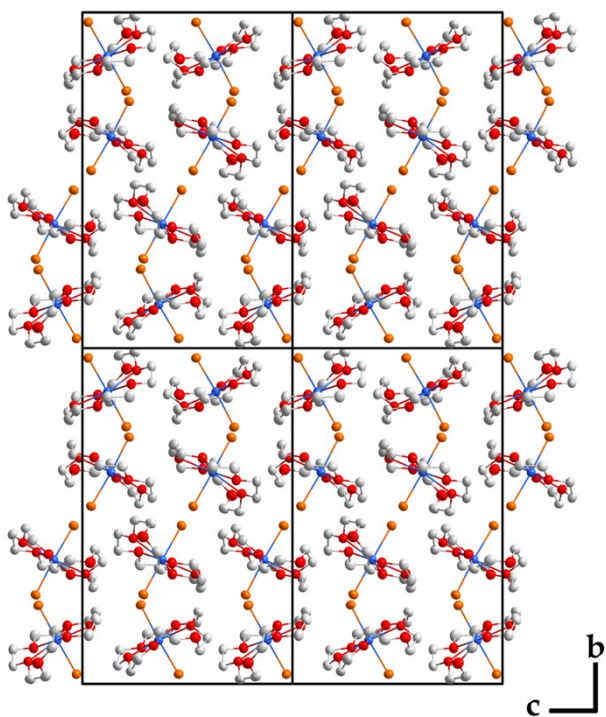


Figure S2. (2×2) unit cells of $\text{MnBr}_2(18\text{-crown-6})$ (**1**) (hydrogen atoms not shown).

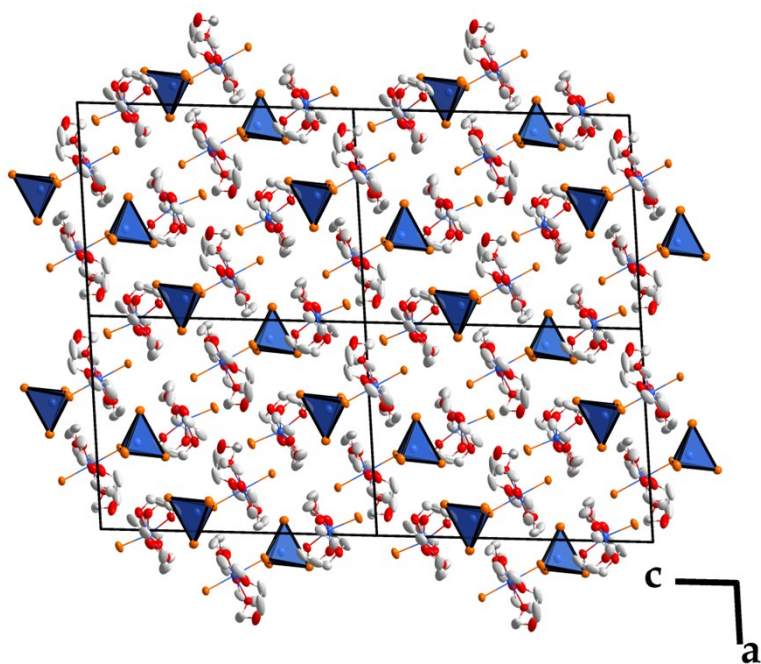


Figure S3. (2×2) unit cells of $\text{Mn}_3\text{Br}_6(18\text{-crown-6})_2$ (**2**) (hydrogen atoms not shown).

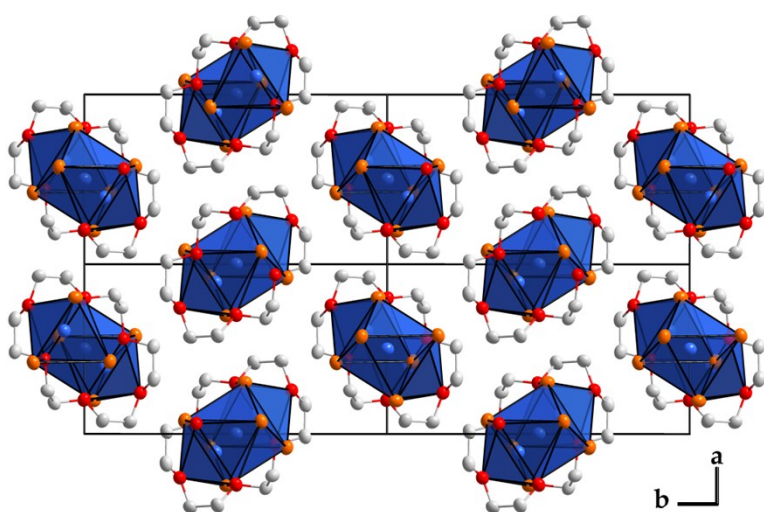


Figure S4. (2×2) unit cells of Mn₃Br₆(18-crown-6) (**3**) (hydrogen atoms not shown).