Polarized Mn K-edge X-ray Absorption Spectroscopy of Binuclear Mn Model Complexes

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Polarized Mn K-edge X-ray absorption (XAS) data have been obtained for binuclear manganese mono- and bis-oxo complexes. Analysis of the 1s to 3d pre-edge splittings and intensities of a Mn(III)-O-Mn(III) complex has been used to determine the relative contributions of each polarization vector to the electric dipole allowed intensity. A ligand field multiplet analysis has been used to estimate the relative electric quadrupole intensity distribution. The experimental results are compared to theoretical predictions from density functional calculations. The presented results should aid in the further interpretation of the 1s to 3d features in other biologically relevant binuclear Mn model complexes, the active site of manganese catalase, and may potentially be applied to the tetranuclear Mn cluster in photosystem II.

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