Supporting Information

for

Structural Investigation of High Valent Manganese Salen Complexes by UV/Vis-, Raman-, XANES- and EXAFS-Spectroscopy


and Helmut Bertagnolli[a]

[a] M.P. Feth, M. Bauer, R. Ramamonjisoa, Prof. Dr. H. Bertagnolli
   Universität Stuttgart, Institut für Physikalische Chemie, Pfaffenwaldring 55,
   70569 Stuttgart (Germany)
   Fax: (+49) 711 685 4443; Tel: (+49) 711 685 4471
   E-mail: m.feth@ipc.uni-stuttgart.de
[b] Prof. Dr. C. Bolm, Dr. J. P. Hildebrand, M. Köhler, Dr. O. Beckmann
   RWTH Aachen, Institut für Organische Chemie, Professor-Pirlet-Strasse 1,
   52056 Aachen (Germany)
   Fax: (+49) 241 809 23 91; Tel: (+49) 241 809 46 75
   E-mail: Carsten.Bolm@oc.rwth-aachen.de

* corresponding author
Supplementary Figures

Figure S1  Comparison of the Raman spectrum of [(salen)Mn$^{III}$Cl] (1) with [(salen)Mn$^{III}$Br] (2).

Figure S2  Comparison of the Raman spectra of 4-PPNO and [(salen)Mn$^{III}$Cl] (1) with the reaction product of 1 with 1 equiv of 4-PPNO (4) and 4-PPNO.
Figure S3  Comparison of the Raman spectra of 4-PPNO and [(salen)Mn$^{III}$Br] (2) with the reaction product of 2 with 1 equiv of 4-PPNO (5) and 4-PPNO.

Figure S4  Comparison of the Raman spectrum of the pure salen ligand with [(salen)Mn$^V$N] (3).
**Figure S5**  Comparison of the IR spectra of 4-PPNO, [(salen)Mn$^{III}$Cl] (1) and [(salen)Mn$^{III}$Br] (2) with the reaction product of 1/2 with 1 equiv of 4-PPNO (4, 5).

**Figure S6**  Comparison of the IR spectrum of the pure salen ligand with [Salen]Mn$^{V}$N (3).
Figure S7  Comparison of the XANES spectra $[(\text{salen})\text{Mn}^{\text{III}}\text{Br}]$ (2) and $[(\text{salen})\text{Mn}^{\text{V}}\text{N}]$ (3) with the reaction products of 2 + 1 equiv or 2 equiv of 4-PPNO (5, 7).

Figure S8  Comparison of the XANES spectra $[(\text{salen})\text{Mn}^{\text{III}}\text{Cl}]$ (1) and $[(\text{salen})\text{Mn}^{\text{V}}\text{N}]$ (3) with the reaction products of 1 + 1 equiv of MCPBA after 0 and 90 minutes (8).
Figure S9  Experimental (solid line) and calculated (dotted line) \( k^3 \chi(k) \) functions a) and their Fourier transforms b) of [(salen)Mn\textsuperscript{III}Cl] (1) + 2 equiv of 4-PPNO (Mn K-edge).

Figure S10  Experimental (solid line) and calculated (dotted line) \( k^3 \chi(k) \) functions a) and their Fourier transforms b) of [(salen)Mn\textsuperscript{III}Br] (2) (Mn K-edge).
Figure S11  Determination of the rate constant $k_1$ of the reaction $[(\text{salen})\text{Mn}^{\text{III}}\text{Cl}]$ (1) + 20 equiv of MCPBA in acetonitrile from the absorbance decrease at 648 nm in the UV/Vis spectra.