

Supplementary Materials

Electrochemical Characterization and CO₂ Reduction Reaction of a family of Pyridazine-Bridged Dinuclear Mn(I) Carbonyl complexes.

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Table S1. Electrochemical and chemical parameters used for the simulation of the cyclic voltammetric curves reported in Figure 2 through the mechanism sketched in Scheme 2.

<u>Redox process</u> or <u>Chemical reaction</u>	<u>Label</u> <u>mechanism</u> <u>process</u>	<u>Kinetic parameters</u>
A / A^-	<i>I</i>	$k_{s0} = 0.1 \text{ cm/s}$; (alpha = 0.5)
A^- / A^{2-}	<i>II</i>	$k_{s1} = 7 \cdot 10^{-4} \text{ cm/s}$; (alpha = 0.45)
A^{2-} / A^{3-}	<i>III</i>	$k_{s2} = 10^4 \text{ cm/s}$; (alpha = 0.45)
$A^{3-} \rightleftharpoons B^{3-}$	<i>k'</i>	$k_{3a} = 10^4 \text{ s}^{-1}$; $k_{3r} = 10^{-4} \text{ s}^{-1}$
B^{2-} / B^{3-}	<i>ReoxI</i>	$k_{s4} = 0.1 \text{ cm/s}$; (alpha = 0.5)
B^- / B^{2-}	<i>ReoxII</i>	$k_{s5} = 3 \cdot 10^{-3} \text{ cm/s}$; (alpha = 0.65)
B / B^-	<i>ReoxIII</i>	$k_{s6} = 0.03 \text{ cm/s}$; (alpha = 0.5)
$B \rightleftharpoons A$	<i>k''</i>	$k_{7a} = 10^4 \text{ s}^{-1}$; $k_{7r} = 10^{-3} \text{ s}^{-1}$

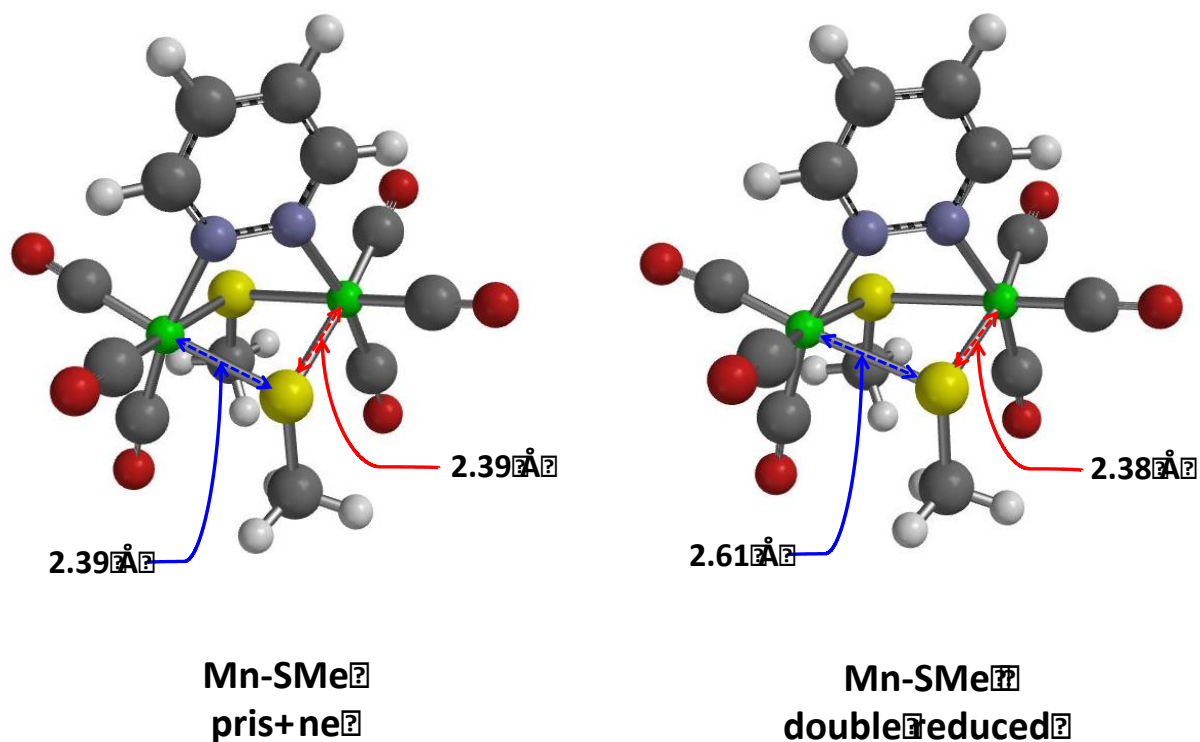


Figure S2. Optimized molecular structures of the complex **Mn-SMe** at M06/3-21G* level of the theory for the pristine species (left) and the double reduced compound (right). The bond length of the ancillary bridging ligand with the two manganese centers are reported for the pristine and the double reduced species showing that one of the two bonds is elongated upon the 2-electron reduction, while the other remain unchanged. The same phenomenon occurs for the other ancillary bridging ligand.