Supplementary Information for:

Encapsulated Transition Metal Catalysts Comprising Peripheral Zn(II)salen Building Blocks: Template-Controlled Reactivity and Selectivity in Hydroformylation Catalysis

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Crystal Structure Determination

X-ray intensities were measured on a Nonius KappaCCD diffractometer with a rotating anode (Mo-Kα, λ = 0.71073 Å) at a temperature of 150 K. The structures were solved with direct methods with the program SHELXS-97\textsuperscript{a} and SIR-97\textsuperscript{b} and refined with the program SHELXL-97\textsuperscript{c} against F\textsuperscript{2} of all reflections. The drawings, structure calculations, and checking for higher symmetry were performed with the program PLATON\textsuperscript{d}

\textsuperscript{a}G. M. Sheldrick, SHELXS-97. Program for crystal structure solution, University of Göttingen, Germany, 1997


\textsuperscript{c}G. M. Sheldrick, SHELXL-97. Program for crystal structure refinement. University of Göttingen, Germany, 1997

UV-vis Titration curves for assemblies $1\bullet P_1$, $(1)_3\bullet P_2$ and $(1)_3\bullet P_3$. 

- **$1\bullet P_1$**: 
  - $1:1$ ratio at $V_{\text{add}} = 65 \mu\text{L}$
  - Graph showing absorbance change with $V_{\text{add}}$.

- **$(1)_3\bullet P_2$**: 
  - $3:1$ ratio at $V_{\text{add}} = 90 \mu\text{L}$
  - Graph showing absorbance change with $V_{\text{add}}$.

- **$(1)_3\bullet P_3$**: 
  - $3:1$ ratio at $V_{\text{add}} = 90 \mu\text{L}$
  - Graph showing absorbance change with $V_{\text{add}}$. 

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S3
Molecular modeling results (PM3 calculations) for assemblies (1)$_3$•P$_2$ (LEFT) and (1)$_3$•P$_3$ (RIGHT)

(Zn = red, Cl = orange, P = yellow, N = blue, C = dark grey, H = light grey)
Displacement ellipsoid plot for assembly (1)•P2 with the adopted numbering scheme.

Selected bond distances (Å) and angles (°): Zn(1)-N(11) = 2.097(3), Zn(1)-N(12) = 2.076(3), Zn(1)-N(41) = 2.138(3), Zn(1)-O(11) = 1.946(3), Zn(1)-O(12) = 1.964(2), Zn(2)-N(21) = 2.085(3), Zn(2)-N(22) = 2.060(3), Zn(1)-N(42) = 2.132(3), Zn(2)-O(21) = 1.953(3), Zn(2)-O(22) = 1.949(2), Zn(3)-N(31) = 2.118(3), Zn(3)-N(32) = 2.069(3), Zn(3)-N(43) = 2.124(3), Zn(3)-O(31) = 1.948(2), Zn(3)-O(32) = 1.975(2), C(43)-P(41)-C(48) = 102.89(16), C(43)-P(41)-C(413) = 98.44(16), C(48)-P(41)-C(413) = 99.40(17).