

Supplementary Materials for

Hydrogen Bonding Directed Self-Assembly of a Binuclear Ag(I) Metallacycle into a 1D Supramolecular Polymer

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1. Experimental data for the complex $[\text{Pd}^{\text{II}}\text{L}_2](\text{SbF}_6)_2$

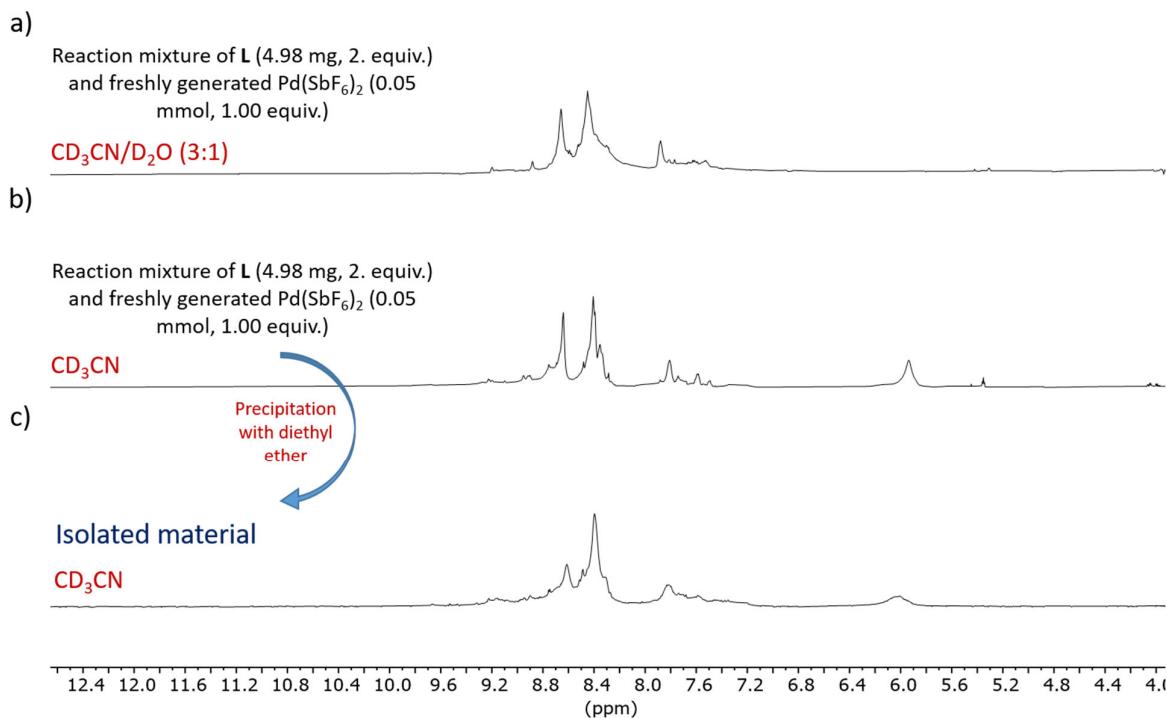


Figure S1. ^1H NMR spectrum (600 MHz) of the reaction mixture $[\text{Pd}^{\text{II}}\text{L}_2](\text{SbF}_6)_2$ (2.0×10^{-2} M). a) in $\text{CD}_3\text{CN}/\text{D}_2\text{O}$ (3:1), b) in CD_3CN , c) isolated material in CD_3CN .

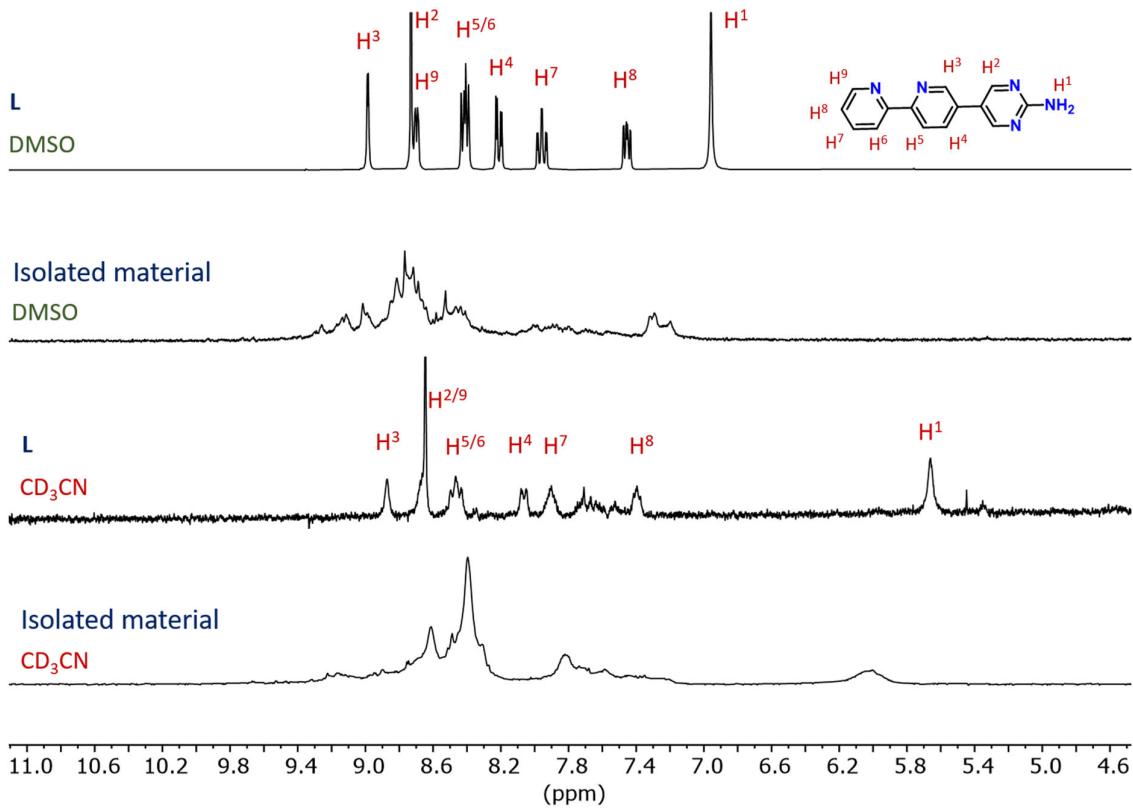


Figure S2. ¹H NMR spectrum (600 MHz) of comparisons free ligand and isolated material (see Figure S1.) in deuterated MeCN and DMSO.

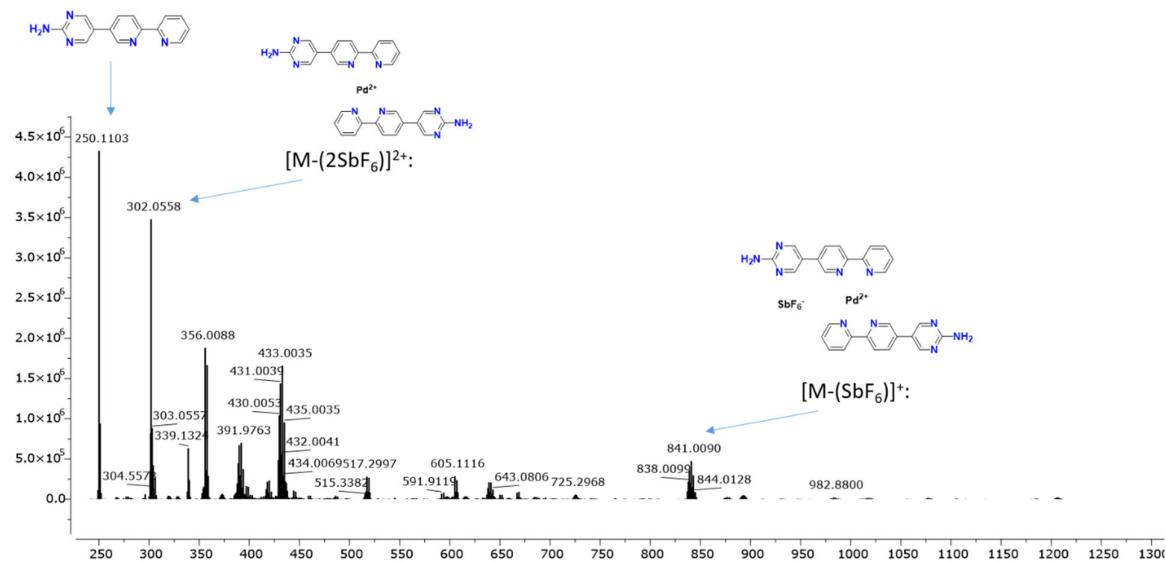


Figure S3. HR-TOF-ESI-MS analysis of the reaction mixture $[\text{Pd}^{\text{II}}\text{L}_2](\text{SbF}_6)_2$.

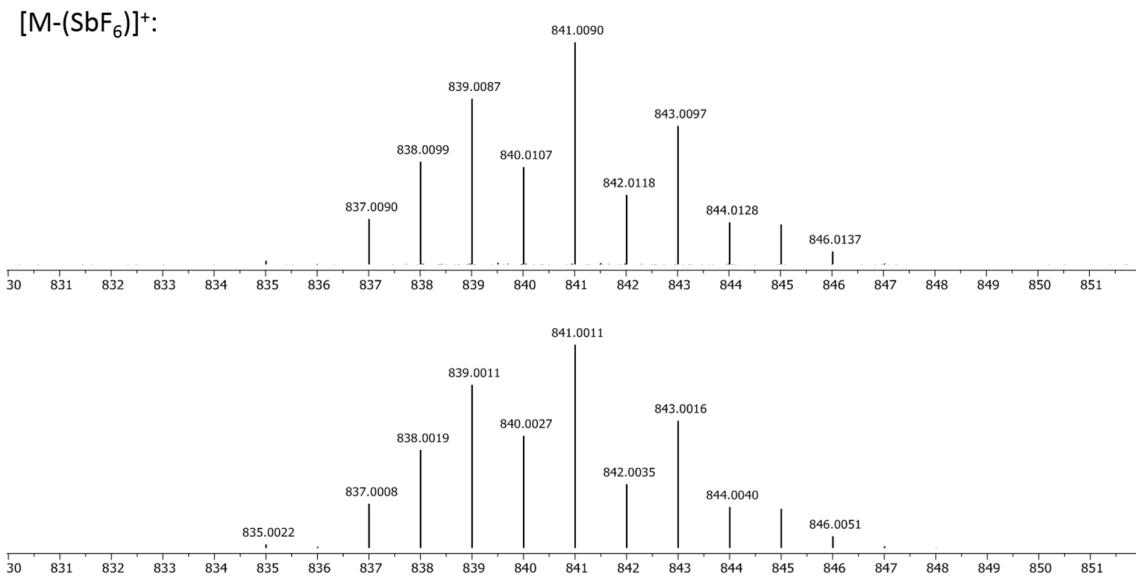


Figure S4. HR-TOF-ESI-MS analysis of the reaction mixture [Pd^{II}L₂](SbF₆)₂, showing the observed data (top) and the theoretical isotope model (bottom).

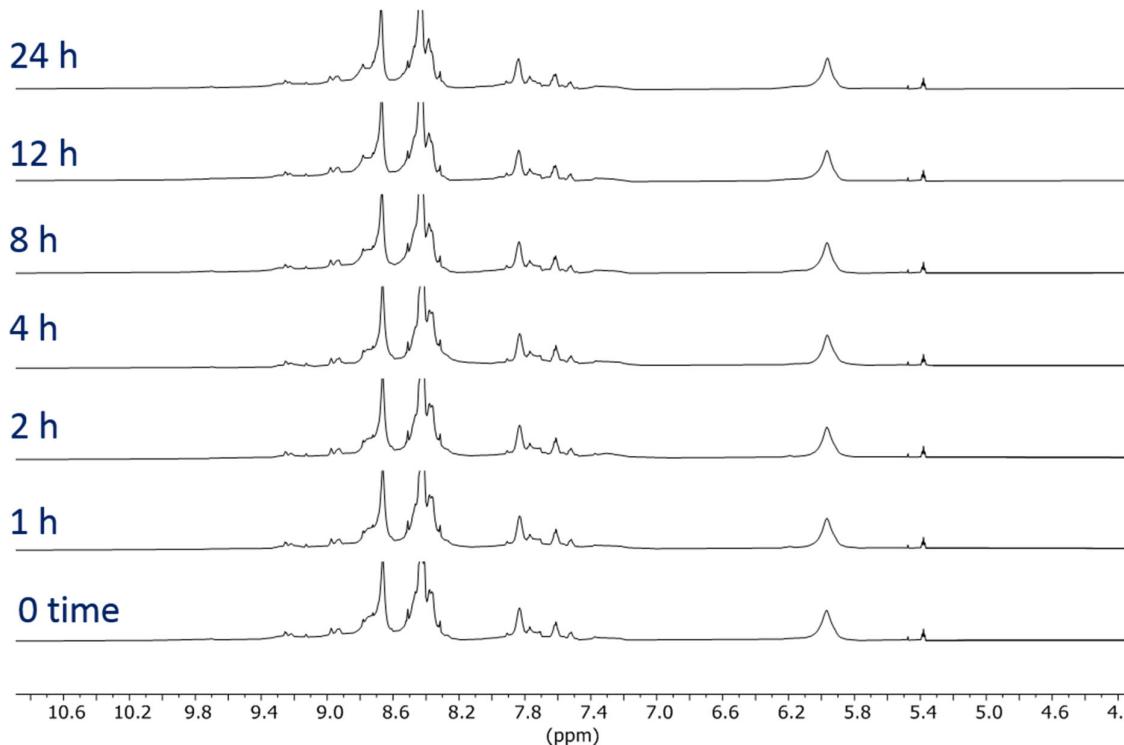


Figure S5. Kinetic ¹H NMR spectrum (600 MHz, CD₃CN) of the reaction mixture [Pd^{II}L₂](SbF₆)₂ (2.0 × 10⁻² M). Reaction component: L (4.98 mg, 2. equiv.), freshly generated Pd(SbF₆)₂ (0.05 mmol, 1.00 equiv.) and 1 mL of acetonitrile-d3.

2. Calculation of void space

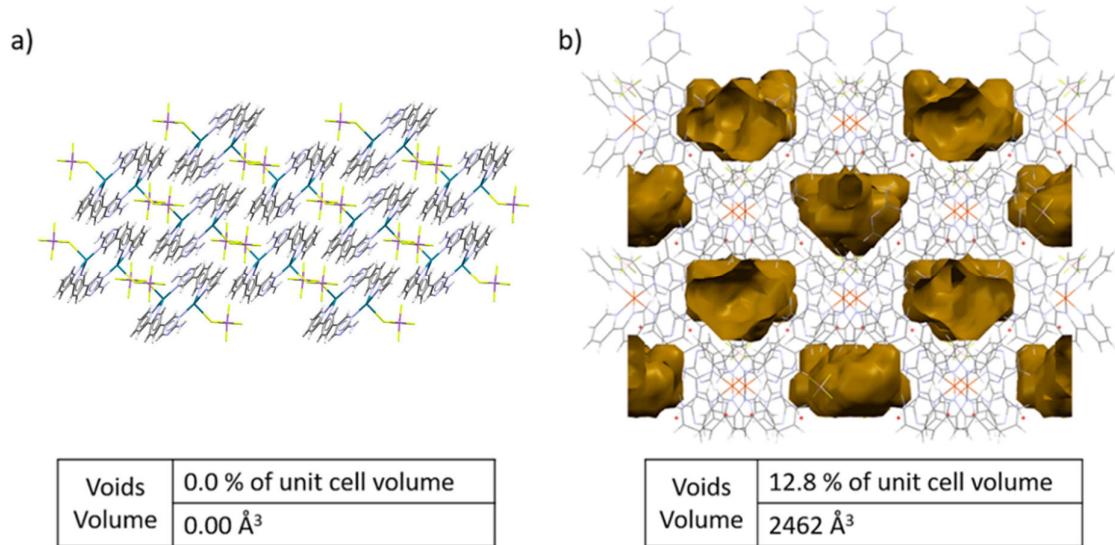


Figure S6. Void analysis of a) complex $[\text{Ag}_2\text{L}_2](\text{SbF}_6)_2$, b) complex $[\text{Fe}^{\text{II}}\text{L}_3](\text{BF}_4)_2 \cdot 9\text{H}_2\text{O}$ performed with MERCURY using a probe radius 1.2 \AA and grid spacing of 0.2 \AA , calculated using the contact surface algorithm.