

Electronic Supplementary Information (ESI)

Host–guest chemistry between cyclodextrin and hydrogen evolution catalyst of cobaloxime

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Table S1. Crystal data and structure refinement for (HNEt₃)[Co^{III}Cl(Hdmg)₂(4-pySO₃)]·MeOH

Chemical formula	C ₂₀ H ₃₈ ClCoN ₆ O ₈ S	
Formula weight	617.00 g/mol	
Temperature	90(0) K	
Wavelength	0.71073 Å	
Crystal size	0.154 x 0.164 x 0.193 mm	
Crystal system	Monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 8.2643(10) Å	<i>α</i> = 90°
	<i>b</i> = 13.2989(17) Å	<i>β</i> = 91.2760(17) °
	<i>c</i> = 25.004(3) Å	<i>γ</i> = 90°
Volume	2747.4(6) Å ³	
<i>Z</i>	4	
Density (calculated)	1.492 g/cm ³	
Absorption coefficient	0.852 mm ⁻¹	
<i>F</i> (000)	1296	
Theta range for data collection	1.63 to 27.07°	
Index ranges	-10 ≤ <i>h</i> ≤ 10, -17 ≤ <i>k</i> ≤ 12, -32 ≤ <i>l</i> ≤ 24	
Reflections collected	15310	
Independent reflections	6014 [<i>R</i> (int) = 0.0857]	
Goodness-of-fit on <i>F</i> ₂	0.996	
Final <i>R</i> indices	<i>R</i> ₁ =0.0542, w <i>R</i> ₂ =0.1154 (3305 data; <i>I</i> > 2σ(<i>I</i>)) <i>R</i> ₁ =0.1253, w <i>R</i> ₂ =0.1582 (all data)	

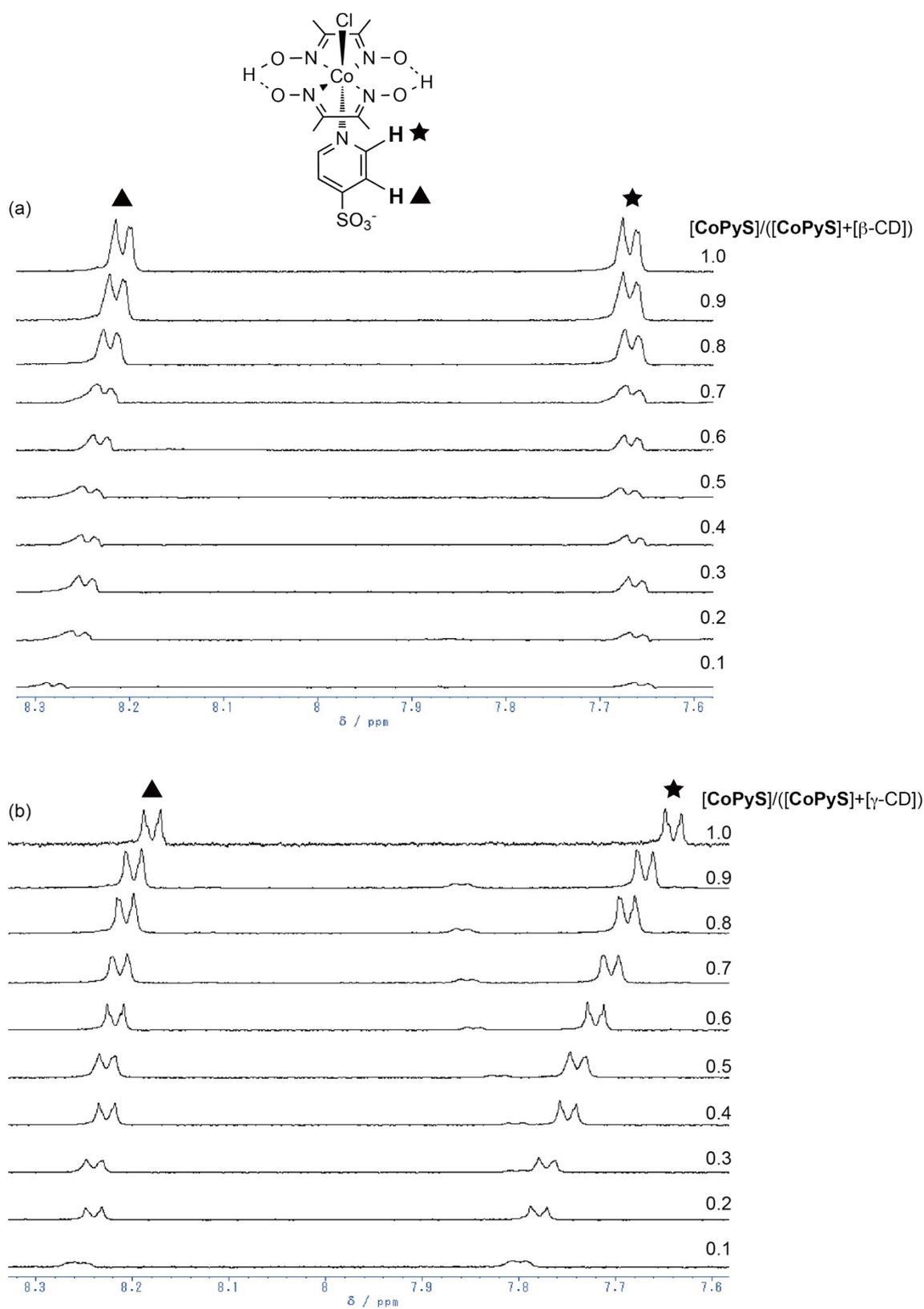


Fig. S1 Proton NMR spectra of **CoPyS** in the aromatic region varying the ratio of (a) [β-CD]: ([β-CD]+[CoPyS]) and (b) [γ-CD]: ([γ-CD]+[CoPyS]) in D₂O.

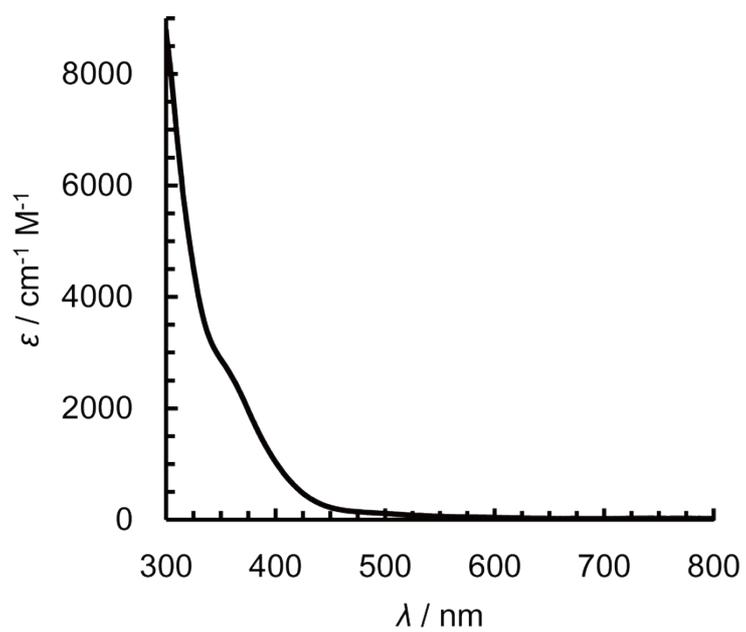


Fig. 2 UV-Vis absorption spectrum of CoPyS (0.32 mM) in water.

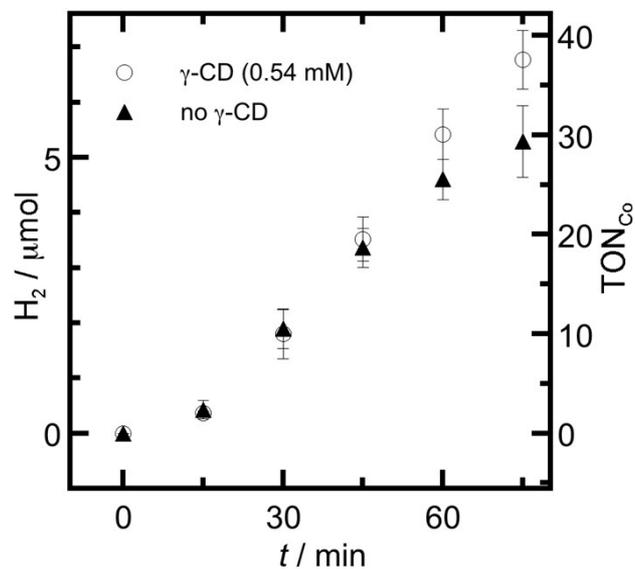


Fig. S3 Time-courses of visible light-driven hydrogen evolution catalyzed by **CoPyS** (0.18 mM) with EY (0.36 mM) in the presence of γ -CD (0.54 mM, open circles) and in the absence of γ -CD (filled triangles) for the determination of quantum yields. A TEOA (0.74 M) buffered aqueous solution at pH 7 was used. The experiments were performed under Ar and visible light irradiation at 520 nm with a light intensity of 10 mW cm⁻².

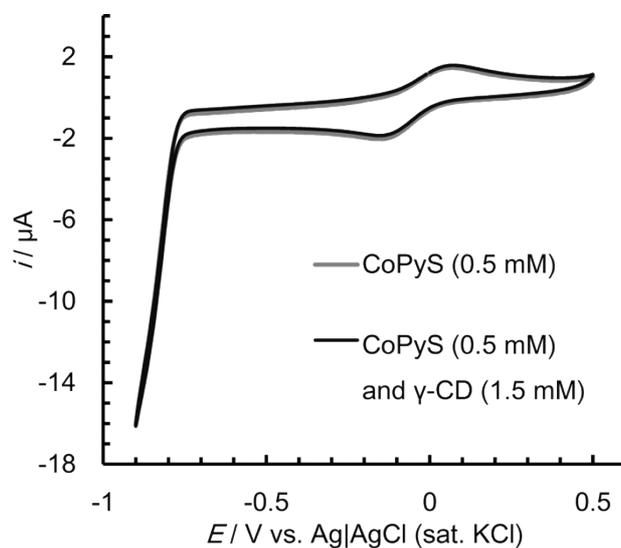


Fig. S4 Cyclic voltammograms of **CoPyS** (0.5 mM) in the presence and absence of γ -CD (1.5 mM). These cyclic voltammograms were recorded in an aqueous solution containing 0.74 M TEOA and 0.1 M NaCl at pH 7 under Ar. A scanning rate was 0.02 V s⁻¹.