Supplementary Information

A pdc-pinched copper complex for sustainable hydrogen production through ligand supported-metal centric proton-coupled electron transfer

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1.1. Chemicals

All chemicals and solvents used in the synthesis were the analytical reagent grade (AR), and of the highest purity available. >98.0% 2,6 pyridine dicarboxylic acid (**pdc**) (TCI, Japan), $Cu(NO_3)_2 \cdot 3H_2O$ (Sigma-Aldrich, USA), $Zn(NO_3)_2 \cdot 6H_2O$ (Sigma-Aldrich, USA) and Potassium chloride (SRL, India) and acidic acid (AcOH), conc. Sulfuric Acid (H_2SO_4), ethanol, double distilled water were purchased from monetary outlets. All the solvents were used as received without further purification.

1.2. Synthesis of [Cu(pdc)(H₂O)₂]

The complex **[Cu(pdc)(H₂O)₂]** was synthesized using previously reported method with slight modifications.[1] The **[Cu(pdc)(H₂O)₂]** was synthesized by the reaction between 0.4 mmol of $Cu(NO_3)_2 \cdot 3H_2O$ and 0.4 mmol of 2,6-pyridine dicarboxylic acid (**pdc**) in 1:1 in an ethanol-water medium at ambient conditions. The resulting solution was kept for slow evaporation under ambient conditions. After a few days, blue-colored crystals were obtained. The single crystal was subjected to SC-XRD.

Yield for **[Cu(pdc)(H₂O)₂]:** 0.078 g (~81% based on metal salt). Anal. Calc. for $C_7H_7NO_6Cu$: C:31.77, H:2.67, N:5.29. Found: C:31.69, H:2.63, N:5.25%. UV–Vis (λ, nm, H_2O): 267, 609.

1.3. Synthesis of [Zn(pdc)₂]

The **[Zn(pdc)₂]** was synthesized under ambient conditions using 0.4 mmol $Zn(NO_3)_2 \cdot 6H_2O$ and 0.4 mmol pdc in a 1:1 ethanol-water mixture. Slow evaporation of the reaction mixture for 4-5 days yielded transparent white crystals of bis-chelated **[Zn(pdc)₂]** complex characterized by SC-XRD. However, the crystals were not of standard quality (not publishable).

Yield for **[Zn(pdc)₂]**: 0.091 g (~77 % based on metal salt). Anal. Calc. for $C_{14}H_6N_2O_8Zn$: C:42.51, H:1.53, N:7.08. Found: C:42.58, H:1.49, N:7.01. UV–Vis (λ, nm, H_2O): 267.

1.4. Physical measurements:

Steady-state absorption spectral data of **[Cu(pdc)(H₂O)₂]** was measured with a HITACHI U-2910 spectrophotometer. A Perkin Elmer 2400 CHN microanalyzer was employed to carry out the elemental analyses of the compounds. The structural characteristics of **[Cu(pdc)(H₂O)₂]** were determined by powder X-ray diffractometer (Rigaku Smart Lab) using Cu-K_α radiation ranging from 10°-80°. A K-Lyte-1.0 potentiostat consisting of a glassy-carbon working electrode, Pt counter electrode, and Ag/AgCl reference was employed to study the electrochemical analysis of the compounds.

1.5. X-ray structural studies and refinement

Suitable single crystals of **[Cu(pdc)(H₂O)₂]** were selected for single-crystal X-ray diffraction studies. The structural diffraction data were collected on a Rigaku XtaLAB SuperNova, Dual, Cu at home/near Pilatus 200 K diffractometer at 100 K cooled with liquid nitrogen. Using Olexsys software, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimization. [2] non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were fixed at calculated positions.

1.6. Electrochemical measurements

The electrochemical study of **[Cu(pdc)(H₂O)₂]** complex was carried using a K-Lyte-1.0 potentiostat electrochemical workstation. A standard three-electrode configuration comprising of a glassy carbon electrode (GCE, 3 mm diameter) as a working electrode, Platinum wire as a counter electrode and Ag/AgCl as a reference electrode was employed. The working electrode

was thoroughly cleaned by polishing it with alumina powder (0.05 Microns) dispersed in distilled water. The recorded cyclic voltammograms (CVs) were referenced against Ag/AgCl (saturated with AgCl) as an internal standard. The electrochemical studies were performed in aqueous acidic medium using 1mM **[Cu(pdc)(H$_2$O)$_2$],** 0.1 M KCl as a supporting electrolyte at a scan rate of 100 mV/S. All glass wares were dried overnight prior to the experiments, and all the experiments were performed under N$_2$ flow to maintain the inertness of the set-up. The solution was purged with N$_2$ to eliminate dissolved oxygen.

The cyclic voltammetry (CV) was recorded by taking 1.3 mg (1 mM) of **[Cu(pdc)(H$_2$O)$_2$]** in 5ml aqueous solution containing 0.1 M KCl as a supporting electrolyte. For acid titrations, a stock solution of 1 M acetic acid (AcOH) was prepared. The subsequent CVs were recorded with the addition of AcOH from the 1 M stock solution in the following amounts of 10 µL, 20 µL, 30 µL, up to 300µL.

1.7. Catalyst concentration dependence study

 1 mM stock solution of **[Cu(pdc)(H$_2$O)$_2$]** was prepared by dissolving 1.3 mg **[Cu(pdc)(H$_2$O)$_2$]** crystals in double distilled water. 5 mL solution of 0.1 M KCl in H$_2$O was prepared in an electrochemical cell. CVs were taken from 0.0 to -1.6 V at 100 mV/s. Fixed amount of AcOH (60 mM) was added to the electrochemical cell. The concentration of **[Cu(pdc)(H$_2$O)$_2$]** was varied using 1 mM, 1.5 mM, 2 mM, 2.5 mM and 3 mM and the corresponding CV measurements were taken.

1.8. EPR analysis for 1e reduction of the AcOH treated-[Cu(pdc)(H$_2$O)$_2$] in water-DMF

An equal amount of cobaltocene was added into an AcOH treated**-[Cu(pdc)(H$_2$O)$_2$]** in water-DMF (v/v, 5/95) under a nitrogen atmosphere in a Glove box. The initial blue solution of the acid-treated **[Cu(pdc)(H$_2$O)$_2$]** solution turned out to be a faint brown-colored solution. An aliquot was syringed out and injected into an EPR tube for EPR analysis.

1.9. Theoretical Calculation

All the structures were optimized by Density functional theory (DFT) by using the B3LYP functional[3] and 6-311G(d,p) basic set.[4] The calculation in water (ε =78.3553) medium using IEFPCM solvation methods.[5] Gauss view was used as a visualization tool, and all the analysis was carried out by Gaussian 09.[6] After obtaining the converged geometry, the vibrational harmonic frequencies were calculated at the same theoretical level to ensure that the imaginary frequency number was zero for the stationary point.

B. Figures
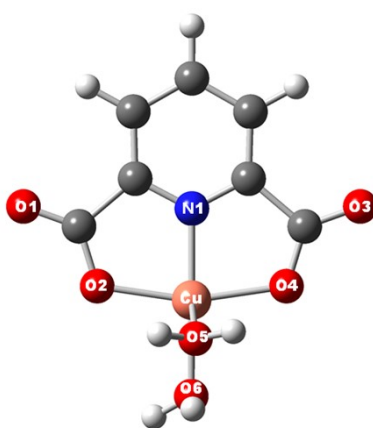
Figure S1: Optimized structure of **[Cu(pdc)(H$_2$O)$_2$]**.
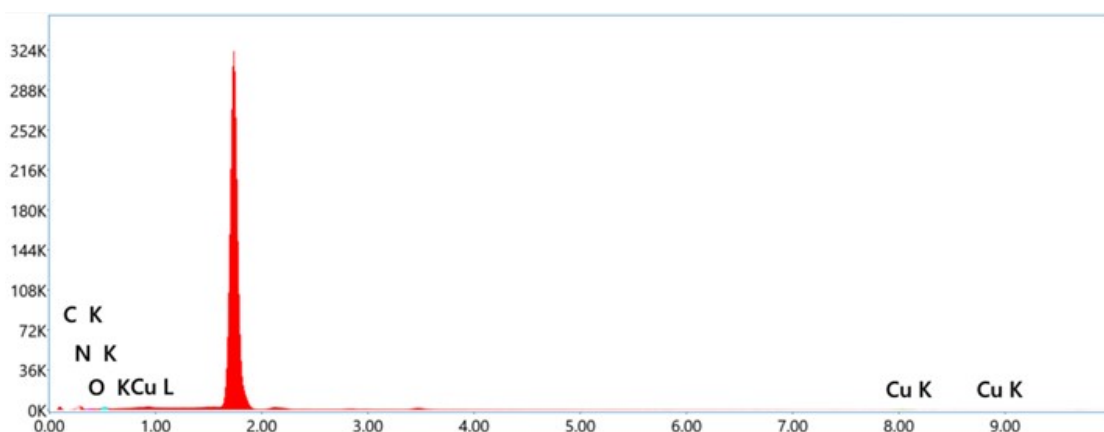
Figure S2: EDX analysis of **[Cu(pdc)(H$_2$O)$_2$]**.
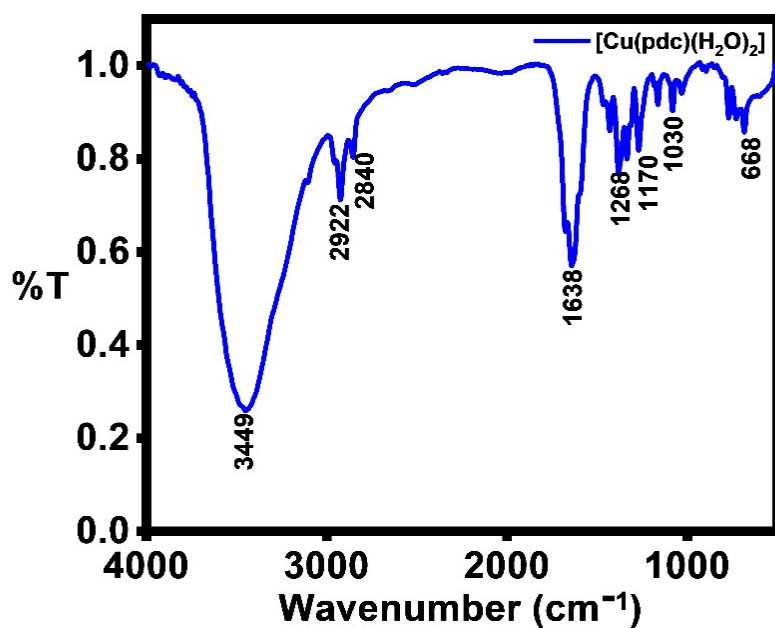
Figure S3: FT-IR spectrum of **[Cu(pdc)(H₂O)₂].**
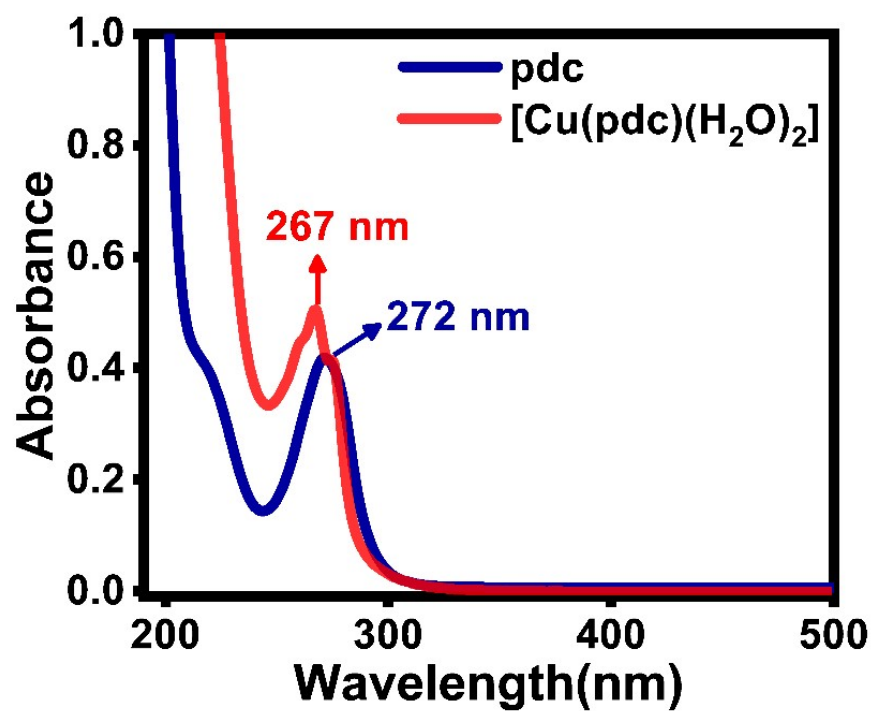
Figure S4: UV-Vis spectra of the ligand **pdc** and **[Cu(pdc)(H₂O)₂]** in water.
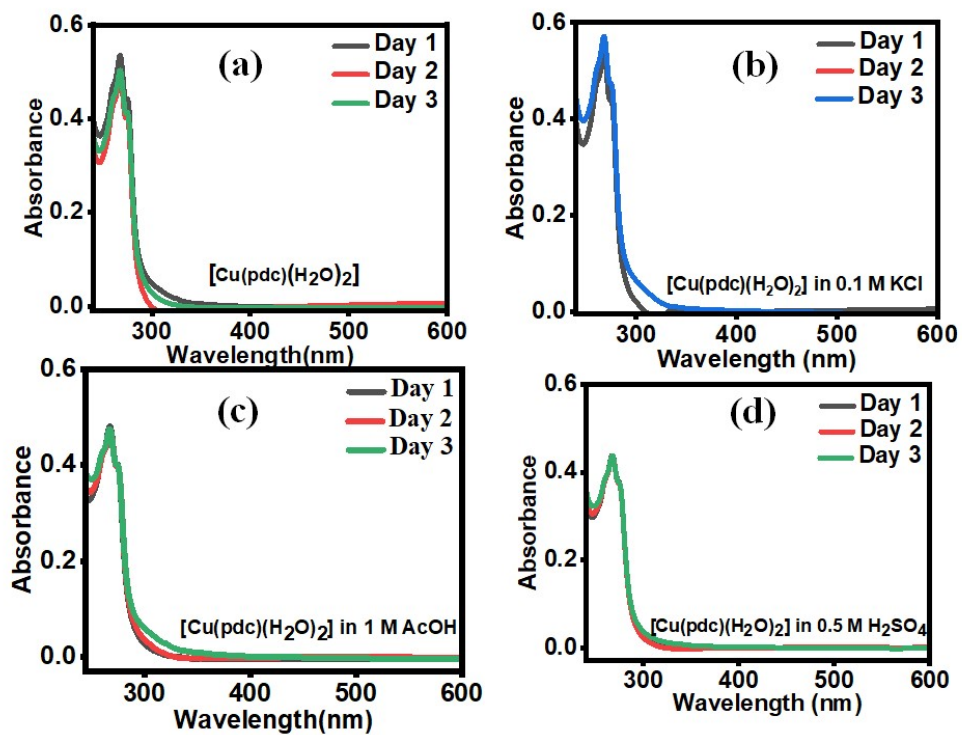
Figure S5: Time dependent UV-Vis spectra of **[Cu(pdc)(H₂O)₂]**; **(a)** in H₂O; **(b)** in aq. 0.1

M KCl; **(c)** in 1 M AcOH; and **(d)** in 0.5 M H₂SO₄.
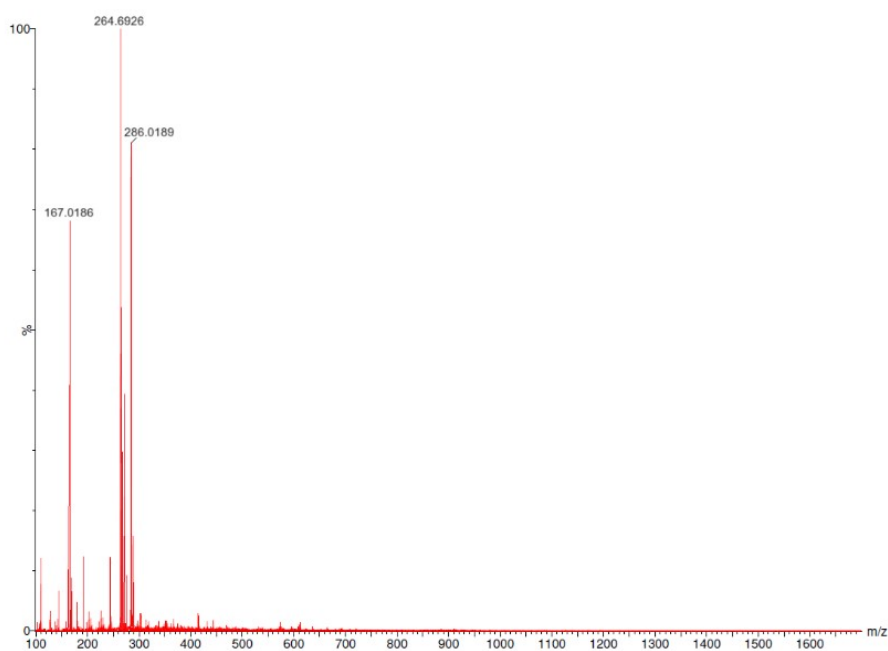
Figure S6: ESI MS spectra of **[Cu(pdc)(H₂O)₂]** in water.
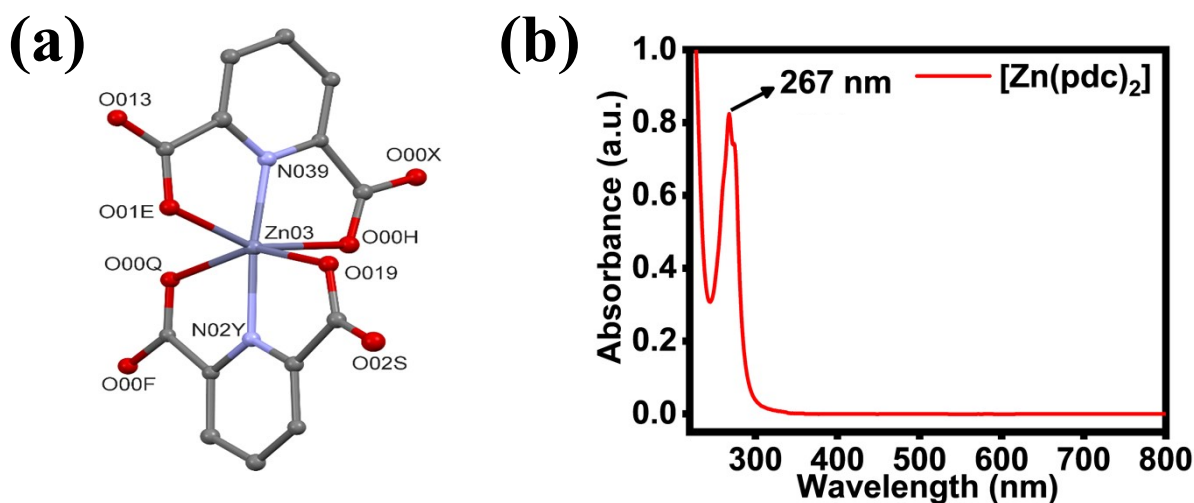
Figure S7: (a) Crystal structure of **[Zn(pdc)₂]** complex; **(b)** UV-Vis spectrum of the ligand

pdc and **[Zn(pdc)₂]** in water.
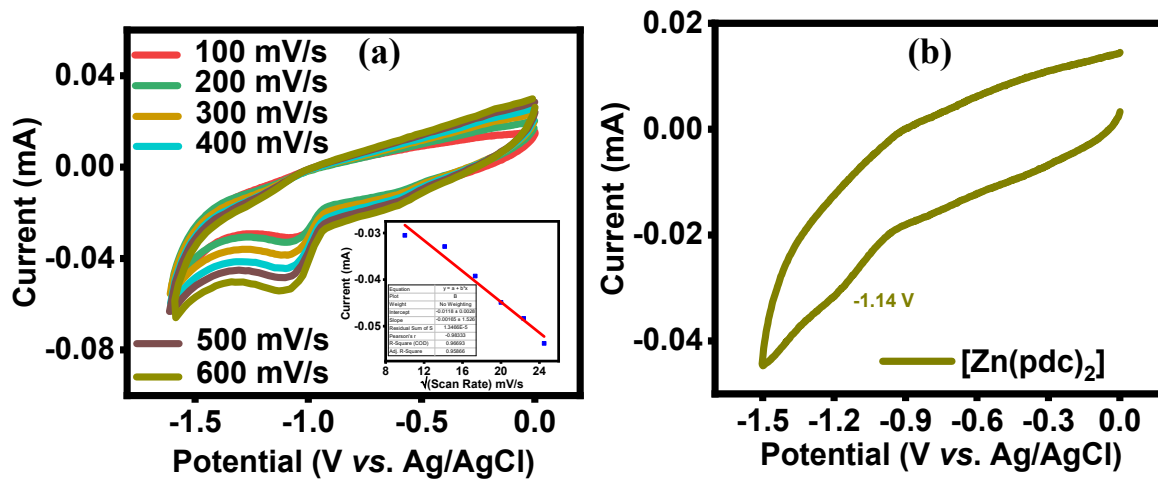
Figure S8: **(a)** CV of **pdc** with various scan rate, 100 mV/s to 600 mV/s recorded in the region

of 0 V to -1.6 V at scan rate of 100 mV/s, inset represents the linear fit of square root of scan

rate vs. peak current obtained from {**Figure S8 (a)**}; **(b)** CV of 1 mM **[Zn(pdc)₂]** complex in

0.1 M aqueous KCl recorded in the region of 0 V to -1.6 V at a scan rate of 100 mV/s.
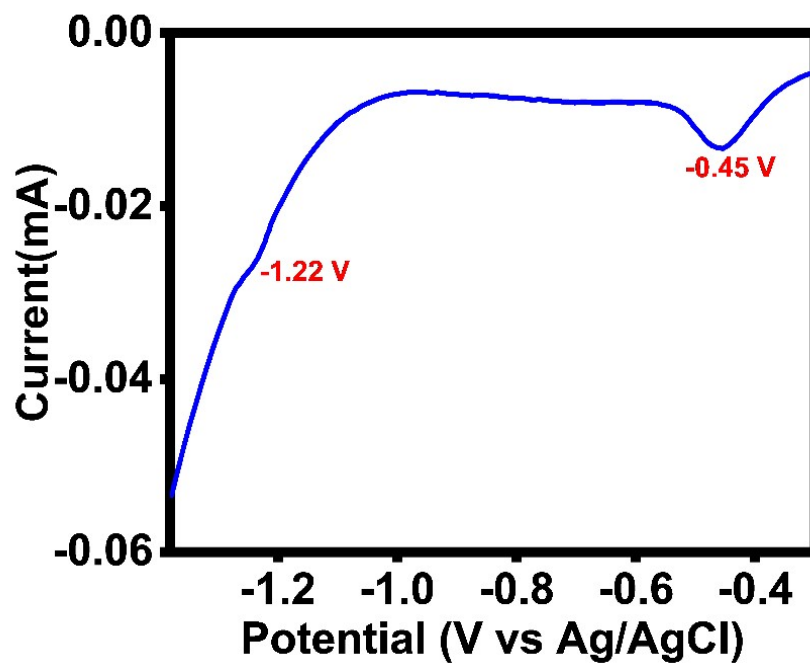
Figure S9: Differential pulse voltammetry (DPV) of **[Cu(pdc)(H₂O)₂],** in 0.1 M aqueous KCl.
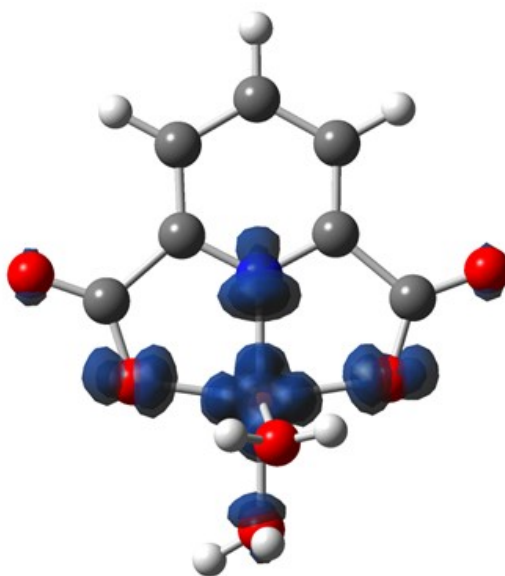
Figure S10: Spin density plot of **[Cu(pdc)(H₂O)₂]** (S=1/2,q=0).
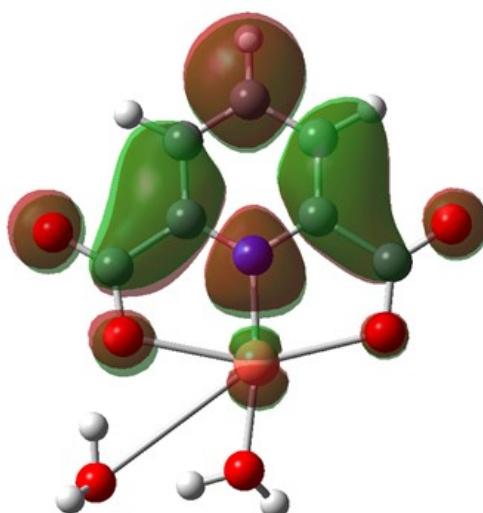
Figure S11: LUMO of singlet-configured reduced **[Cu(pdc)(H₂O)₂].**
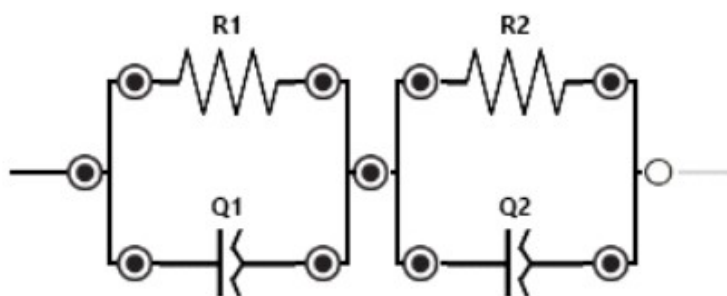
Figure S12: Circuit diagram for impedance spectral study.
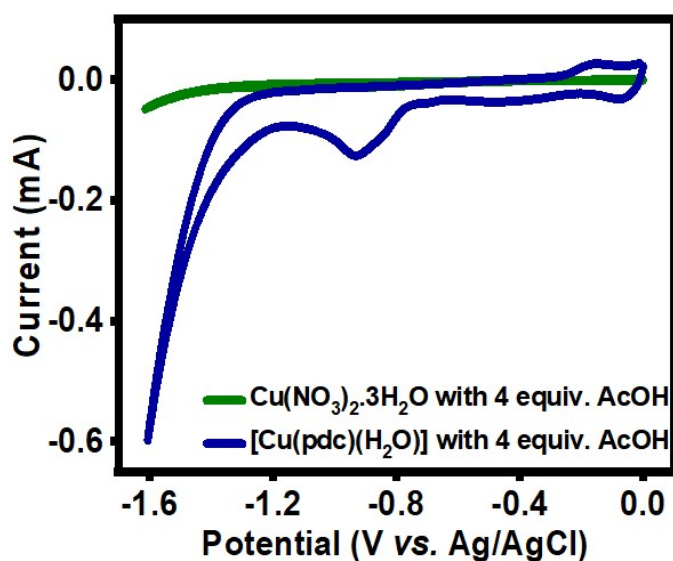
Figure S13: Comparison of CV of **Cu(NO₃)₂.3H₂O** and **[Cu(pdc)(H₂O)₂]** in 0.1 M aqueous KCl with 4 equiv. AcOH addition was recorded in the region of 0 V to -1.6 V at a scan rate of 100 mV/s.
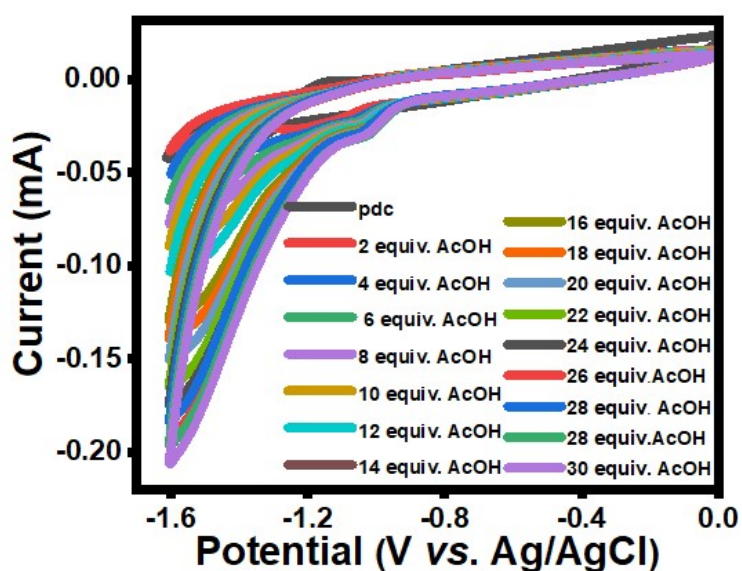
Figure S14: (a) CV of ligand, **pdc** in 0.1 M aqueous KCl with sequential AcOH addition (0-30 equiv.), recorded in the region of 0 V to -1.6 V at a scan rate of 100 mV/s.

Equation	y = a + b*x
Plot	B
Weight	No Weighting
Intercept	-0.12759 ± 0.00327
Slope	-0.00577 ± 8.98182E-5
Residual Sum of Squares	4.6984E-4
Pearson's r	-0.99843
R-Square (COD)	0.99686
Adj. R-Square	0.99662
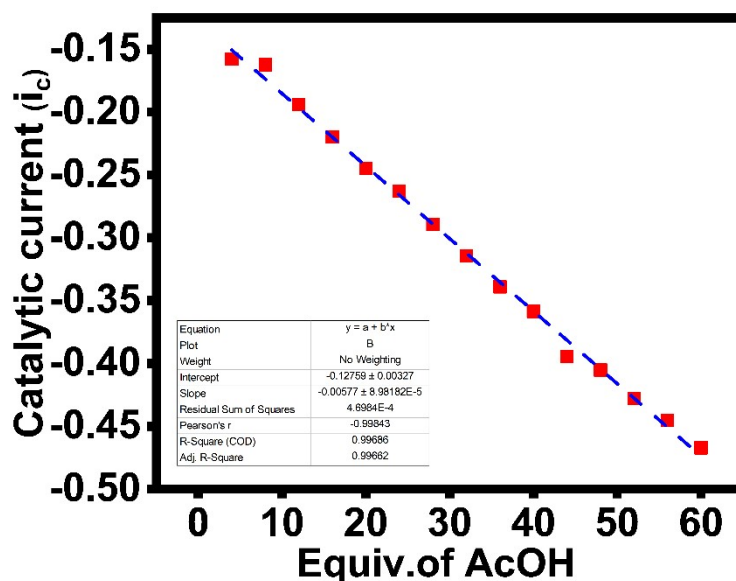
Figure S15: Plot of concentration of AcOH vs. catalytic current obtained from **{Figure 3(b)}.**

(a) legend:
1mM [Cu(pdc)(H$_2$O)$_2$] + 60 eq. AcOH
1.5mM [Cu(pdc)(H$_2$O)$_2$]+ 60 eq. AcOH
2 mM [Cu(pdc)(H$_2$O)$_2$]+60 eq. AcOH
2.5 mM [Cu(pdc)(H$_2$O)$_2$] + 60 eq. AcOH
3 mM [Cu(pdc)(H$_2$O)$_2$] + 60 eq. AcOH

(b) table:

Equation	y = a + b*x
Plot	B
Weight	No Weighting
Intercept	-0.54864 ± 0.0026
Slope	-0.03102 ± 0.0012
Residual Sum of Square	1.1747E-5
Pearson's r	-0.99757
R-Square (COD)	0.99514
Adj. R-Square	0.99352
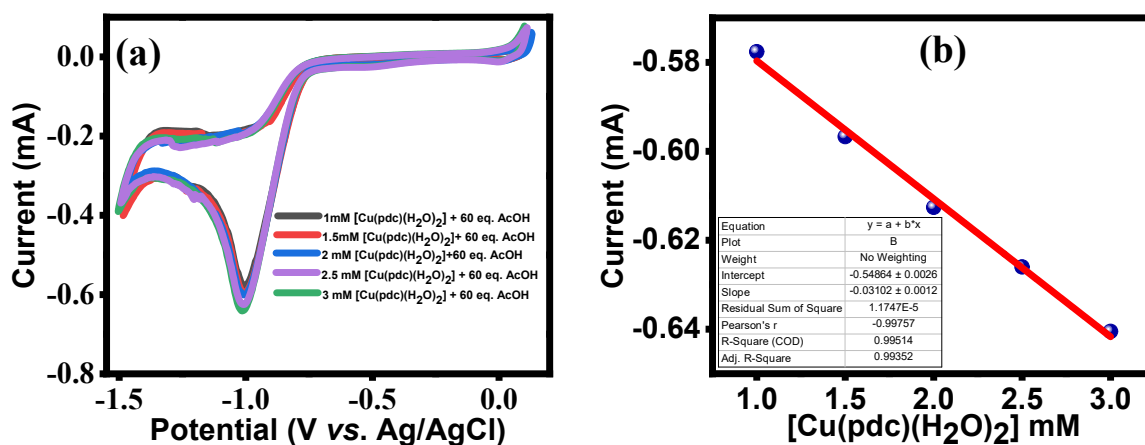
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gure S16: (a) CV of different concentrations of **[Cu(pdc)(H$_2$O)$_2$]** (1 mM to 3 mM) recorded in 0.1 M aqueous KCl with 60 equiv. AcOH addition in the region of 0 V to -1.6 V (V *vs*. Ag/AgCl) at scan rate of 100 mV/s and **(b)** Plot of concentration of **[Cu(pdc)(H$_2$O)$_2$]** *vs*. peak current obtained from {**Figure S16(a)**}.
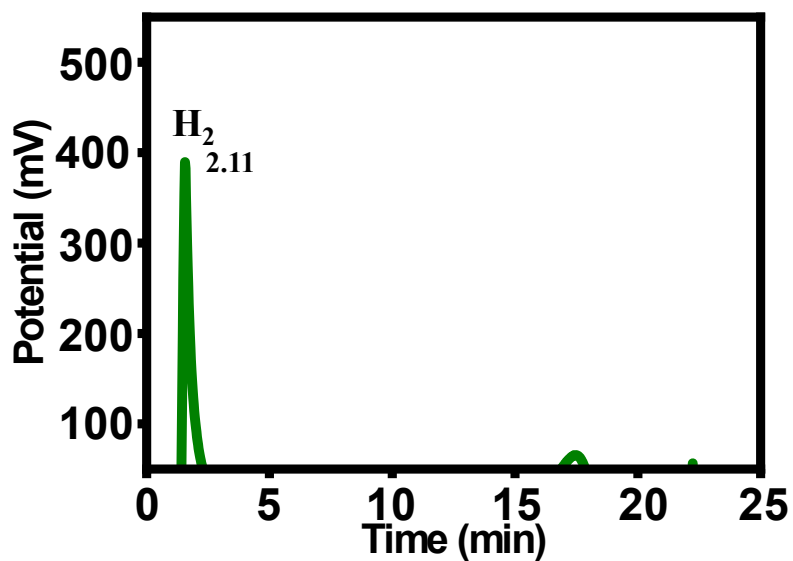
Figure S17: Hydrogen gas detection by gas chromatography (GC).
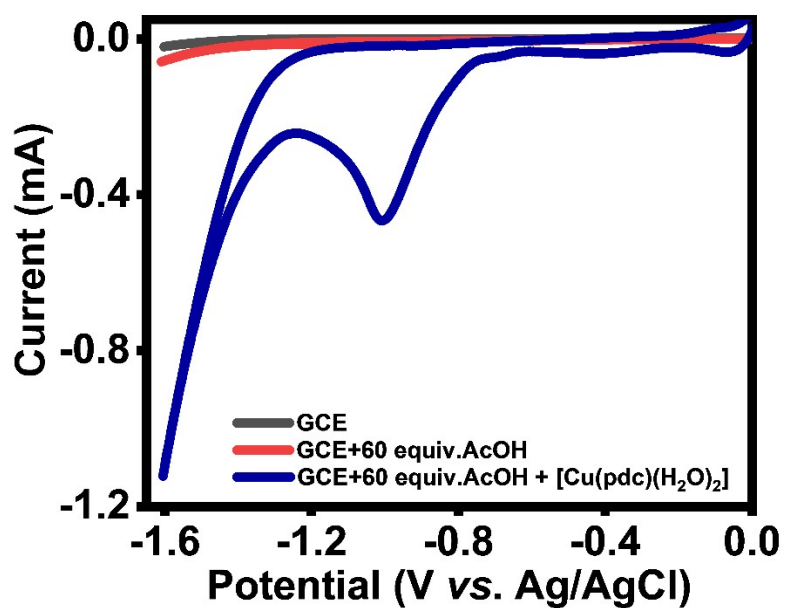
Figure S18: Comparison of CV of bare GCE (black); dipped GCE, rinsed and dipped in 0.1M KCl and 60 equiv. AcOH(red) and dipped GCE with 0.1 M KCl and 1 mM **[Cu(pdc)(H₂O)₂]** in water(blue).
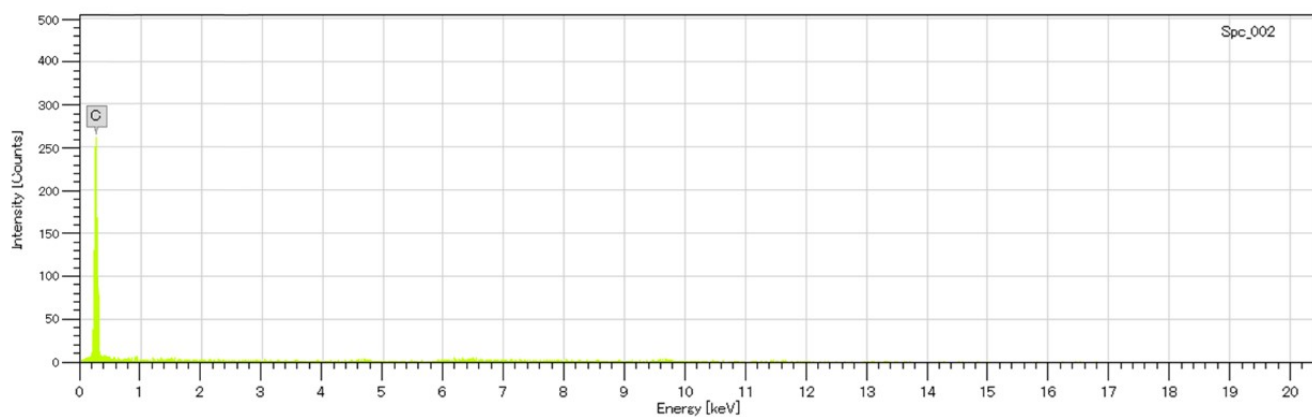
Figure S19: EDX of the electrode-wiped carbon tape after CPE.
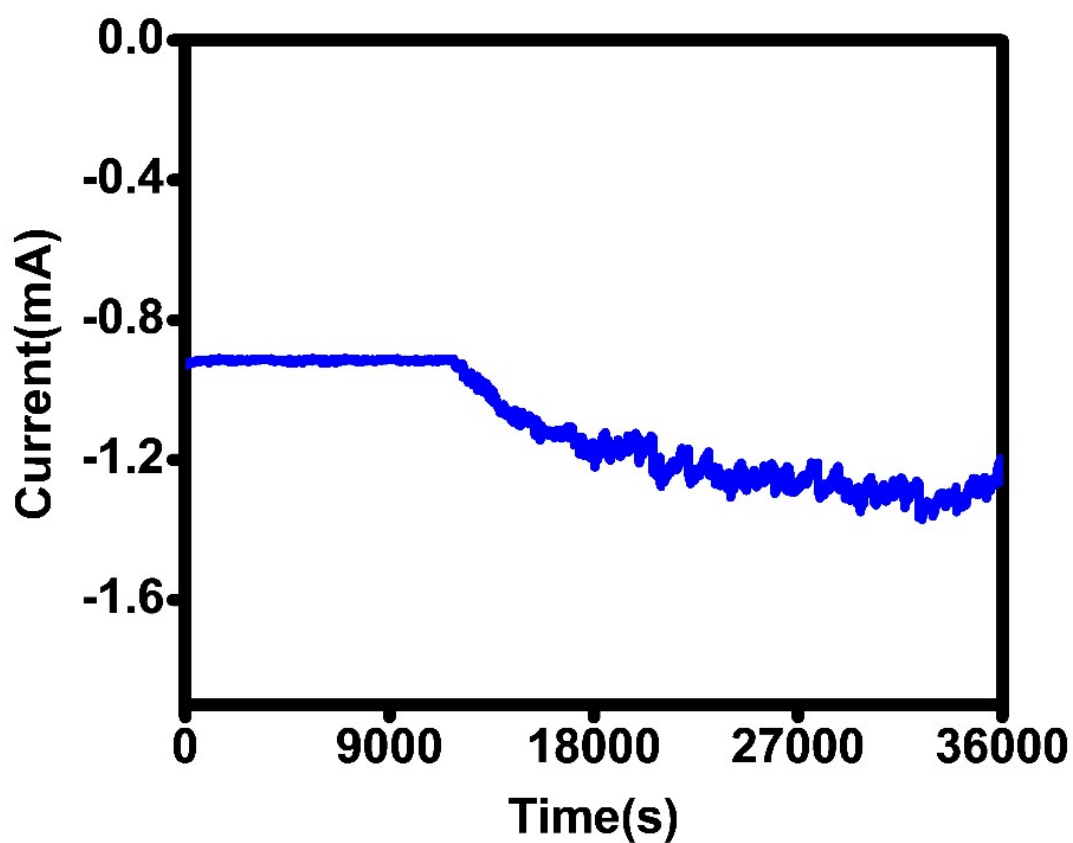
Figure S20: CPE of **[Cu(pdc)(H₂O)₂]** for 10 hours , in 0.1 M aqueous KCl with 60 equiv.

AcOH addition at -1.2 V .
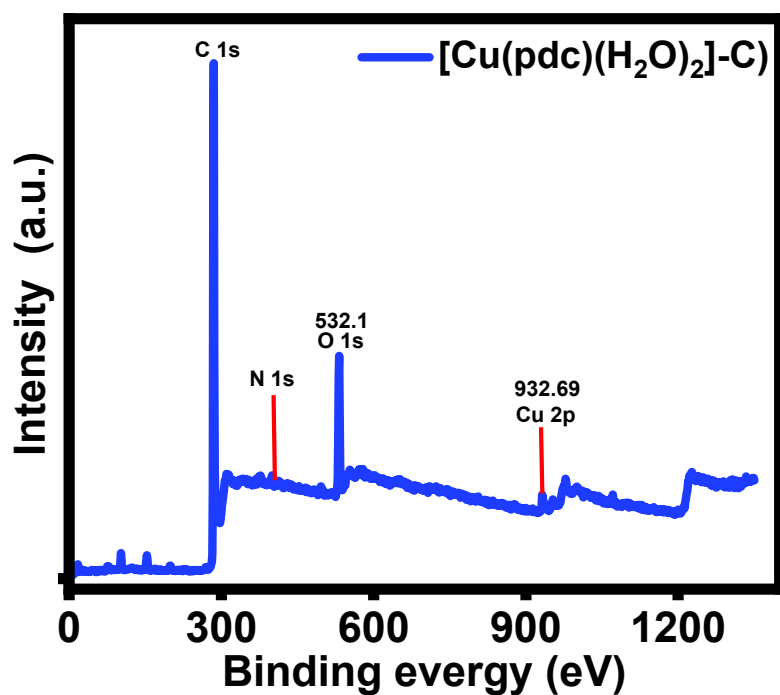
Figure S21: Full XPS spectra of the deposited species after 10 hrs CPE, revealing the presence

of C 1s, N 1s, O 1s and Cu 2p.
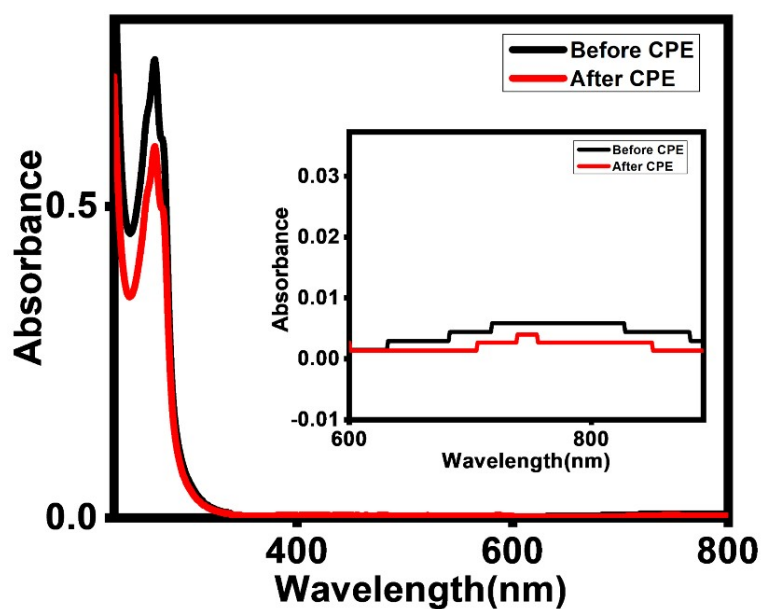
Figure S22:UV-Vis spectra of the **[Cu(pdc)(H$_2$O)$_2$]** before and after CPE (10 hours), Inset:

Comparison of the d-d bands of the **[Cu(pdc)(H$_2$O)$_2$]** before and after CPE.
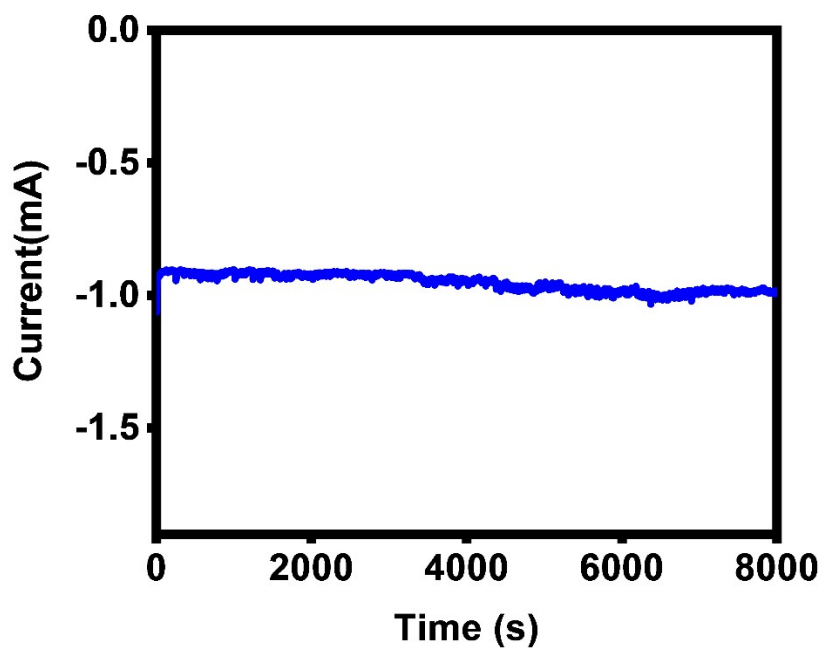
Figure S23: Post CPE durability study, CPE for 3.5 hours using a fresh electrode.
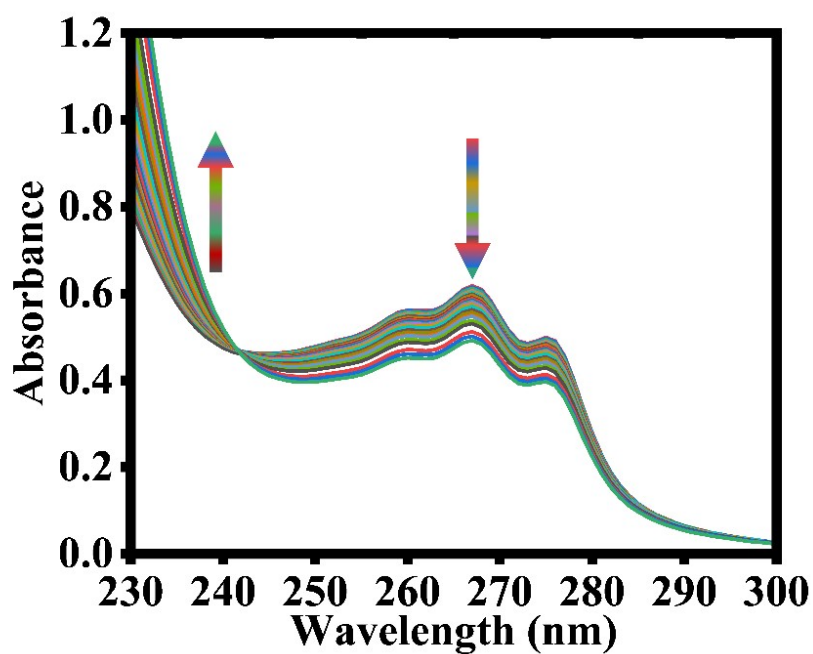
Figure S24: Spectrophotometric titration of **[Cu(pdc)(H$_2$O)$_2$]** in 1 M AcOH in H$_2$O under ambient conditions.
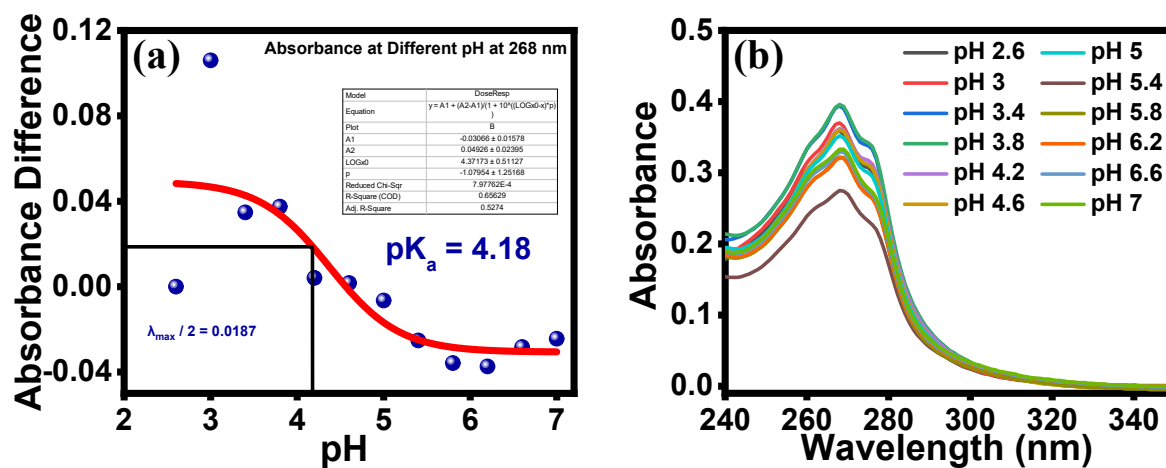
Figure S25: pH-dependent spectrophotometric study for calculation of pKa value in citrate-phosphate buffer in the pH range 2.6 -7.
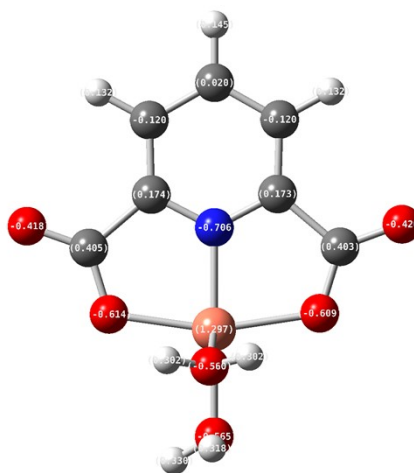
Figure S26: Mulliken charge distribution of **[Cu(pdc)(H₂O)₂].**
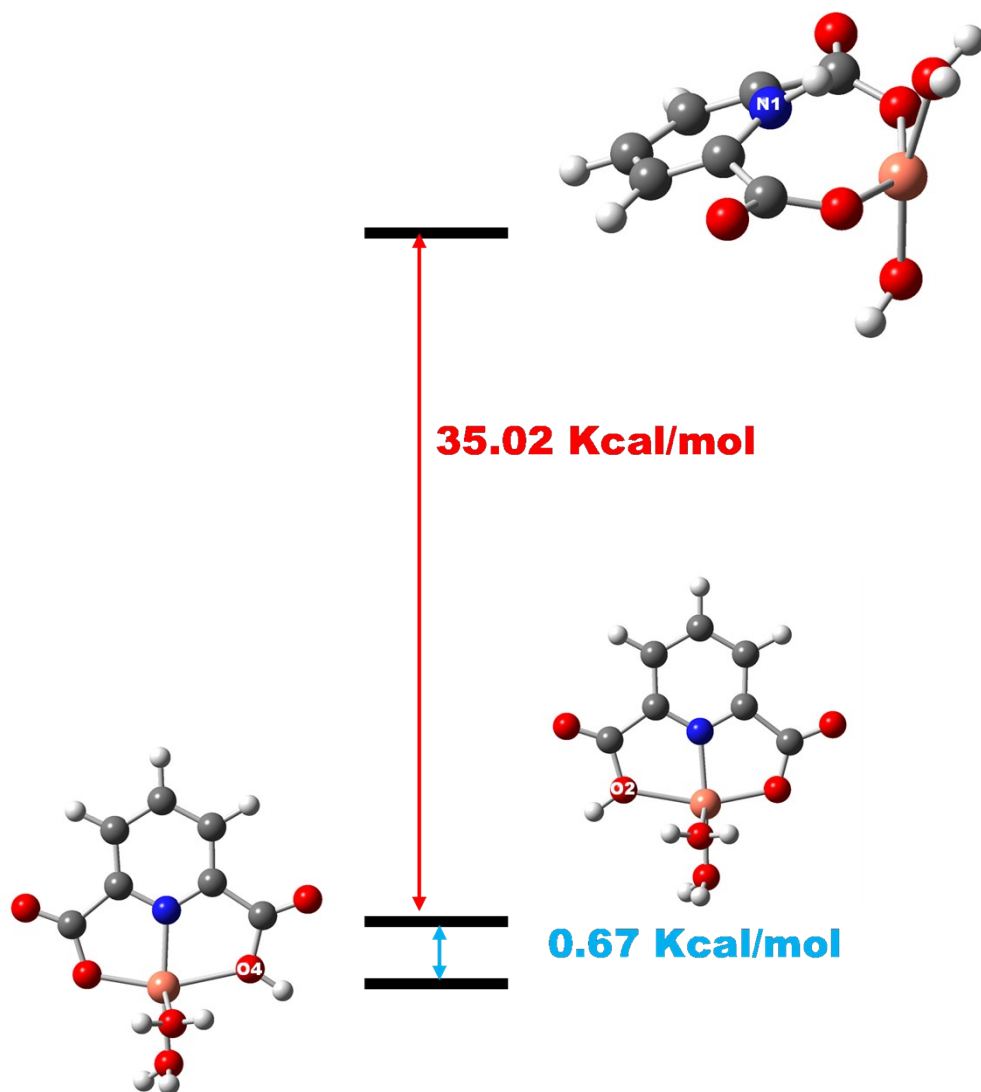
Figure S27: The energy difference between the protonation sites of O(4), O(2), and N(1).
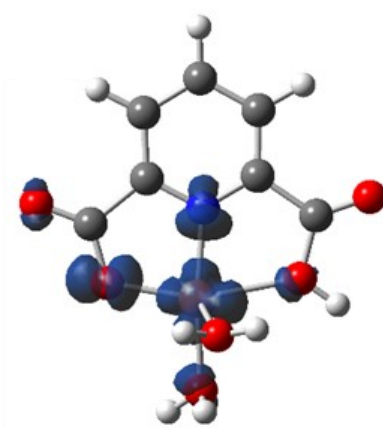
Figure S28: Spin density plot of protonated **[Cu(pdc)(H₂O)₂]** intermediate**(B).**
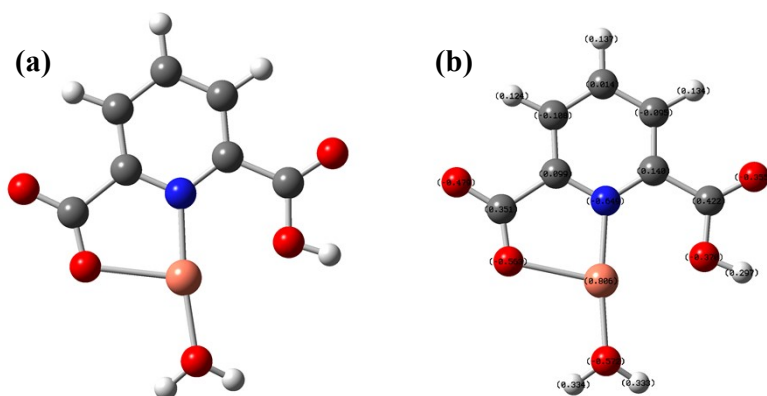
Figure S29:(a) Optimized structure of intermediate **(C), (b)** Mulliken charge distribution of intermediate **(C).**
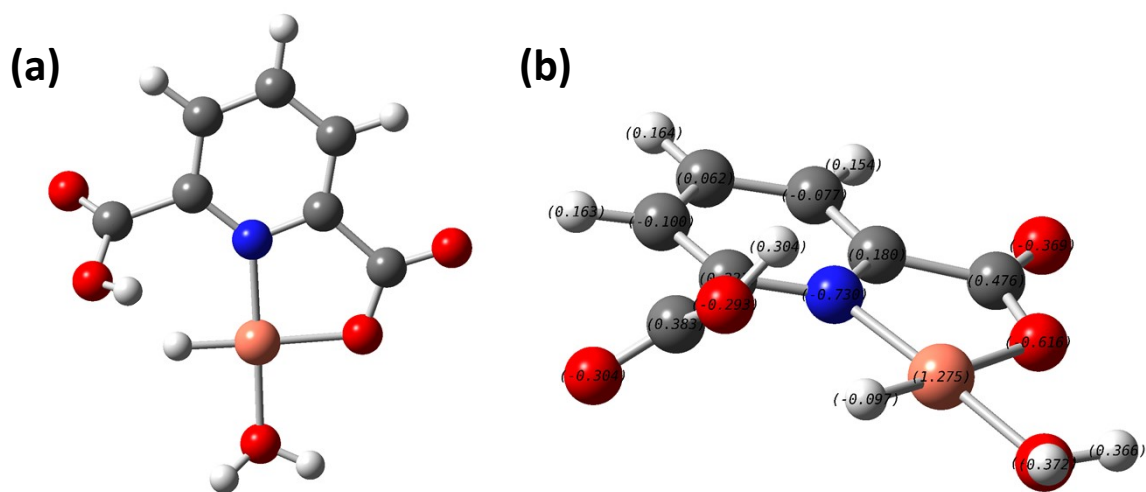
Figure S30: (a) Optimized structure of intermediate **(D); (b)** Mulliken charge distribution of intermediate **(D).**
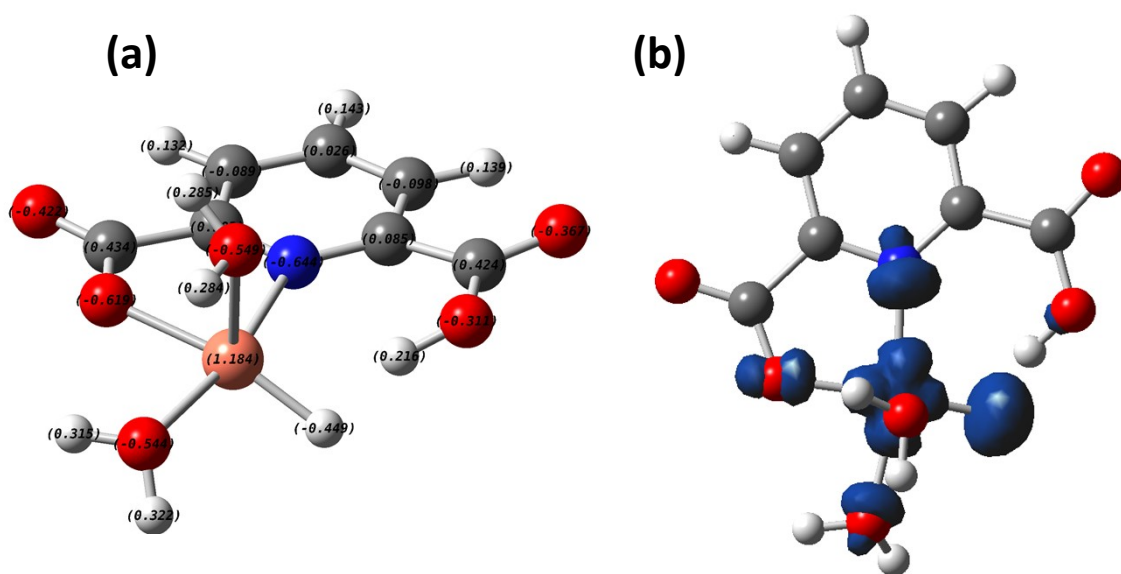
Figure S31: (a) Mulliken charge distribution of intermediate **(E); (b)** Spin density plot of intermediate **(E).**
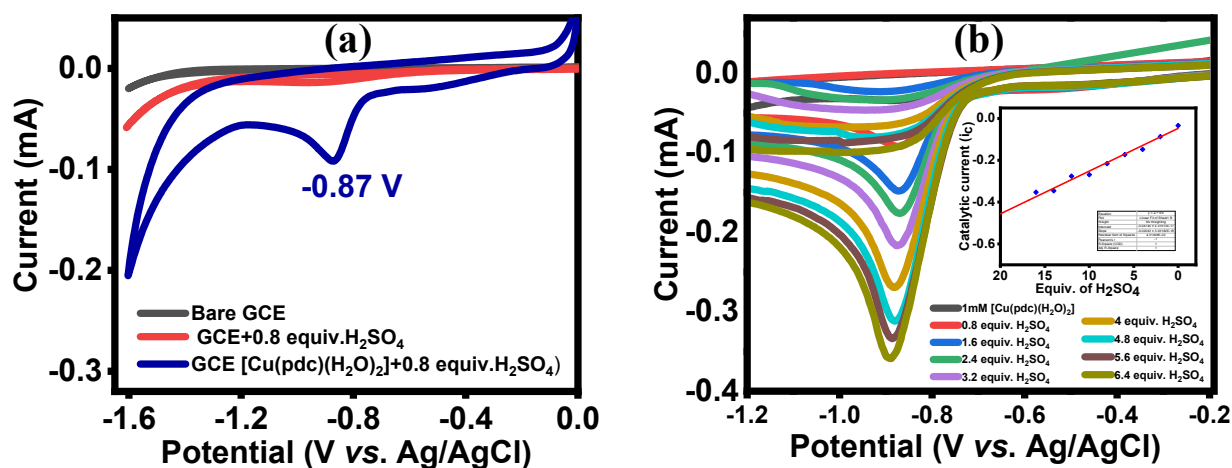
Figure S32: (a) CV comparison of electrolyte solution (blank, grey), electrolyte solution after addition of 0.8 equiv. of H_2SO_4 (red) and **[Cu(pdc)(H₂O)₂]** with addition of 0.8 equiv. of H_2SO_4 addition (blue) recorded; **(b)** CV of **[Cu(pdc)(H₂O)₂]** in 0.1 M aqueous KCl with sequential H_2SO_4 addition (0-6.4 equiv.),inset represents the plot of concentration H_2SO_4 vs. catalytic current obtained from **{Figure S32(a)}.**
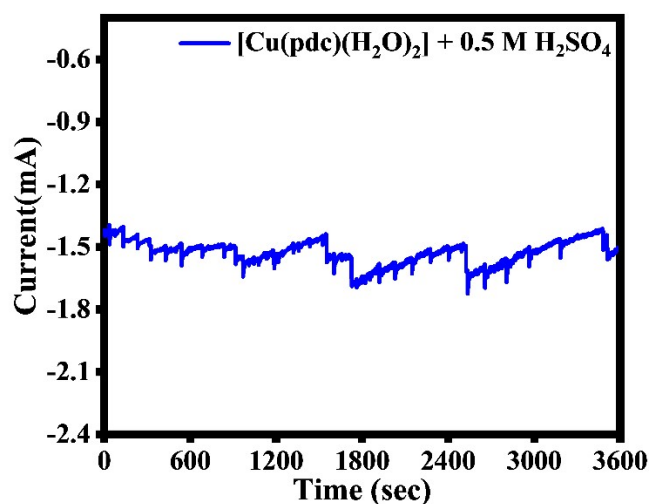
Figure S33: CPE of **[Cu(pdc)(H₂O)₂]** in the presence of 6.4 equiv. H_2SO_4 at constant potential of -1.2 V (V vs. Ag/AgCl) for 1 hour .
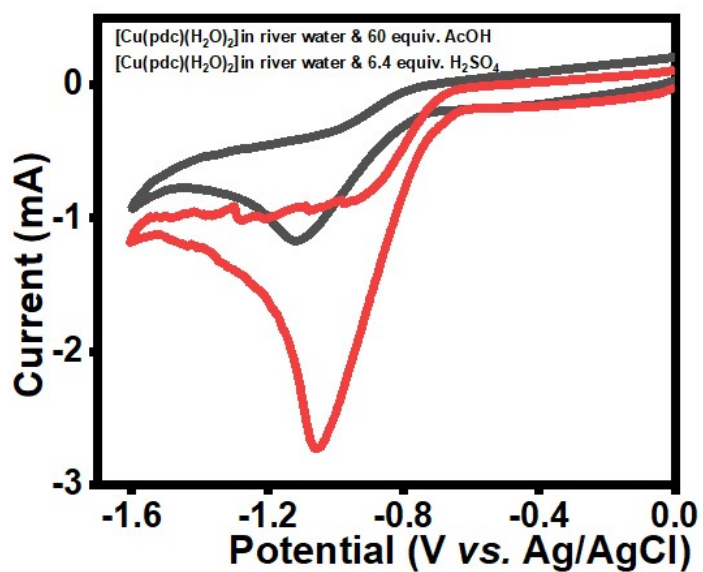
Figure S34: CV of **[Cu(pdc)(H₂O)₂]** in river water with 60 equiv. AcOH addition (black) and

6.4 equiv.), H₂SO₄ addition (red) (recorded in the region of 0 V to -1.6 V (V *vs*. Ag/AgCl) at

scan rate of 100 mV/s.

C. Tables

Table S1. Crystallographic structural parameters of [Cu(pdc)(H₂O)₂]	
Parameters	**[Cu(pdc)(H₂O)₂]**
CCDC	2369860
Empirical formula	$C_7H_7NO_6Cu$
Formula weight	264.68
T (K)	293K
Wavelength (Å)	1.54184
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit Cell Dimensions	0.24 x 0.26 x 0.28
a (Å)	4.6917(3)
b (Å)	8.9149(5)
c (Å)	10.3084(5)
α (°)	80.248(4)
β (°)	85.172(4)
γ (°)	83.783(4)
V (Å³)	421.48(4)
Z	2
ρ (g cm⁻³)	2.086
Absorption coefficient (mm⁻¹)	3.844
F(000)	266
Theta range for data collection	4.4 to 79.9
Index ranges (h, k, l)	$-5 \leq h \leq 5$, $-9 \leq k \leq 11$, $-10 \leq l \leq 13$
Reflections collected	7212
Independent reflections	1772
R(int)	0.031
Final R indices [I>2sigma(I)]	$R_1 = 0.0305$, $wR_2 = 0.0820$

Table S2. Selected bond distances (Å) and angles (°) of [Cu(pdc)(H₂O)₂]:

	Exp.	DFT		Exp.	DFT
Cu(1) − O(2)	2.0099(15)	1.98	∠O(2) − Cu(1) − N(1)	80.51(6)	81.70
Cu(1) − O(4)	2.01(15)	1.99	∠O(4) − Cu(1) − O(5)	96.64(6)	91.06
Cu(1) − O(5)	2.1508(15)	2.39	∠O(4) − Cu(1) − O(6)	97.15(6)	98.56
Cu(1) − O(6)	1.9770(15)	1.99	∠O(4) − Cu(1) − N(1)	80.36(6)	81.47
Cu(1) − N(1)	1.9161(17)	1.89	∠O(5) − Cu(1) − O(6)	92.79(6)	74.28
∠O(2) − Cu(1) − O(4)	160.45(6)	163.08	∠O(5) − Cu(1) − N(1)	108.97(6)	110.80
∠O(2) − Cu(1) − O(5)	93.37(6)	96.48	∠O(6) − Cu(1) − N(1)	158.23(6)	174.91
∠O(2) − Cu(1) − O(6)	99.10(6)	98.04	∠Cu(1) − O(2) − C(1)	114.94(12)	115.42
∠Cu(1) − O(5) − H(5A)	110	120.11	∠Cu(1) − O(4) − C(7)	115.20(12)	115.40
∠Cu(1) − O(5) − H(5B)	111(2)	120.04	∠Cu(1) − N(1) − C(2)	118.31(13)	117.62
∠Cu(1) − O(6) − H(6B)	115(3)	122.04	∠Cu(1) − N(1) − C(6)	118.60(13)	117.87
∠Cu(1) − O(6) − H(6A)	109.00	120.11			

Table S3. Hydrogen bond lengths (Å) and angles (°) for [Cu(pdc)(H₂O)₂]:

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry
O(5)– H(5A)···O(3)	0.85	1.85	2.703(2)	178	2-x,1-y,2-z
O(5)– H(5B)···O(4)	0.82(3)	2.00(3)	2.751(2)	152(3)	-1+x,y,z
O(6)–H(6A)···O(1)	0.85	1.92	2.731(2)	160	1-x,1-y,1-z
O(6)–H(6B)···O(2)	0.75(3)	2.29(3)	2.925(2)	144(3)	1+x,y,z
O(6)–H(6B)···O(2)	0.75(3)	2.39(3)	3.026(2)	143(3)	2-x,1-y,1-z
C(3)–H(3)···O(1)	0.93	2.38	3.299(2)	169	-x,2-y,1-z
C(5)–H(5)···O(3)	0.93	2.41	3.310(2)	162	2-x,2-y,2-z

Table S4. Electrochemical experimental results from a typical AcOH titration of [Cu(pdc)(H₂O)₂] obtained using (Equation S3):

[Cu(pdc)(H₂O)₂] (mM)	AcOH (eq)	i_c (mA)	i_p (mA)	$i_{cat}i_p$	Scan rate ($\vartheta,mV/s$)	k_{obs} (s⁻¹)
1	4	-0.15783	-0.03414	4.623023	100	9.28
1	8	-0.11624	-0.03414	3.404804	100	9.83
1	12	-0.1941	-0.03414	5.685413	100	14.04
1	16	-0.2198	-0.03414	6.438196	100	18.7
1	20	-0.24498	-0.03414	7.175747	100	22.37
1	24	-0.26299	-0.03414	7.703281	100	25.78
1	28	-0.28933	-0.03414	8.47481	100	31.2
1	32	-0.31439	-0.03414	9.208846	100	36.84

1	36	-0.339053	-0.03414	9.931254	100	42.85
1	40	-0.358688	-0.03414	10.50639	100	47.96
1	44	-0.39474	-0.03414	11.56239	100	58.09
1	48	-0.40528	-0.03414	11.87112	100	61.23
1	52	-0.42791	-0.03414	12.53398	100	68.26
1	56	-0.44915	-0.03414	13.15612	100	73.87
1	60	-0.46724	-0.03414	13.686	100	81.38

D. Calculations:

1. **Determination of the diffusion coefficient (D) of [Cu(pdc)(H$_2$O)$_2$] in 0.1 M KCl aqueous solution:**

The Diffusion Coefficient (D) was derived from the theoretical slope using the equation below-

$$Slope = [0.4463nFAC^0\left(\frac{nFD}{RT}\right)^{\frac{1}{2}}] \ldots\ldots\ldots\ldots \textbf{(Equation S1)}$$

$$D = \left(\frac{slope}{0.4463\ n\ FA\ C^0}\right)^2\frac{RT}{nF} \ldots\ldots\ldots\ldots\ldots\ldots \textbf{(Equation S2)}$$

Slope = -0.00215

Area of the glassy carbon electrode (A) =0.071 cm^2

Concentration of the analyte (C) = 1 × 10^{-3} moles

Faraday constant (F) = 96485 C/mole

R = ideal gas constant, and T = 298 K

$$\textbf{D = 5.7 x10}^{-4}\textbf{ cm}^2\textbf{ s}^{-1}$$

2. **Calculation of net charge based on Control potential Electrolysis (CPE) in aqueous 0.1M KCl solution:**

Total charge = $Q_{with\ cat} - Q_{blank} = Q_{net}$

=10.6056 C – 0.046 C = 10.5596

3. **Calculation of theoretical moles of hydrogen made via total charge**
    a) Moles of Hydrogen produced using AcOH:

Moles of H_2 produced(theoretical) =10.6056 $\times$ (1 mol e⁻ /96485 C) x (1 mol H_2 /2 mol e⁻)

= **5.5×10⁻⁵** moles H_2 based on the charge from electrolysis.

    b) Moles of Hydrogen produced using H_2SO_4:

Moles of H_2 produced(theoretical) = 17.06 $\times$ (1 mol e⁻ / 96485 C) x (1 mol H_2 / 2 mol e⁻)

= **8.819×10⁻⁵** moles H_2 based on the charge from electrolysis.

4. **Calculation of the catalytic turnover frequency (TOF):**

Assuming two electrons are passed for each H_2 molecule produced (n=2), and the acid concentration does not change significantly during the measurement, the catalytic turnover frequency (k_{obs}) can be calculated using (**Equation S3**)

$$\frac{i_{cat}}{i_p} = \frac{n}{0.4463}\sqrt{\frac{RTKobs}{Fv}}$$ …………………..(**Equation S3**)

E. Co-ordinates of the intermediates and the adduct involved in the mechanistic cycle of [Cu(pdc)(H₂O)₂] catalyzed HER

A

Cu 4.882   6.237   7.263

O 1.843   7.764   5.15

O 3.44   6.383   5.871

O 6.833   8.491   9.954

O 6.248   6.768   8.639

O 3.679   5.019   8.565

H 4.182   4.62   9.128

H 3.047   5.449   8.859

O 5.855   4.674   6.541

H 5.333   4.218   6.049

H 6.47   4.836   6.143

N 4.397   8.074   7.504

C 2.844   7.519   5.827

C 3.44   8.582   6.728

C 3.1   9.924   6.829

H 2.428   10.288   6.3

C 3.798   10.713   7.749

H 3.594   11.616   7.833

C 4.8   10.151   8.542

H 5.27   10.666   9.158

C 5.073   8.799   8.383

C 6.145   7.979   9.077

B

Cu 4.882   6.237   7.263

O 1.843   7.764   5.15

O 3.44   6.383   5.871

O 7.00749   8.4998   9.84905

O 6.248   6.768   8.639

O 3.679   5.019   8.565

H 4.182   4.62   9.128

H 3.047   5.449   8.859

O 5.855   4.674   6.541

H 5.333   4.218   6.049

H 6.47   4.836   6.143

N 4.397   8.074   7.504

C 2.844   7.519   5.827

C 3.44   8.582   6.728

C 3.1   9.924   6.829

H 2.428   10.288   6.3

C 3.798   10.713   7.749

H 3.594   11.616   7.833

C 4.8   10.151   8.542

H 5.27   10.666   9.158

C 5.073   8.799   8.383

C 6.18056   7.96642   9.11672

H 6.86197   6.29223   9.20317

C

Cu -0.81694   -0.9274   0.02515

O -1.30757   3.24281   -0.06654

O -1.93323   1.08443   0.11658

O 3.43001   -2.00547   -0.01683

O 1.21524   -2.38135   -0.00538

O -2.35164   -2.07319   0.05074

H -3.18068   -1.53004   -0.03602

H -2.42271   -2.81381   -0.55833

N 0.66959   0.26386   0.01034

C -1.09421   2.02693   0.01844

C 0.38653   1.58393   0.0098

C 1.3975   2.5434   -0.00416

H 1.10699   3.58439   -0.00938

C 2.72794   2.14686   -0.01223

H 3.52587   2.87899   -0.01986

C 3.01708   0.78703   -0.01254

H 4.03225   0.4161   -0.0212

C 1.96447 -0.12217 -0.0031

C 2.29773 -1.58346 -0.00906

H 1.52283 -3.30214 -0.00939

D

Cu 0.88951 -1.07059   0.01906

O 2.68205   2.33328   0.03806

O 2.25945   0.15608   0.17531

O -3.56699 -1.14091   0.02118

O -1.5301   -2.2684   0.10981

O 2.05978 -2.4774   0.03505

H 2.84266 -2.23672   0.53582

H 1.64008 -3.23815   0.44335

N -0.27754   0.38177 -0.02453

C 1.8811   1.3629   0.0584

C 0.36035   1.53284 -0.04544

C -0.315   2.75035 -0.1416

H 0.21987   3.6761   -0.18396

C -1.71476   2.72287 -0.17685

H -2.2749   3.6316   -0.24999

C -2.37198   1.48129 -0.11241

H -3.44096   1.43603 -0.12373

C -1.61327   0.29887 -0.03481

C -2.3105   -1.07257   0.03314

H -1.02272 -2.26769   0.92477

H -0.21592 -2.02683 -0.13754

E

Cu -1.26288 -0.62077 -0.39561

O -1.19088 3.28452 0.2495

O -1.89341 1.1598   0.07067

O 3.29385 -2.1239   0.15377

O 1.15506 -2.61159 -0.07395

O -3.2656 -1.0646 -0.62265

H -3.78368 -0.25056 -0.56832

H -3.57854 -1.54105 -1.40039

N 0.60739 0.23457 -0.08971

C -0.9996   2.08132 0.10803

C 0.43501 1.57076 -0.01679

C 1.50208 2.4611 -0.00733

H 1.2875   3.51902 0.05186

C 2.79528 1.96255 -0.06846

H 3.64905 2.62867 -0.07587

C 2.97497 0.58573 -0.09254

H 3.95831 0.13905 -0.09589

C 1.86337 -0.25632 -0.09461

C 2.15327 -1.74729 -0.01172

H 0.2839 -2.21717 -0.39007

H -0.84046 -1.90578 -1.13256

O -1.67857 -1.34874 1.80095

H -2.57265 -1.70892 1.76445

H -1.74157 -0.61411 2.42166

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