Electronic Supplementary Information

An electrocatalytic hydrogen production activity with a copper(II) complex supported by dipyridylamine ligand in acidic water

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A. Experimental

Physical measurements

FT-IR spectra of **$[Cu(dpa)_2(N_3)]Cl\cdot 4H_2O$** were recorded using an FTIR-8400S SHIMADZU spectrometer in the 400-3600 cm^{-1} range. Steady-state absorption spectral data of **$[Cu(dpa)_2(N_3)]Cl\cdot 4H_2O$** 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 **$[Cu(dpa)_2(N_3)]Cl\cdot 4H_2O$** were determined by powder X-ray diffractometer (Rigaku SmartLab) using Cu-K_α radiation ranging from 10°-80°. An RVL PG-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.

HER by $[Cu(dpa)_2(N_3)]^+$

To investigate the hydrogen evolution activity, CV was recorded by taking 11.1 mg (1 mM) of **$[Cu(dpa)_2(N_3)]^+$** in 0.1 M KCl, a supporting electrolyte in 20 ml aqueous solution. The 1 M acetic acid (AcOH) in a 10 ml volumetric flask was prepared as a stock solution to monitor the acid titration. The subsequent CVs were recorded with the addition of AcOH from the 0.1 M stock solution in the following amounts of 100 µL, 200 µL, 300 µL, 400 µL and so on. The pH of the solution of 1 mM **$[Cu(dpa)_2(N_3)]^+$** in 0.1 M KCl was 6.20, recorded using Eutech pH 700 meter. In the same solution, with the addition of 14 mM AcOH and 18 mM AcOH, the pH was 3.56 and 3.17, respectively.

Catalyst concentration dependence study

A 0.1 M stock solution of **$[Cu(dpa)_2(N_3)]^+$** was prepared by dissolving 0.555 g **$[Cu(dpa)_2(N_3)]Cl\cdot 4H_2O$** crystals with H_2O in a 10 mL volumetric flask. A 20 mL solution of 0.1 M KCl in H_2O was prepared in an electrochemical cell. 14 mM AcOH was added to the cell and

purged with nitrogen. CVs were taken from 0.0 to -1.6 V at 100 mV/s with the addition of 50 µL, 100 µL, 150 µL, 200 µL, and 250 µL of the **$[Cu(dpa)_2(N_3)]^+$**stock solution.

DFT study

All the structures were optimized by Density functional theory (DFT) by using the B3LYP functional[1] and 6-311g(d,p) basic set. The calculation in water (**ε** =78.3553) medium using IEFPCM solvation methods. Gauss view was used as a visualization tool, and all the analysis was carried out by Gaussian 16.[2] 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

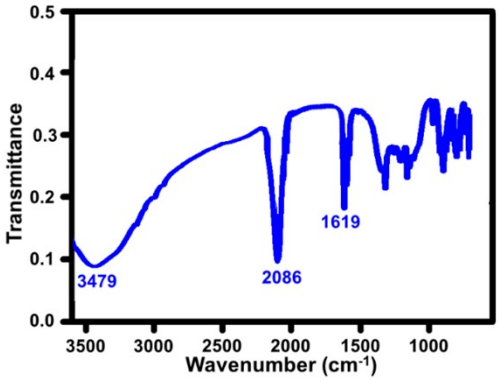

Figure S1. FT-IR spectra of **$[Cu(dpa)_2(N_3)]Cl{\cdot}4H_2O$.**

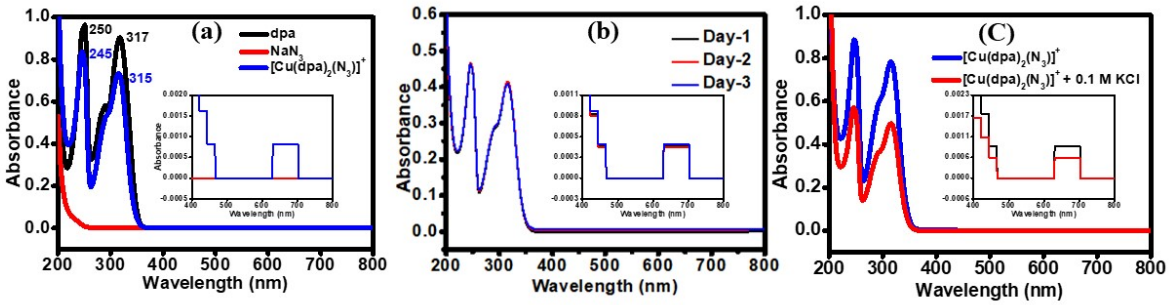

Figure S2. (a) UV-Vis spectra of **$[Cu(dpa)_2(N_3)]^+$** in water; **(b)** UV-Vis spectra of **$[Cu(dpa)_2(N_3)]^+$** in water for stability test over 3 days; **(c)** UV-Vis spectra of **$[Cu(dpa)_2(N_3)]^+$** in water and the presence of 0.1 M KCl in water media.

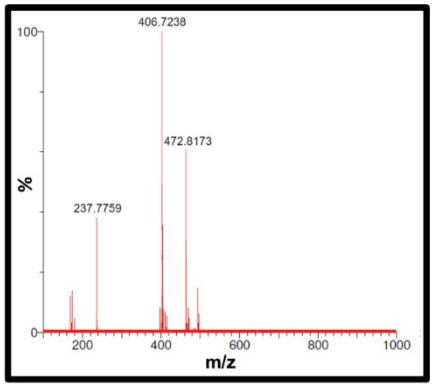

Figure S3. ESI-MS of **$[Cu(dpa)_2(N_3)]^+$** in water.

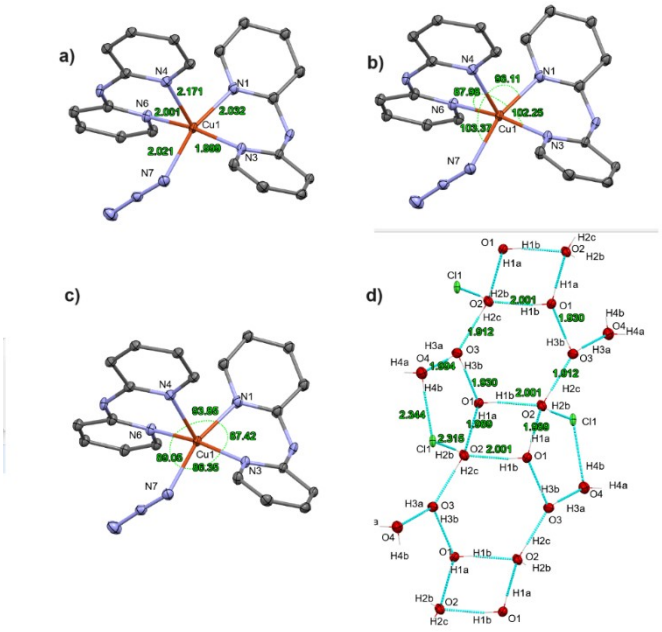

Figure S4. Structural validity of the copper complex with crystallographic bond distance and bond angle measurement.

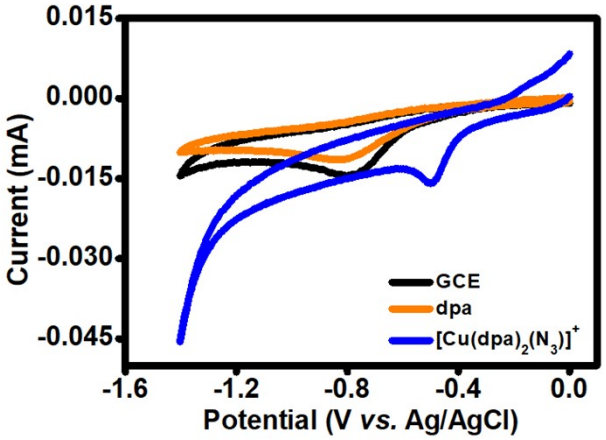

Figure S5. CVs of GCE (**black**), dpa (**orange**), and (**blue**) $[Cu(dpa)_2(N_3)]^+$. Peak around -0.8 V vs. Ag/AgCl is due to dissolved O_2**.**

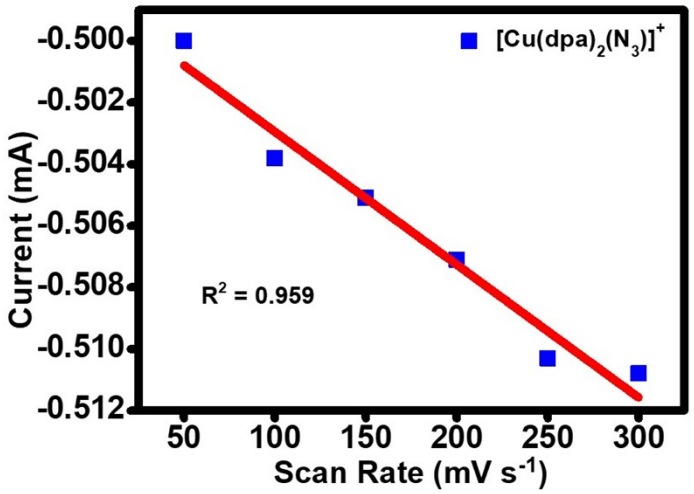

Figure S6. Plot of current *vs*. scan rate of **$[Cu(dpa)_2(N_3)]^+$.**

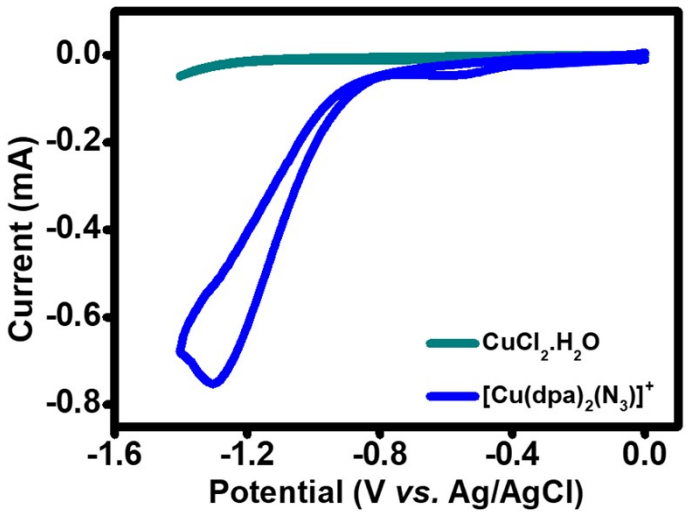

Figure S7. Comparison of CV of $CuCl_2.2H_2O$ salt and **$[Cu(dpa)_2(N_3)]^+$** with addition of 14 mM AcOH.

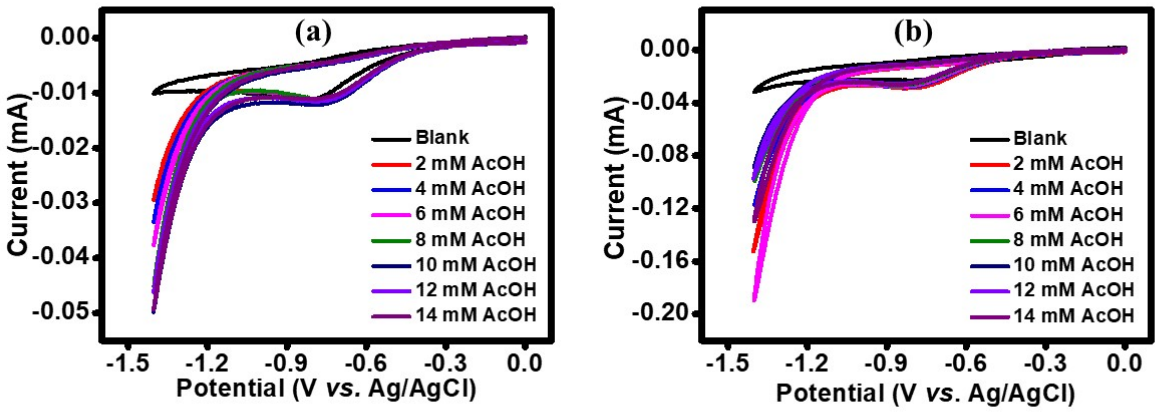

Figure S8. (a) dpa titration with AcOH in 0.1 M KCl; **(b)** only 0.1 M KCl titration with AcOH. (the appearance of a peak at around -0.8V (V vs. Ag/AgCl) is due to the presence of oxygen.)

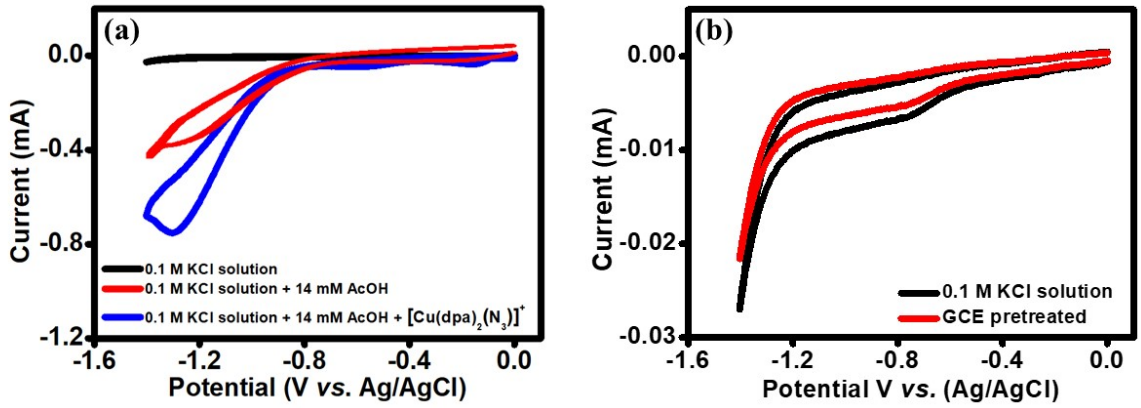

Figure S9. (**a).** CVs run in 0.1 M KCl as an electrolyte in aqueous solution (black), in the presence of 14 mM AcOH (red) and the presence of **$[Cu(dpa)_2(N_3)]^+$** with 14 mM AcOH (blue). **(b)** CVs were recorded in an electrolyte-only solution using a freshly polished GCE (black trace) and an electrode after CPE in a solution of 1mM **$[Cu(dpa)_2(N_3)]^+$** and 14 mM AcOH for 3 h (red trace).

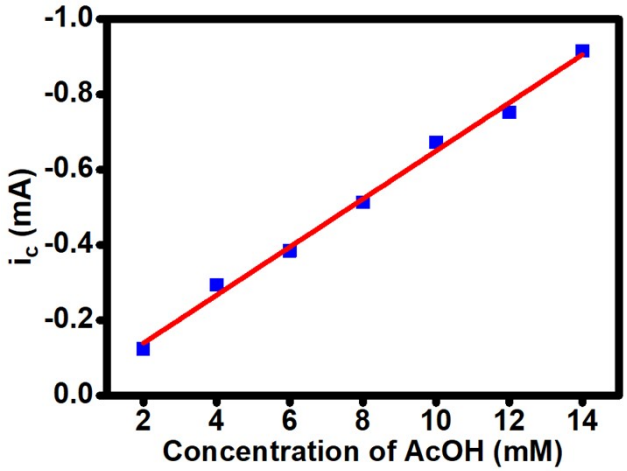

Figure S10. Plot of catalytic current (i_c) *vs.* concentration of AcOH.

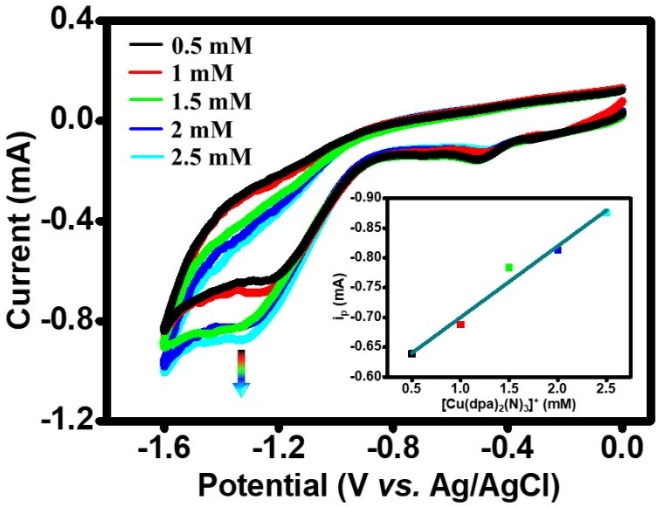

Figure S11. CVs in 0.1 M KCl aqueous solution containing 14 mM AcOH with different concentrations of **$[Cu(dpa)_2(N_3)]^+$** at a scan rate of 100 mV/s. Inset i_p vs. **$[Cu(dpa)_2(N_3)]^+$** fitted with a linear correlation exhibiting an R^2 value of 0.99.

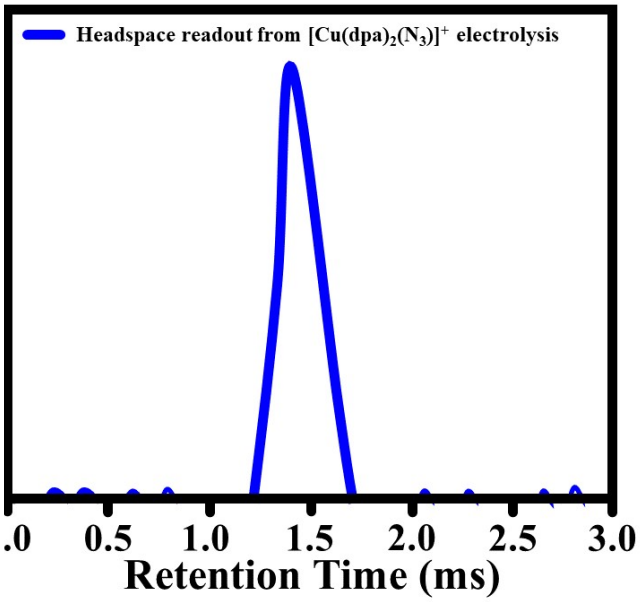

Figure S12. Hydrogen gas detection by gas chromatography (GC).

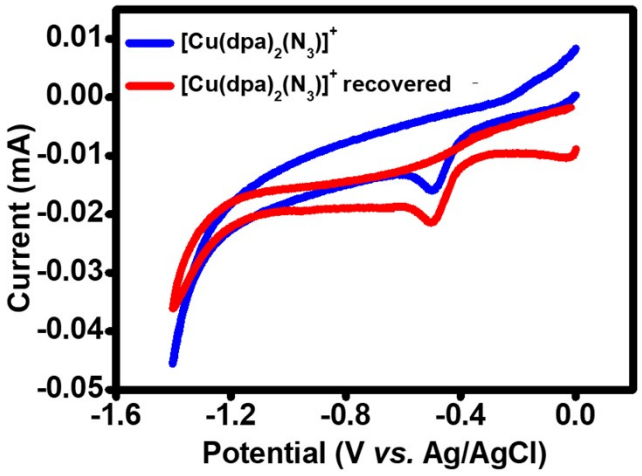

Figure S13. CV of complex and recovered complex.

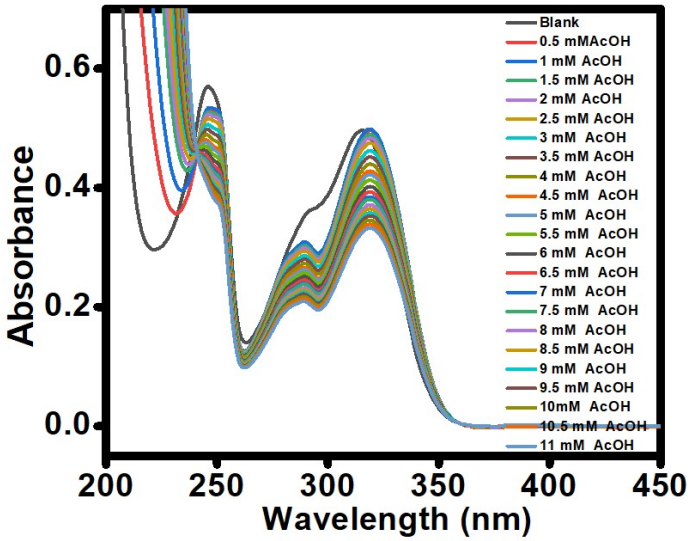

Figure S14. UV-Vis titration of $[Cu(dpa)_2(N_3)]^+$ using 0.5 to 11 mM of AcOH.

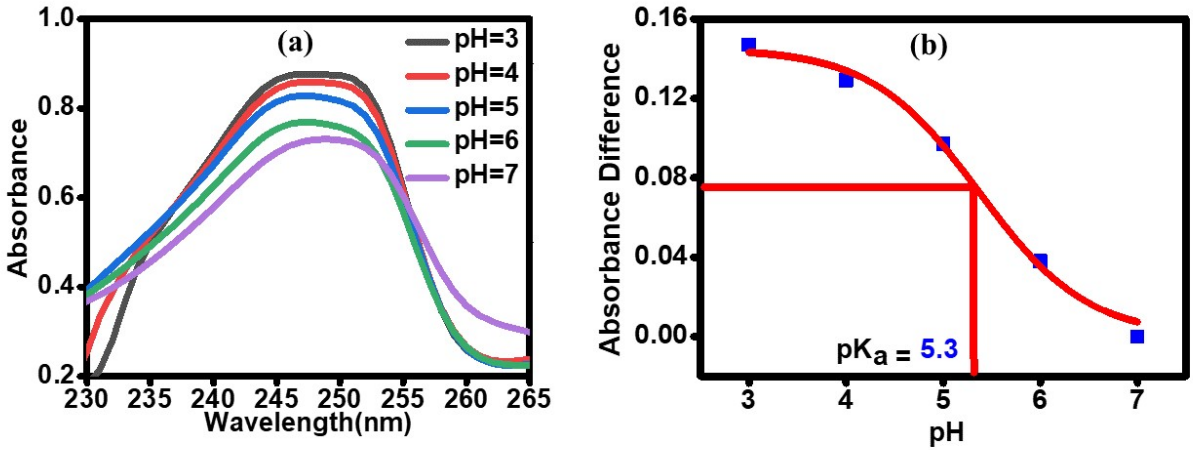

Figure S15. (a)UV-Vis plot of $[Cu(dpa)_2(N_3)]^+$ in a citrate-phosphate buffer in the pH range of 3-7. **(b)** Plot of absorbance *vs*. pH at 345 nm.

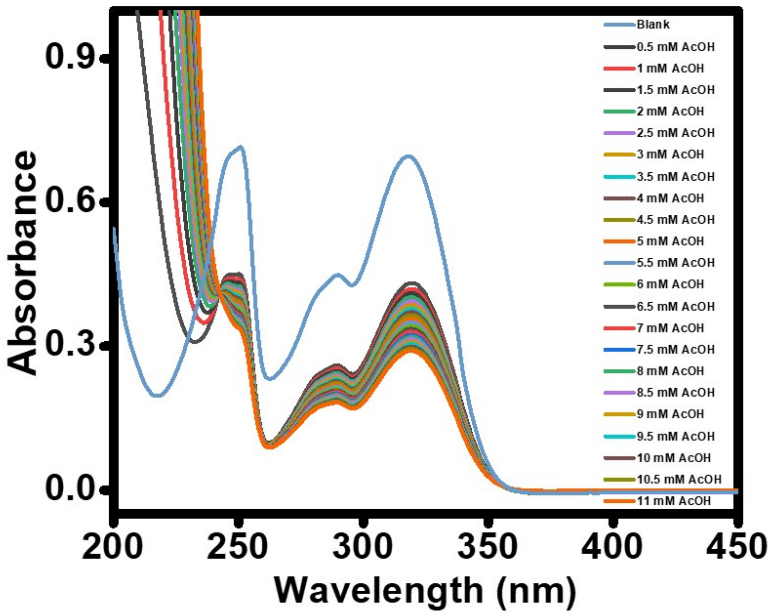

Figure S16. UV-Vis titration of **dpa** using 0.5 to 11 mM of AcOH.

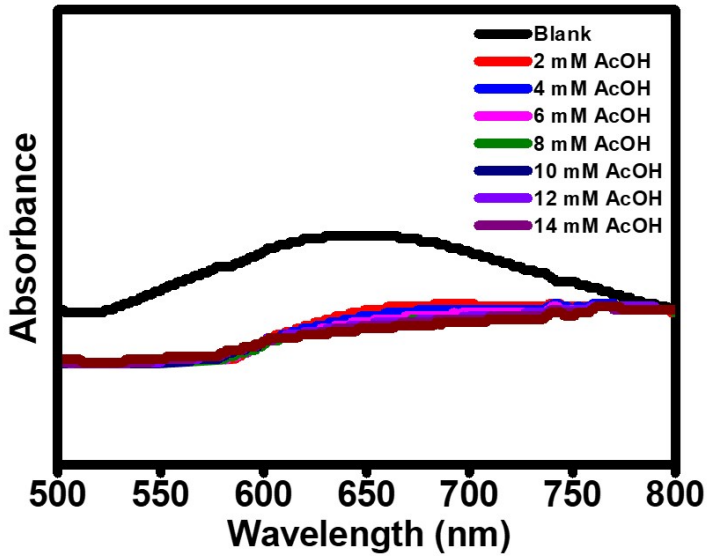

Figure S17. Decrement of the d-d band of the $\mathbf{[Cu(dpa)_2(N_3)]^+}$. A high concentration of complex was used to clarify the d-d band.

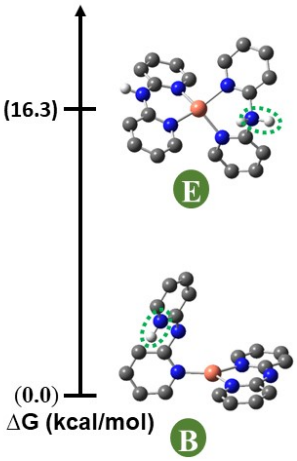

Figure S18. Energy profile of different N-protonated species using DFT calculation.

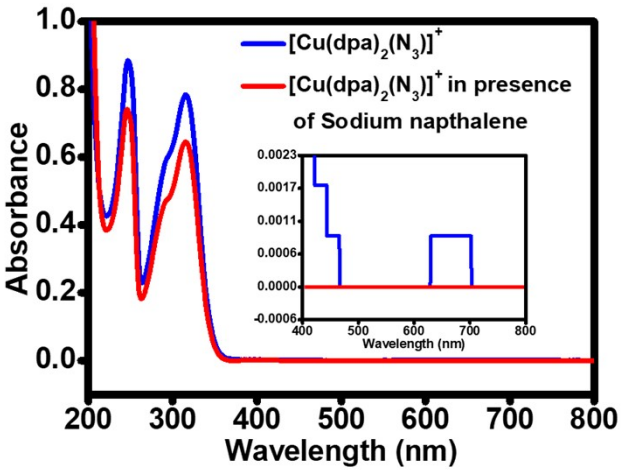

Figure S19. UV-Vis spectra of **$[Cu(dpa)_2(N_3)]^+$** in water (blue) and after one equivalent sodium naphthalene as one electron reductant (red). Inset: Diminishing nature of d-d band.

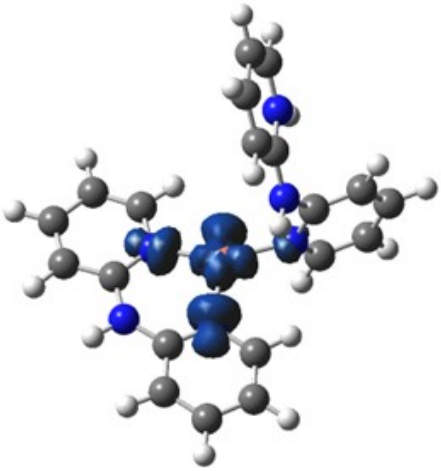

Figure S20. The spin density plot of N-site protonated intermediate (B) at an isovalue of 0.003.

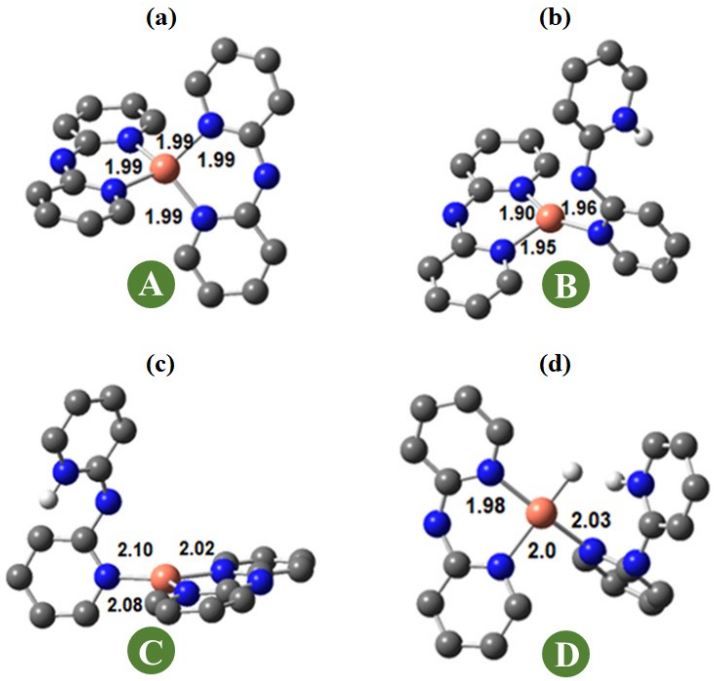

Figure S21: Optimized structure of intermediates a) N-site protonation of Cu(II) state, b) N-site protonation of Cu(I) state, c) doubly protonated Cu(II) intermediate state in Tafel step of $[Cu(dpa)_2(N_3)]^+$ electrocatalyst.

C.CALCULATION

1. Determination of the diffusion coefficient (D) of $[Cu(dpa)_2(N_3)]^+$ in 0.1 M KCl aqueous solution

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

$$Slope = [0.4463nFAC^0\left(\frac{nFD}{RT}\right)^{\frac{1}{2}}] \quad \text{.....(S1)}$$

$$D = \left(\frac{slope}{0.4463\ n\ FA\ C^0}\right)^2 \frac{RT}{nF} \quad \text{.....(S2)}$$

Slope ≡ 3.65×10^{-3}

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

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

Faraday constant (F) = 96485 C/mole e^-

R = ideal gas constant, and T = 298 K

$$\mathbf{D_0} = 4.432 \times 10^{-3}\ cm^2 / s$$

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

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

=8.143 C – 0.04568 C = 8.09732 C

3. Calculation of theoretical Moles of Hydrogen Made via Total Charge

Moles H_2 theoretical = 8.143 x (1 mol e^- / 96485 C) x (1 mol H_2 / 2 mol e^-)

= 4.196×10^{-5} moles H_2 based on the charge from electrolysis

4. Calculation of turnover number (TON)

$$TON = \frac{Moles\ of\ H_2\ produced}{Moles\ of\ [Cu(dpa)_2(N_3)]^+\ used}$$

$$\text{TON} = \frac{4.196 \times 10^{-5}\ moles\ H_2\ produced}{0.000001\ moles\ [Cu(dpa)_2(N_3)]^{+}\ used}$$

TON = 41.96

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 (kobs = k[H+]) can be calculated using equation

$$\frac{i_{cat}}{i_p} = \frac{n}{0.4463}\sqrt{\frac{RT(K\ [H^+])}{Fv}} \quad \text{.....(S3)}$$

The apparent rate constant (k_{app}) associated with acid and catalyst is calculated using the **equation S4**.

$$i_C = nFAC_{cat}\left(Dk_{app}C_{acid}\right)^{1/2} \quad \text{.....(S4)}$$

D. Tables

Table S1. Crystallographic structural parameters of $[Cu(dpa)_2(N_3)]Cl{\cdot}4H_2O$	
Parameters	**$[Cu(dpa)_2(N_3)]Cl{\cdot}4H_2O$**
CCDC	**2299272**
Empirical formula	$C_{20}H_{26}ClCuN_9O_4$
Formula weight	555.49
T (K)	250K
Wavelength (Å)	1.54184
Crystal system	Monoclinic
Space group	*P21/c*
Unit Cell Dimensions	
a (Å)	7.0295(4)
b (Å)	27.8164(16)
c (Å)	12.8722(7)
α (°)	90.00
β (°)	99.071(5)
γ (°)	90
V (Å^3)	2485.5(2)
Z	4
ρ (g cm^{-3})	1.485
Absorption coefficient (mm^{-1})	1.032
F(000)	1148
Theta range for data collection	2.7 to 32.8
Index ranges (h, k, l)	$-8 \leq h \leq 8$, $-29 \leq k \leq 30$, $-14 \leq l \leq 9$
Reflections collected	16212
Independent reflections	4195

R(int)	0.021
Final R indices [I>2sigma(I)]	R_1 = 0.0605, wR_2 = 0.1593
Largest diff. peak and hole	1.45/-1.13 e. Å-3

Table S2. Selected bond distances (Å) and angles (°) of $[Cu(dpa)_2(N_3)]Cl{\cdot}4H_2O$.

	Exp.	**DFT**		**Exp.**	**DFT**
Cu1-N3	1.999(3)	2.0692	Cu1-N8	2.033(3)	2.0783
Cu1-N4	2.170(3)	2.2837	Cu1-NC	2.021(3)	1.9547
Cu1-N5	2.001(3)	2.0624			
∠N3-Cu1-N4	102.27(10)	107.02	∠N3-Cu1-NC	86.33(11)	87.38
∠N3-Cu1-N5	169.51(11)	167.73	∠N4-Cu1-N5	87.97(10)	85.23
∠N3-Cu1-N8	87.40(11)	86.52	∠N4-Cu1-N8	96.15(11)	94.29
∠N4-Cu1-NC	103.38(11)	97.29	∠N5-Cu1-NC	89.09(11)	90.82
∠N5-Cu1-N8	93.84(11)	92.95	∠N8-Cu1-NC	160.34(11)	168.06

Table S3. Hydrogen bond lengths (Å) and angles (°) for $[Cu(dpa)_2(N_3)]Cl{\cdot}4H_2O$.					
D–H···A	***d*(D–H)**	***d*(H···A)**	***d*(D···A)**	**∠(DHA)**	**Symmetry**
O1--H1B..Cl5	0.85	2.31	3.156(3)	171	x,y,1+z
NA--HA..Cl5	0.86	2.55	3.251(2)	139	x,y,1+z
O2--H2B..Cl5	0.85	2.34	3.193(4)	177	-1+x,y,z
O3--H3A..O4	0.85	1.93	2.781(4)	175	-x,1-y,2-z
O3--H3B..O2	0.85	1.99	2.842(4)	177	x,y,1+z
O4--H4A..O1	0.85	1.99	2.842(4)	177	1-x,1-y,2-z
CN--HN..NC	0.93	2.59	3.464(4)	156	x,3/2-y,1/2+z

Table S4. X···π bond lengths (Å) and angles (°) for $[Cu(dpa)_2(N_3)]Cl{\cdot}4H_2O$		
X···Cg(*I*)	***d*[X···Cg(*I*)]**	**∠[CHCg(*I*)]**
N9-NL[1] -> Cg5	3.357(4)	8.76

Table S5. Electrochemical experimental results from a typical AcOH titration of $[[Cu(dpa)_2(N_3)]^+$obtained using equation S3.						
$[[Cu(dpa)_2(N_3)]^+$ (mM)	**AcOH (mM)**	**i_c (mA)**	**i_p (mA)**	i_{cat}/i_p	**Scan rate** $(\vartheta, V/s)$	**k_{obs} (s^{-1})**
1	2	-0.124	-0.0569	2.17	0.1	0.90
1	4	-0.2944	-0.0569	5.166	0.1	5.15
1	6	-0.3847	-0.0569	6.75	0.1	8.79
1	8	-0.5132	-0.0569	9.006	0.1	15.65

Table S7. Comparison of homogeneous HER activity with reported Copper complexes.

S. No	Electrocatalyst	TOF / TON	Electrochemical media/proton source		Stability/Durability	
1	10	-0.6727	-0.0569	11.80	0.1	23.68
1	12	-0.7517	-0.0569	13.19	0.1	33.56
1	14	-0.9157	-0.0569	16.07	0.1	49.81
1	[(**bztpen**)**Cu**](**BF4**)$_2$[3]	10000 s^{-1}	Acidic aqueous buffer.		Not explicitly discussed	
2	[**Cu**(**TMPA**)**Cl**]**Cl** (**1**) and [**Cu**(Cl-**TMPA**)**Cl$_2$**] (**2**)[4]	(**1**) 6108 TON and (**2**) 10014 TON in 6 h	CH_3CN/H_2O solution (9:1, v/v) with Ir complex as PS and triethylamine (TEA) as sacrificial reductant (SR).		After electrolysis for 2 h, characteristic NIR absorption of Cu(II) species was diminished.	
3	[**Cu**(**QCl-tpy**)(**OAc**)(**Cl**)] (**1**), and [**Cu**(**4Ql-tpy**)(**OAc**)(**OH$_2$**)]**Cl** (**2**)[5]	(**1**) 1153 s^{-1} (**2**) 1682 s^{-1}	95:5 DMF/H_2O (v/v) in the presence of AcOH as a proton source.		Not explicitly discussed	
4	[**Cu**(**tpen**)](**PF$_6$**)[6]	3415 s^{-1}	95:5 DMF/H_2O (v/v) in the presence of AcOH as a proton source.		1)After electrolysis for 2 h, some minor spectral changes were observed in the UV– vis spectra. 2)FESEM and EDX analyses revealed a slight decomposition of copper on working electrode.	

Table S6. Approximate catalytic rate constants, *k*app, with AcOH, were obtained using equation S4.

k_{app} (2 mM) $M^{-1}s^{-1}$	k_{app} (4 mM) $M^{-1}s^{-1}$	k_{app} (6 mM) $M^{-1}s^{-1}$	k_{app} (8 mM) $M^{-1}s^{-1}$	k_{app} (10 mM) $M^{-1}s^{-1}$	k_{app} (12mM) $M^{-1}s^{-1}$	k_{app} (14mM) $M^{-1}s^{-1}$
9.214	26.04	29.64	39.56	54.39	56.59	71.99

5	[{**(OAc)$_2$Cu(3py-tpy)**}$_2$**Cu(OAc)$_2$(H$_2$O)$_2$**] (**1**), {[**Cu(4pytpy)(OAc)**]**Cl**}$_n$ (**2**) and [**Cu(Ph-tpy)(OAc)$_2$**] (**3**)[7]	(**1**) 1473 s^{-1} (**2**) 700 s^{-1} (**3**) 926 s^{-1}	95:5 DMF/H_2O (v/v) in the presence of AcOH as a proton source.	No substantial change in the CV and UV-vis spectrum recorded before and after the bulk electrolysis.
6	**Cu(II)L**,[8]	10000 $s^{-1}$and TON 52 in ACN and 5100 $s^{-1}$and TON 73 in DMF	ACN and DMF with AcOH as a proton source.	CPE reveals no sign of degradation over 23 h.
7	**[Cu(dpa)$_2$(N$_3$)]$^+$ This work**	241.75 s^{-1} and TON 73.06	AcOH in 0.1 M KCl water.	CPE reveals no sign of degradation over 1.6 h, PXRD, UV-vis spectrum displays negligible change after electrolysis.

Table S8. Computational coordinates using B3LYP/6-311g(d,p) in water.

[Cu(dpa)$_2$(N$_3$)]$^+$

Cu	0.15354	-0.04865	-0.43176
N	2.04503	-0.8642	-0.62854
N	0.8458	-1.09566	1.33476
N	-1.61447	1.00169	-0.58804
N	-2.97803	-0.69098	0.39302
H	-3.92057	-1.04878	0.36296
N	1.04564	1.41737	0.74062
N	3.11906	1.23032	-0.37668
H	3.99588	1.70485	-0.53196

C	3.16034	-0.12685	-0.70001
C	- 2.1384	-1.41543	1.23658
C	-2.82717	0.48993	-0.31667
C	-2.70956	-2.46581	1.97881
H	-3.76068	-2.7061	1.8699
C	2.281	1.88954	0.51131
C	4.38883	-0.67407	-1.10142
H	5.26937	-0.04575	-1.16212
C	-0.08507	-1.78824	2.2028
H	0.95486	-1.48409	2.25464
C	4.45422	-2.02167	-1.39913
H	5.39435	-2.46346	-1.70688
C	-1.5469	2.15954	-1.28671
H	-0.54808	2.53494	-1.47407
C	0.28786	2.03921	1.67228
H	-0.68297	1.59575	1.84264

C	-4.00322	1.1301	-0.75693
H	-4.96751	0.69424	-0.52591
C	2.1245	-2.18165	-0.91836
H	1.18418	-2.71402	-0.88899
C	-1.90783	-3.17518	2.85137
H	-2.32734	-3.98734	3.4329
C	3.30037	-2.80063	-1.2911
H	3.30834	-3.85879	-1.51436
C	-0.55957	-2.82734	2.98033
H	0.09853	-3.35285	3.65923
C	-2.65041	2.83982	-1.74836
H	-2.53279	3.75643	-2.31003
C	2.76243	3.04717	1.15017
H	3.75928	3.41042	0.93071
C	-3.91306	2.29917	-1.47872
H	-4.81224	2.79225	-1.82743
C	0.69701	3.16125	2.36039

H	0.04643	3.6183	3.09352
C	1.96088	3.68738	2.0724
H	2.31955	4.57525	2.57911

E			
Cu	-0.00001	-0.00013	0.00004
N	1.36091	1.27771	0.69414
N	-1.36029	1.27841	-0.69394
N	-1.36113	-1.27792	0.6938
N	-3.23793	0.00044	-0.00082
H	-3.84142	0.43446	0.66808
N	-1.36055	-1.27875	-0.6934
H	4.2481	-0.0004	-0.00054
C	2.68775	1.06124	0.68852

C	2.68719	1.06219	-0.68901
C	-2.68794	-1.06122	0.6881
C	-3.56984	1.92165	-1.37146
H	-4.63398	1.72683	-1.34043
C	2.68737	-1.06215	-0.6886
C	3.57089	1.92035	1.37078
H	4.63499	1.72534	1.33917
C	-0.87579	2.33051	-1.40445
H	0.1989	2.44856	-1.39645
C	3.06395	2.99009	2.0737
H	3.73463	3.65515	2.60316
C	-0.87736	-2.32983	1.40505
H	0.1973	-2.44824	1.39769
C	0.87625	-2.33085	-1.40402
H	-0.1984	-2.44922	-1.39584
C	-3.57125	-1.92008	1.37046

H	-4.6353	-1.72485	1.33884
C	0.87693	2.32965	1.40524
H	-0.19774	2.44791	1.39777
C	-3.06237	2.99154	-2.07378
H	-3.73267	3.65687	-2.60336
C	1.67987	3.20151	2.10069
H	1.23986	4.02188	2.64997
C	-1.67824	3.20274	-2.1
H	-1.23781	4.02322	-2.64878
C	-1.68047	-3.20149	2.10056
H	-1.24061	-4.02188	2.64995
C	3.57018	-1.9212	-1.37137
H	4.63427	-1.72607	-1.34047
C	-3.06452	-2.98983	2.07351
H	-3.73532	-3.6547	2.60304
C	1.67885	-3.20272	-2.09986

H	1.2386	-4.02323	-2.64874
C	3.06292	-2.99108	-2.07385
H	3.73332	-3.65609	-2.6037
H	-3.84045	-0.43368	-0.67053
B			
Cu	-0.00001	-0.00013	0.00004
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N	-1.36029	1.27841	-0.69394
N	-1.36113	-1.27792	0.6938
N	-3.23793	0.00044	-0.00082
H	-4.2481	0.0006	-0.0011
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N	3.23794	-0.00047	-0.00016
H	4.2481	-0.0004	-0.00054
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C	-2.68719	1.06219	-0.68901
C	-2.68794	-1.06122	0.6881

C	-3.56984	1.92165	-1.37146
H	-4.63398	1.72683	-1.34043
C	2.68737	-1.06215	-0.6886
C	3.57089	1.92035	1.37078
H	4.63499	1.72534	1.33917
C	-0.87579	2.33051	-1.40445
H	0.1989	2.44856	-1.39645
C	3.06395	2.99009	2.0737
H	3.73463	3.65515	2.60316
C	-0.87736	-2.32983	1.40505
H	0.1973	-2.44824	1.39769
C	0.87625	-2.33085	-1.40402
H	-0.1984	-2.44922	-1.39584
C	-3.57125	-1.92008	1.37046
H	-4.6353	-1.72485	1.33884
C	0.87693	2.32965	1.40524

H	-0.19774	2.44791	1.39777
C	-3.06237	2.99154	-2.07378
H	-3.73267	3.65687	-2.60336
C	1.67987	3.20151	2.10069
H	1.23986	4.02188	2.64997
C	-1.67824	3.20274	-2.1
H	-1.23781	4.02322	-2.64878
C	-1.68047	-3.20149	2.10056
H	-1.24061	-4.02188	2.64995
C	3.57018	-1.9212	-1.37137
H	4.63427	-1.72607	-1.34047
C	-3.06452	-2.98983	2.07351
H	-3. 73532	-3.6547	2.60304
C	1.67885	-3.20272	-2.09986
H	1.2386	-4.02323	-2.64874
C	3.06292	-2.99108	-2.07385
H	3.73332	-3.65609	-2.6037
H	-0.74308	0.67785	-0.18563

C			
Cu	-0.66152	-0.27456	-0.63694
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N	1.9313	-0.56059	0.83156
H	1.39113	-0.8833	1.62547
N	-2.02467	-1.08632	0.50166
N	-3.27777	0.92962	0.67801
H	-4.07585	1.33886	1.14356
C	-2.67493	1.76661	-0.2337
C	2.82968	0.43068	1.10839
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C	2.96096	0.97992	2.39268
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C	-3.236	3.03714	-0.45472
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C	-2.65037	3.88074	-1.37228
H	-3.07694	4.85956	-1.55126
C	0.75616	-2.36649	-2.04373

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H	3.91134	-3.57343	-2.02378
C	-2.75409	-3.0574	1.65634
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C	-3.839	-2.34361	2.17952
H	-4.55206	-2.82674	2.83539

H	3.49922	0.57482	-0.82437
D			
Cu	-0.00001	-0.00013	0.00004
N	1.36091	1.27771	0.69414
N	-1.36029	1.27841	-0.69394
N	-1.36113	-1.27792	0.6938
N	-3.23793	0.00044	-0.00082
H	-4.2481	0.0006	-0.0011
N	1.36055	-1.27875	-0.6934
N	3.23794	-0.00047	-0.00016
H	4.2481	-0.0004	-0.00054
C	2.68775	1.06124	0.68852
C	-2.68719	1.06219	-0.68901
C	-2.68794	-1.06122	0.6881
C	-3.56984	1.92165	-1.37146
H	-4.63398	1.72683	-1.34043
C	2.68737	-1.06215	-0.6886
C	3.57089	1.92035	1.37078
H	4.63499	1.72534	1.33917
C	-0.87579	2.33051	-1.40445
H	0.1989	2.44856	-1.39645
C	3.06395	2.99009	2.0737

H	3.73463	3.65515	2.60316
C	-0.87736	-2.32983	1.40505
H	0.1973	-2.44824	1.39769
C	0.87625	-2.33085	-1.40402
H	-0.1984	-2.44922	-1.39584
C	-3.57125	-1.92008	1.37046
H	-4.6353	-1.72485	1.33884
C	0.87693	2.32965	1.40524
H	-0.19774	2.44791	1.39777
C	-3.06237	2.99154	-2.07378
H	-3.73267	3.65687	-2.60336
C	1.67987	3.20151	2.10069
H	1.23986	4.02188	2.64997
C	-1.67824	3.20274	-2.1
H	-1.23781	4.02322	-2.64878
C	-1.68047	-3.20149	2.10056
H	-1.24061	-4.02188	2.64995
C	3.57018	-1.9212	-1.37137
H	4.63427	-1.72607	-1.34047
C	-3.06452	-2.98983	2.07351
H	-3.73532	-3.6547	2.60304
C	1.67885	-3.20272	-2.09986
H	1.2386	-4.02323	-2.64874

C	3.06292	-2.99108	-2.07385
H	3.73332	-3.65609	-2.6037
H	-0.74308	0.67785	-0.18563

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