Supplementary Information for

Electrocatalytic Hydrogen Evolution by Robust Square Planar Nickel Complexes in a S_2P_2 Coordination Environment

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Figure S16. CVs of 0.25 mM **2** in DMF with different TFA concentrations (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat}/i_{pc} against the square root of TFA concentration.

Figure S17. CVs of 0.25 mM **3** in DMF with different TFA concentrations (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat}/i_{pc} against the square root of TFA concentration.

Figure S18. CVs of 0.25 mM **4** in DMF with different TFA concentrations (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat}/i_{pc} against the square root of TFA concentration.

Figure S19. CVs of 0.25 mM **5** in DMF with different TFA concentrations (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat}/i_{pc} against the square root of TFA.

Figure S20. CVs of different TFA concentrations without complex in DMF (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat}/i_{pc} against the square root of TFA concentration.

Figure S21. Red: Cyclic voltammogram of 67.32 mM TFA without **1** in DMF. Black: Cyclic voltammogram of 0.25 mM **1** with 67.32 mM TFA in DMF. Conditions: 0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; 100 mV s^{-1} scan rate.

Figure S22. CVs of 0.05-0.25 mM **2** in DMF with 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Insert: Plot of the i_{cat} against the complex **2** concentration.

Figure S23. CVs of 0.05-0.25 mM **3** in DMF with 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Insert: Plot of the i_{cat} against the complex **3** concentration.

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Figure S25. CVs of 0.05-0.25 mM **5** in DMF with 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Insert: Plot of the i_{cat} against the complex **5** concentration.

Figure S26. Plot of log k_{obs} versus overpotential of 0.25 mM **2** in DMF in the presence of 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; a glassy carbon working electrode).

Figure S27. Plot of log k_{obs} versus overpotential of 0.25 mM **3** in DMF in the presence of 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; a glassy carbon working electrode).

Figure S28. Plot of log k_{obs} versus overpotential of 0.25 mM **4** in DMF in the presence of 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; a glassy carbon working electrode).

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Figure S35. Cyclic voltammograms of **2** (0.25 mM) in DMF with 26.92 mM TFA (red) and a subsequent CV using the same electrode after rinsing and transfer to fresh in DMF of 26.92 mM TFA without adding **2** (blue). For comparison, CV of 26.92 mM TFA without **2** is shown in grey (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

Figure S36. Simulated and experimental UV-vis absorption spectra of complex **1**.

Figure S37. Cumulative coulombs in the presence of 53.8 mM TFA electrolysis for 18 h at a constant potential of -2.00 V (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode).

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Figure S40. Cyclic voltammograms of 0.25 mM **3** with 26.93 mM TFA before and after electrolysis. Inset: Amperometric i-t curve of **3** at a constant potential of -2.00 V. (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

Figure S41. Cyclic voltammograms of 0.25 mM **4** with 26.93 mM TFA before and after electrolysis. Inset: Amperometric i-t curve spectra of **4** at a constant potential of -2.00 V. (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

Figure S42. Cyclic voltammograms of 0.25 mM **5** with 26.93 mM TFA before and after electrolysis. Inset: Amperometric i-t curve spectra of **5** at a constant potential of -2.00 V. (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

Figure S43. SEM images of the surface of the rinsed glassy carbon electrode after 18 hours of CPE testing at 0.25 mM 1 and 53.8 mM TFA.

Figure S44. EDS diagrams of the surface of the rinsed glassy carbon electrode after 18 hours of CPE testing at 0.25 mM **1** and 53.8 mM TFA.

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Figure S46. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **1**.

Figure S47. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **2**.

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Figure S50. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **5**.

Figure S51. Molecular structure of **[1**(L-H)**]**$^-$ after DFT optimization.

Figure S52. Energy shown in the output file after DFT optimization of [**1**(Ni-H)].

Instrumental Details

Elemental analyses were performed on an Elementar Vario EL cube analyzer. FTIR spectra were recorded out on a NICOLET 6700 infrared spectrophotometer using samples prepared as KBr pellets at room temperature. ^{1}H NMR spectra were conducted on a Brucker AV400 NMR spectrometer by using $CDCl_3$ as the solvent at room temperature. UV-Vis absorption spectra were carried out on a TU-1950 ultraviolet-visible spectrophotometer at room temperature. SEM / EDS were measured at a Zeiss Sigma 300 scanning electron micrograph.

Single crystal X-ray diffraction

The single crystals of **2** and **4**·CH_2Cl_2 were obtained by slow evaporation of CH_2Cl_2 / hexane solution under low temperature, respectively. The crystal structural data were collected on a Bruker APEX-II CCD diffractometer with a graphite monochromator utilizing Mo-K_α radiation sealed X-ray tube (λ = 0.71073 Å) in the ω scanning mode at 100.15 K. The molecular structures were solved by means of direct methods using the SHELXS-97 program and refined by full-matrix least-square techniques (SHELXL-97) on F^2. [1, 2] All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were placed in geometrically calculated positions and refined as the riding ones.

Electrochemical measurements

Cyclic voltammetry and controlled potential electrolysis were implemented in DMF solution on a CHI 660E instrument equipped with a three-electrode cell consisting of 3 mm diameter glassy carbon working electrode, Ag^+/Ag reference electrode, and platinum wire counter electrode. Before conducting electrochemical experiments, the glassy carbon working electrode was polished with alumina water slurry, and then carefully cleaned. The solution was purged for about 20 min with N_2 atmosphere prior to electrochemical measurements. All the potentials were calibrated by measuring the Fc^+/Fc couple in the cell at the end of each experiment and reported against this reference system. For the CPE experiments, the evolved gas in the cell at the end of the electrolysis was confirmed by using GC7980 gas chromatograph. All of the electrochemical measurement was maintained at room temperature.

Computational method

Density functional theory calculations were conducted by using Gaussian 09 program. [3] Based on the energetic minima results, geometry optimized and vibrational frequencies were analyzed with B3LYP functional [4, 5] in association with Def2-TZVP basis set. [6, 7] The dispersion corrections for accurately computing the London dispersion interactions were carried out by using DFT-D3 model. Simulating the effect of DMF solvent in the reaction was performed with SMD solvation model. [8]

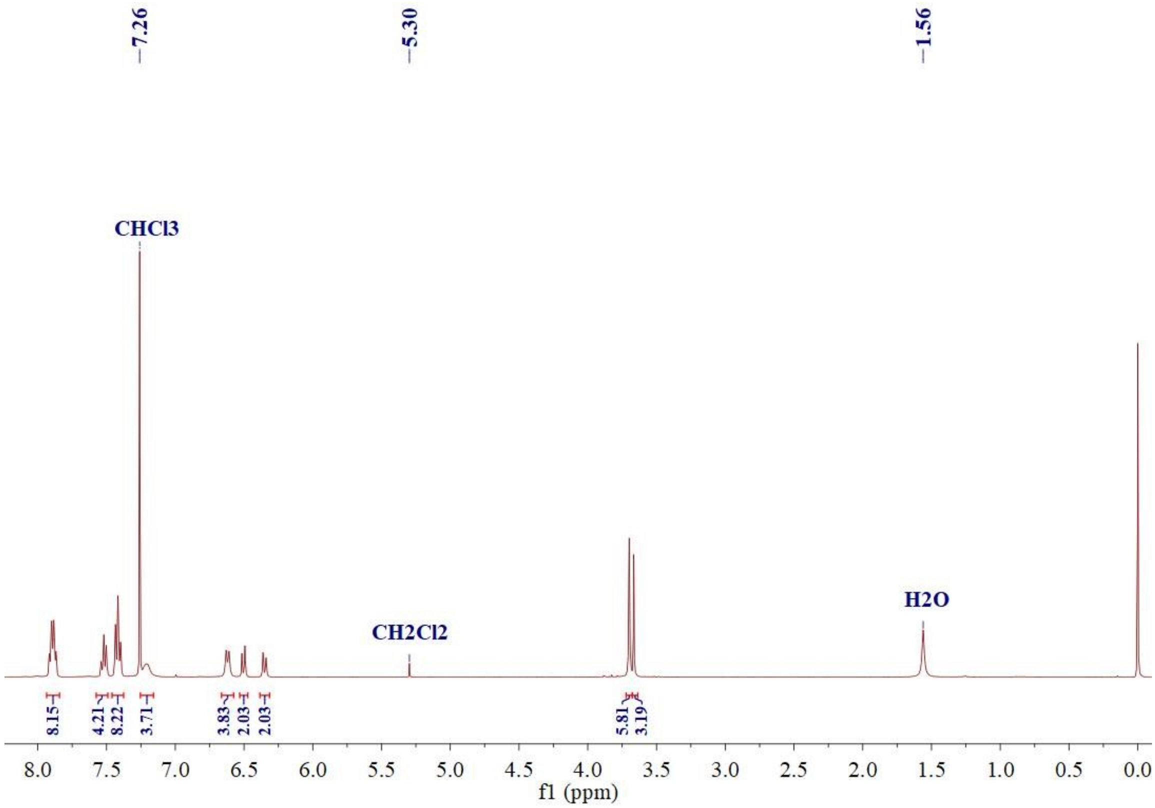


Figure S1. [1]H NMR spectrum of **1** in $CDCl_3$.

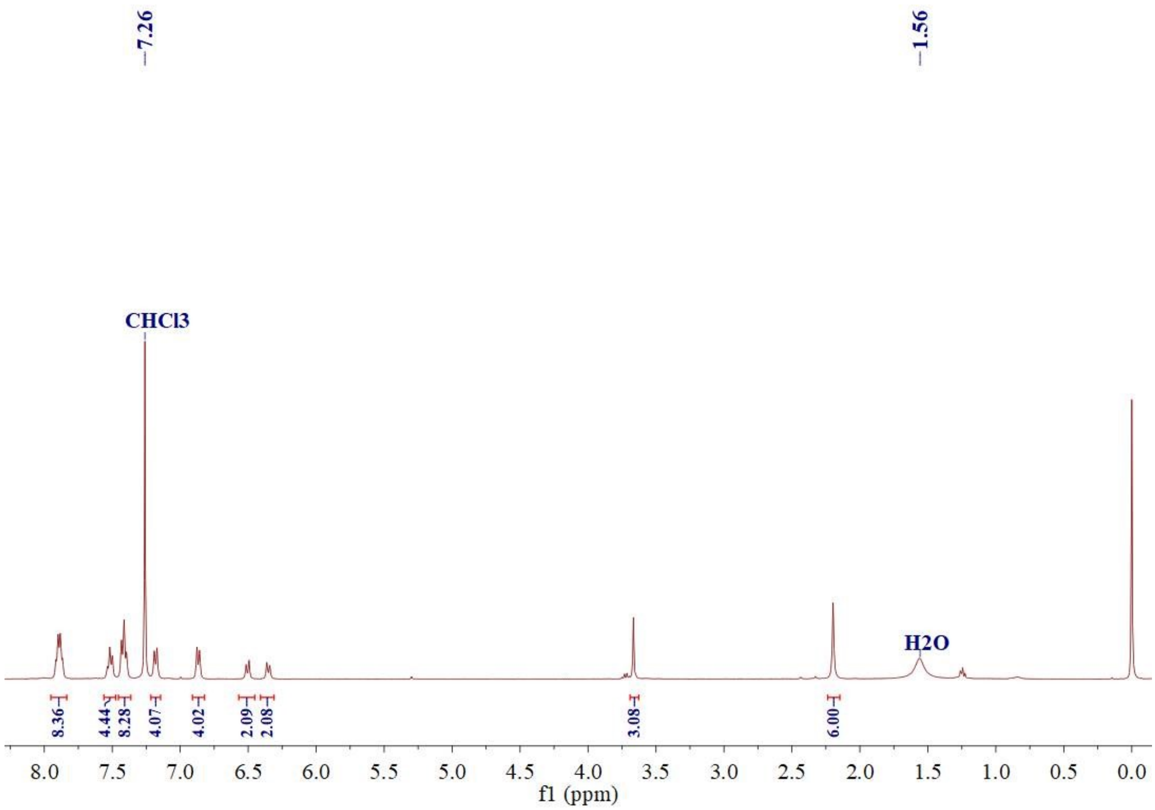


Figure S2. [1]H NMR spectrum of **2** in $CDCl_3$.

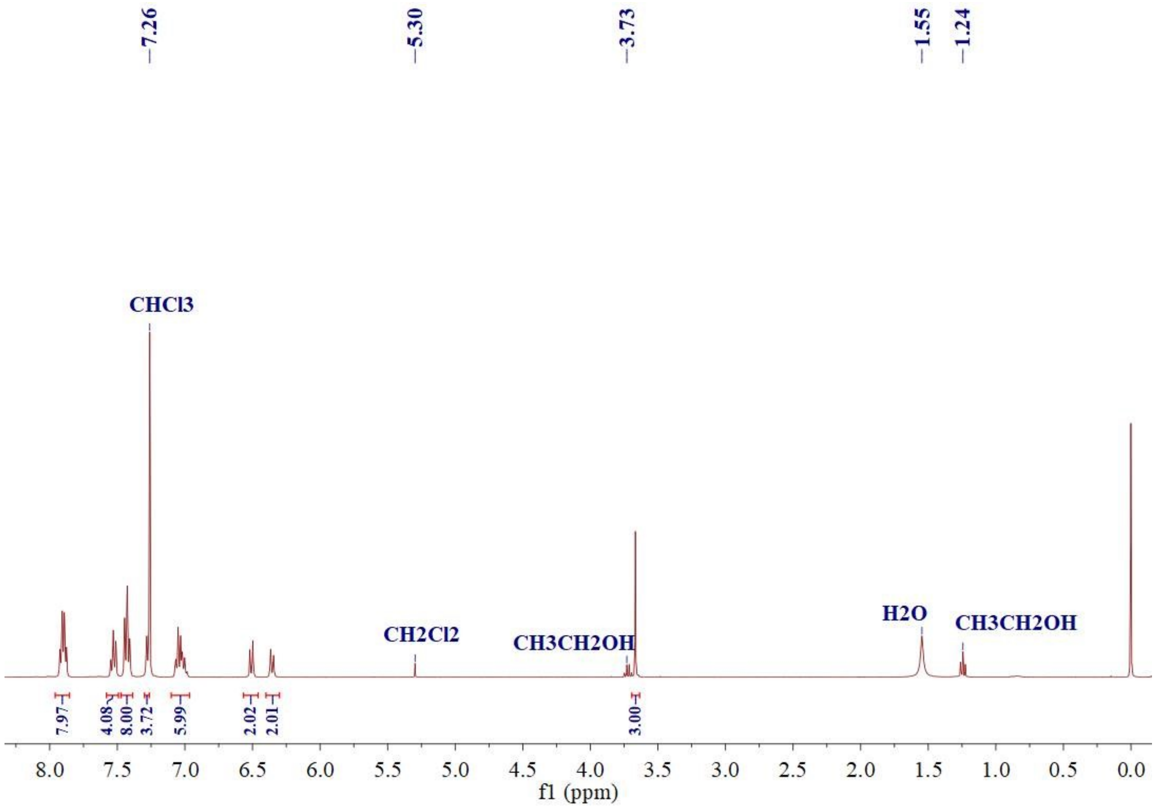


Figure S3. ^{1}H NMR spectrum of **3** in $CDCl_3$.

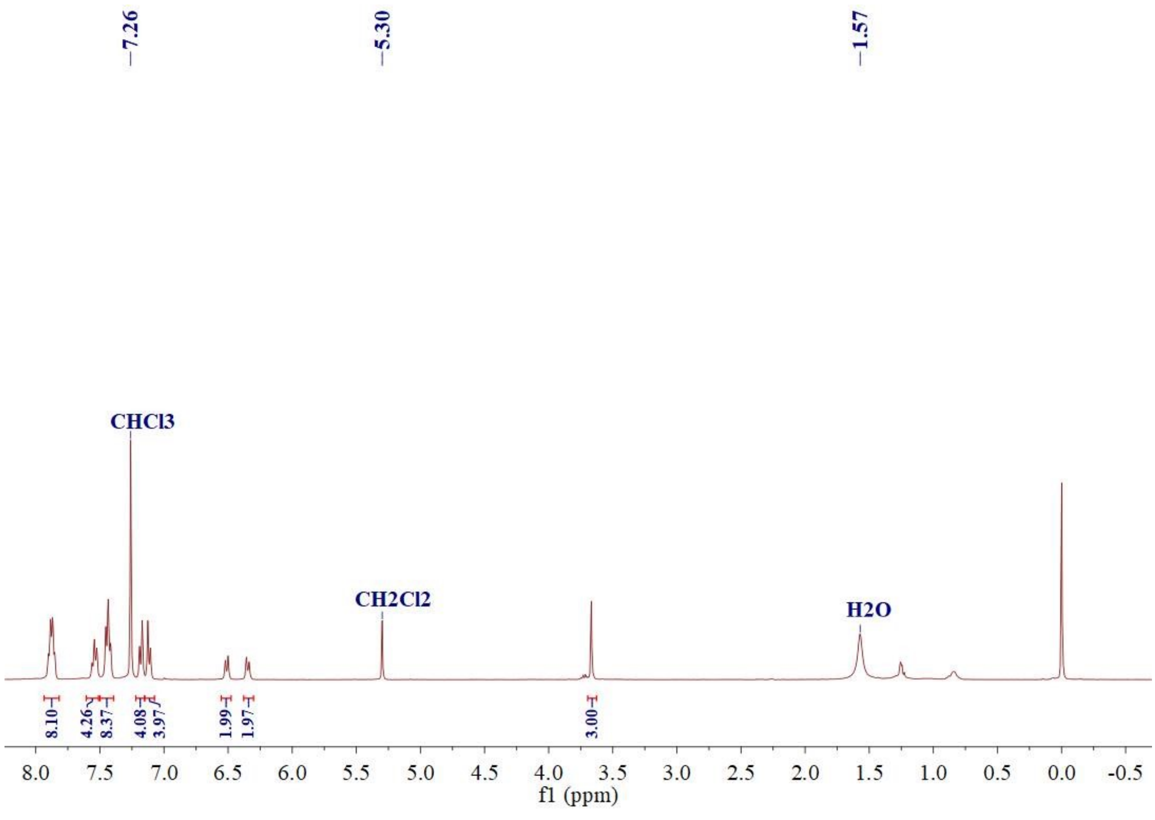


Figure S4. ^{1}H NMR spectrum of **4** in $CDCl_3$.

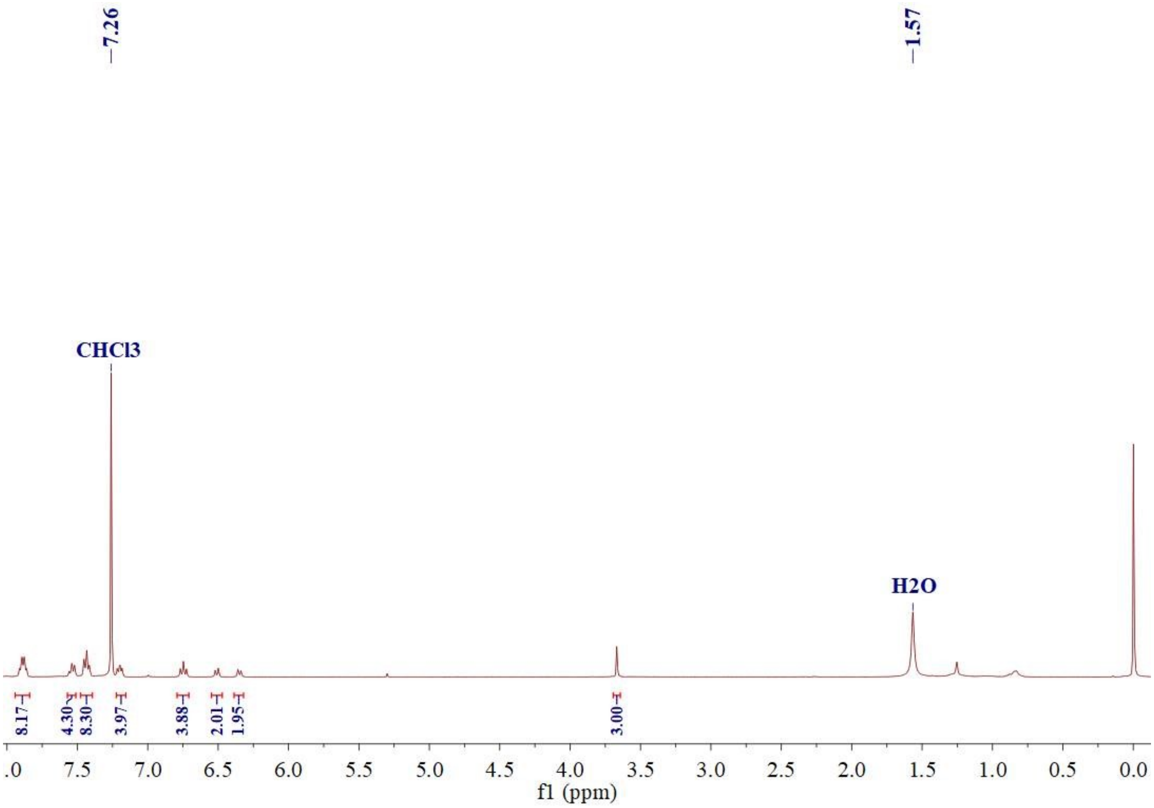


Figure S5. ^{1}H NMR spectrum of **5** in $CDCl_3$.

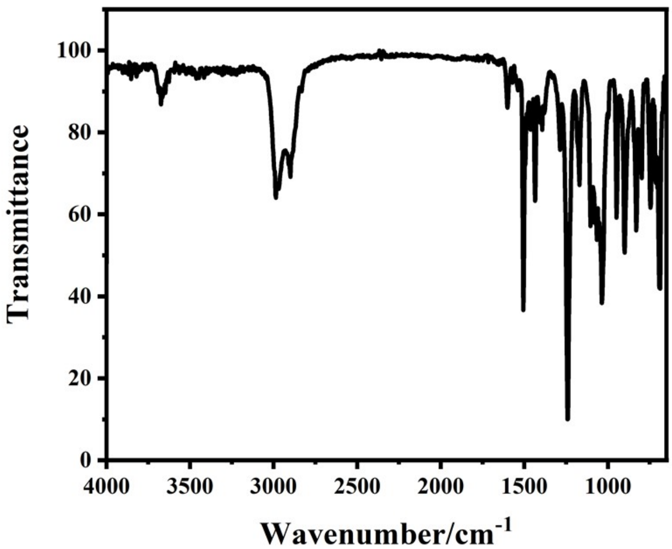


Figure S6. FTIR spectrum of **1**.

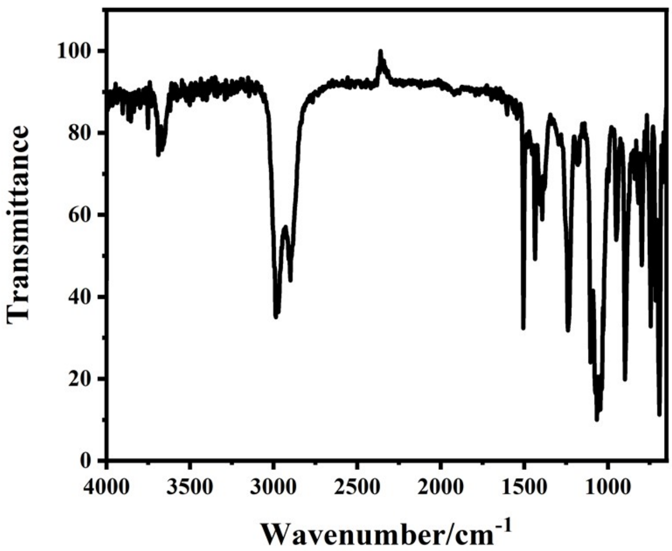


Figure S7. FTIR spectrum of **2**.

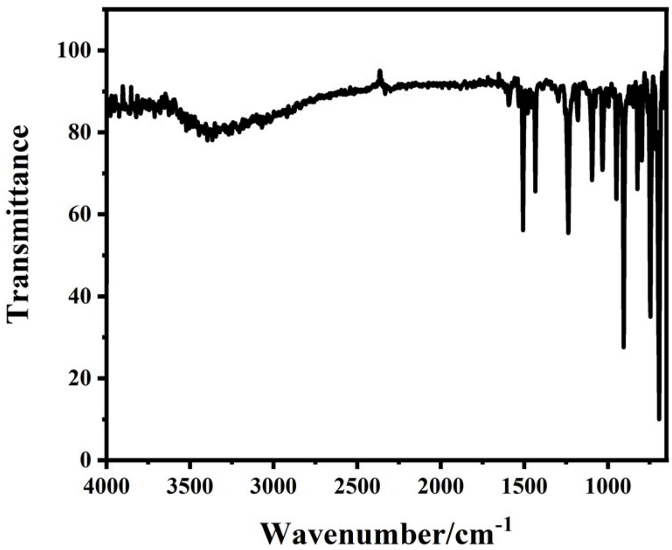


Figure S8. FTIR spectrum of **3**.

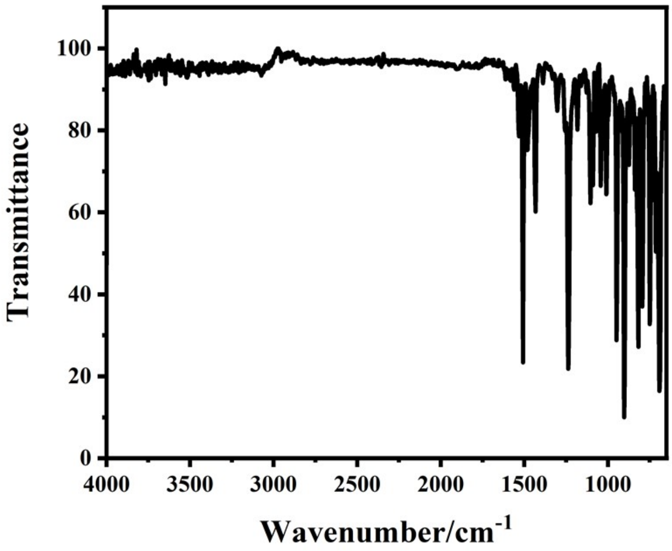


Figure S9. FTIR spectrum of **4**.

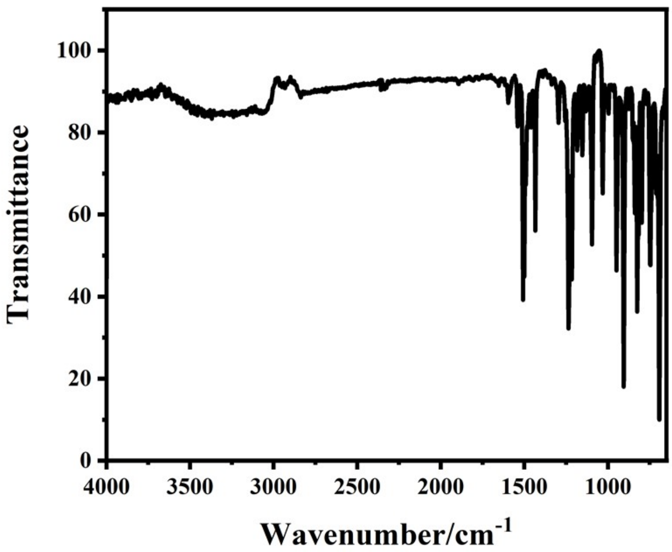


Figure S10. FTIR spectrum of **5**.

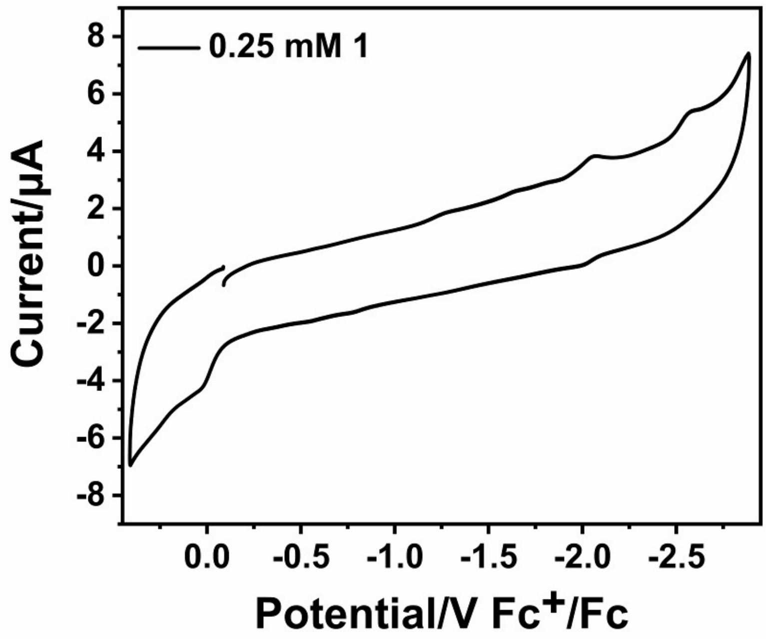


Figure S11. Cyclic voltammogram of 0.25 mM **1** recorded at 100 mV s^{-1} scan rates in DMF solution with 0.1 M n-Bu_4NPF_6 as the supporting electrolyte and using a glassy carbon working electrode.

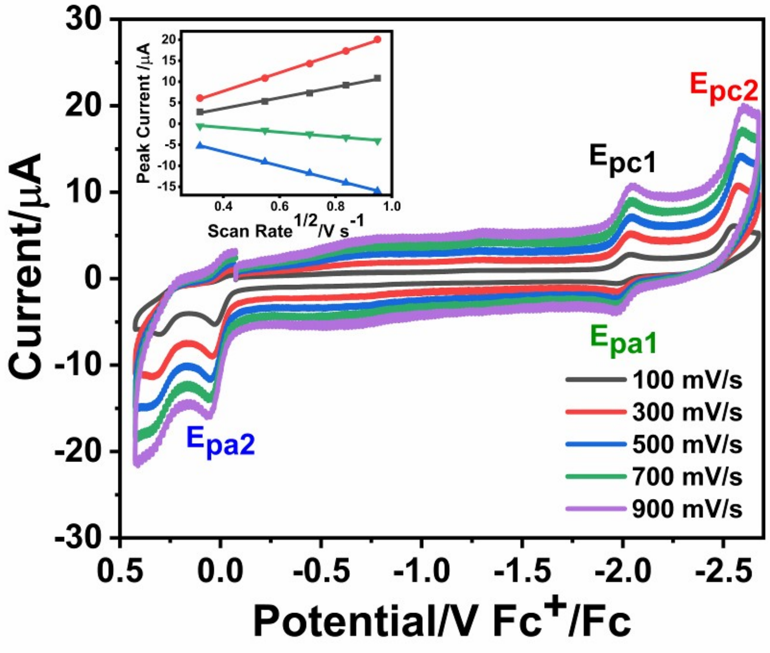


Figure S12. CVs of **2** recorded at scan rates from 100 mV s^{-1} to 900 mV s^{-1} in DMF solution with 0.1 M n-Bu_4NPF_6 as the supporting electrolyte and using a glassy carbon working electrode. Inset: Plots of peak current versus the square root of scan rate.

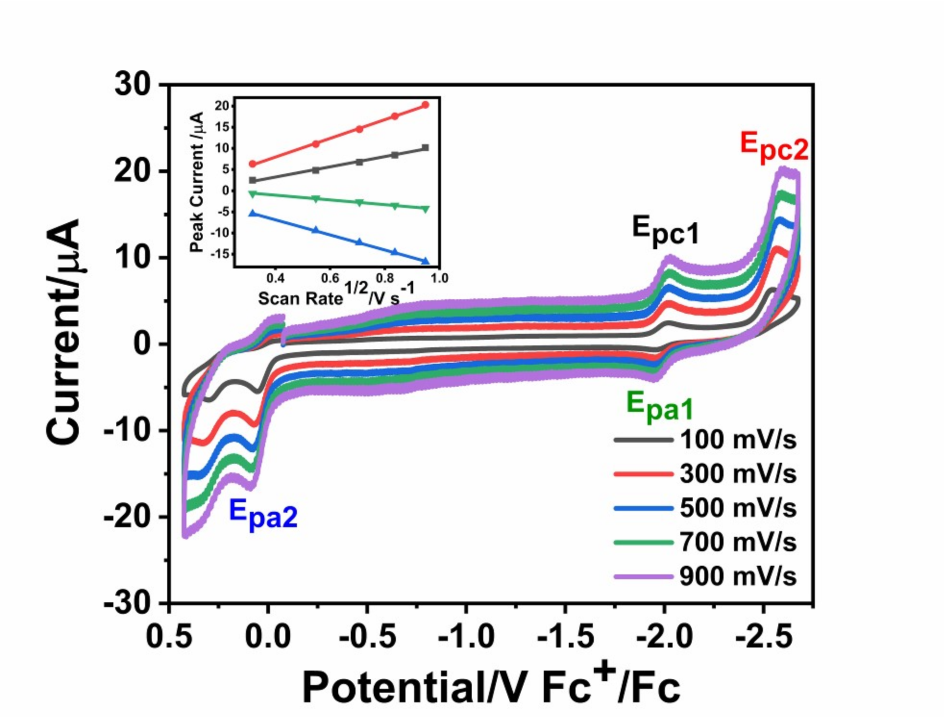


Figure S13. CVs of **3** recorded at scan rates from 100 mV s^{-1} to 900 mV s^{-1} in DMF solution with 0.1 M n-Bu_4NPF_6 as the supporting electrolyte and using a glassy carbon working electrode. Inset: Plots of peak current versus the square root of scan rate.

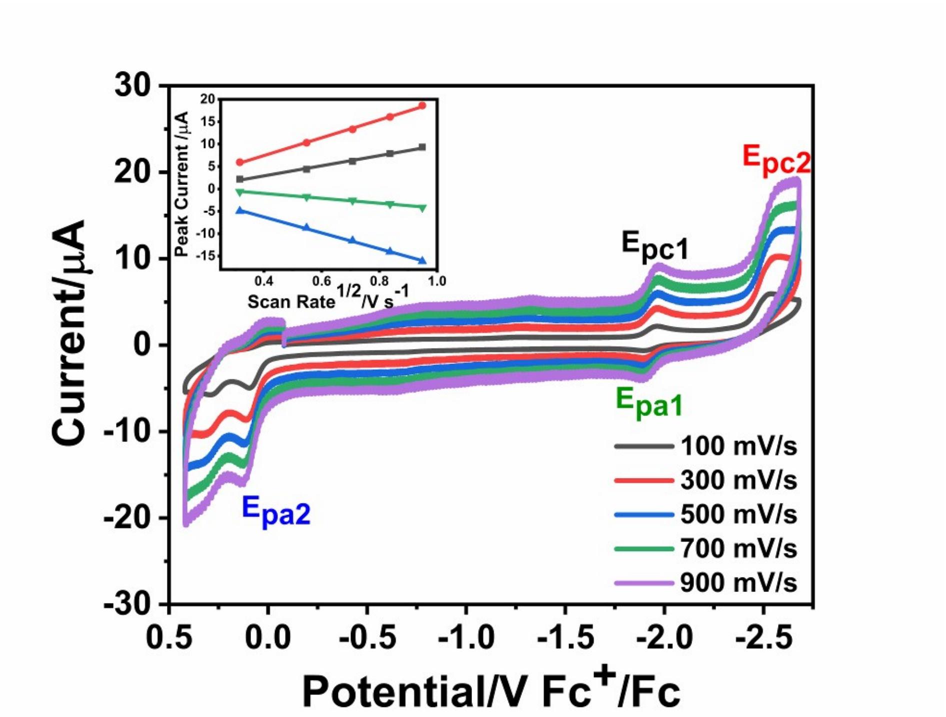


Figure S14. CVs of **4** recorded at scan rates from 100 mV s^{-1} to 900 mV s^{-1} in DMF solution with 0.1 M n-Bu_4NPF_6 as the supporting electrolyte and using a glassy carbon working electrode. Inset: Plots of peak current versus the square root of scan rate.

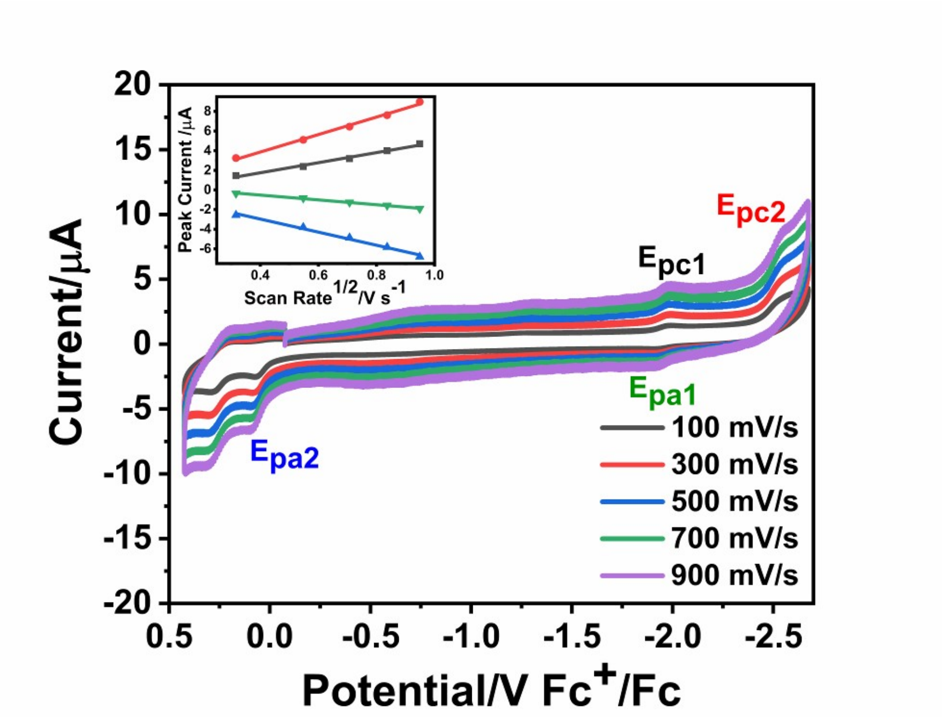


Figure S15. CVs of **5** recorded at scan rates from 100 mV s^{-1} to 900 mV s^{-1} in DMF solution with 0.1 M n-Bu_4NPF_6 as the supporting electrolyte and using a glassy carbon working electrode. Inset: Plots of peak current versus the square root of scan rate.

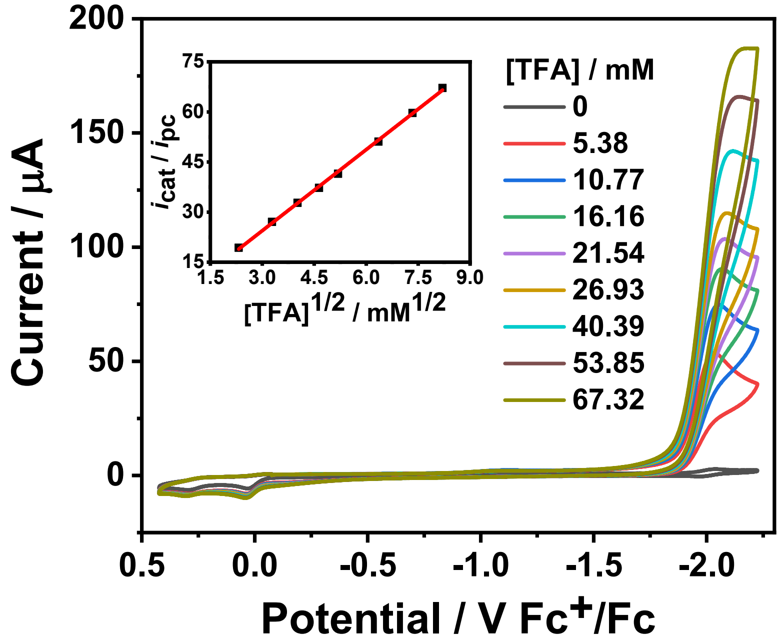


Figure S16. CVs of 0.25 mM **2** in DMF with different TFA concentrations (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat} /i_{pc} against the square root of TFA concentration.

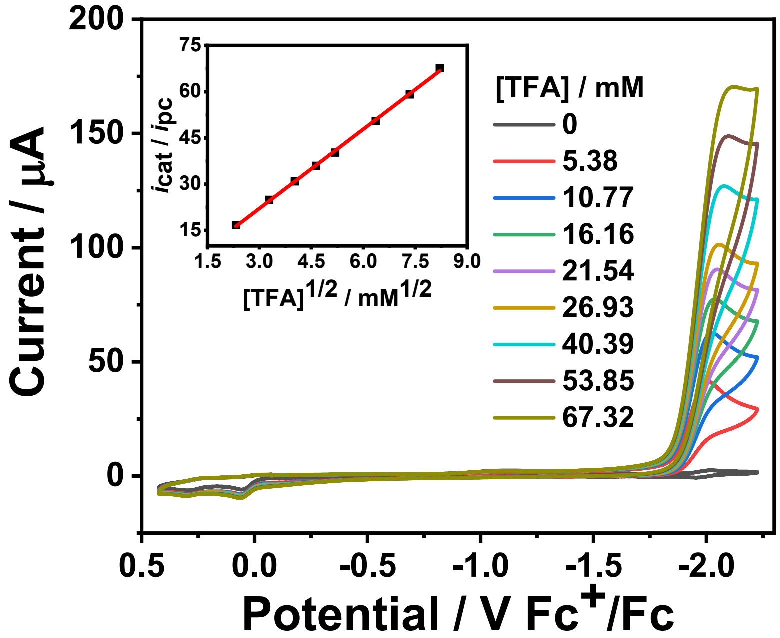


Figure S17. CVs of 0.25 mM **3** in DMF with different TFA concentrations (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat} /i_{pc} against the square root of TFA concentration.

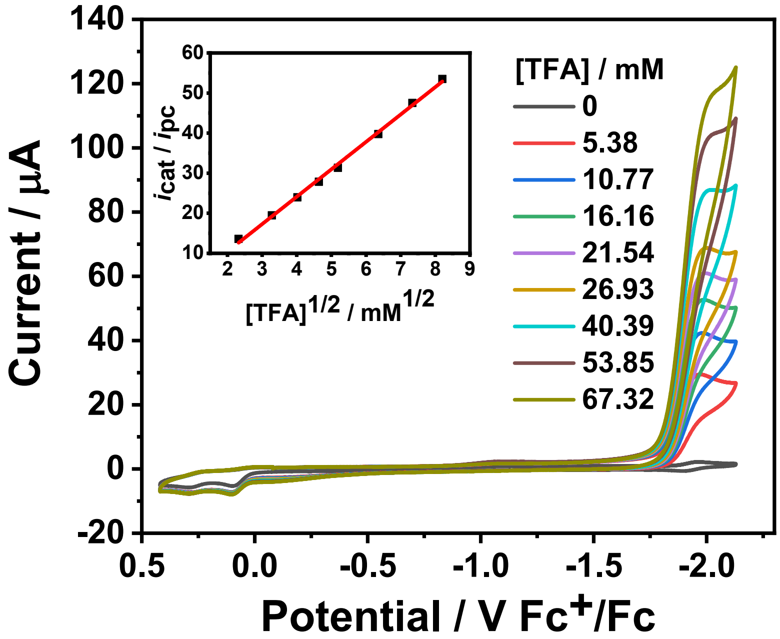
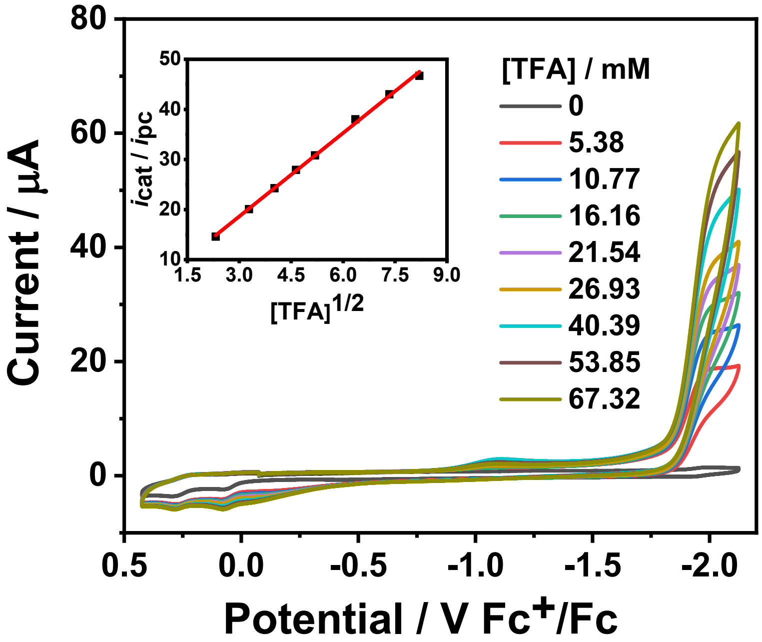


Figure S18. CVs of 0.25 mM **4** in DMF with different TFA concentrations (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat} /i_{pc} against the square root of TFA concentration.



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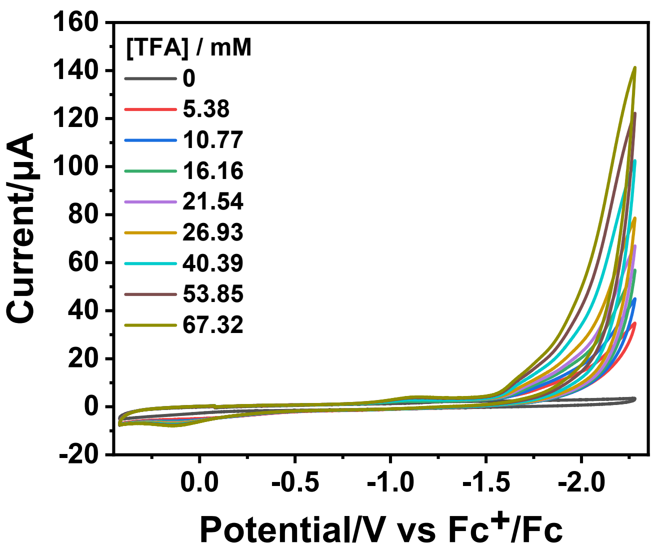


Figure S20. CVs of different TFA concentrations without complex in DMF (0, 5.38, 16.15, 21.54, 26.92, 40.39, 53.85, and 67.32 mM) at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Inset: Plot of the i_{cat} /i_{pc} against the square root of TFA concentration.

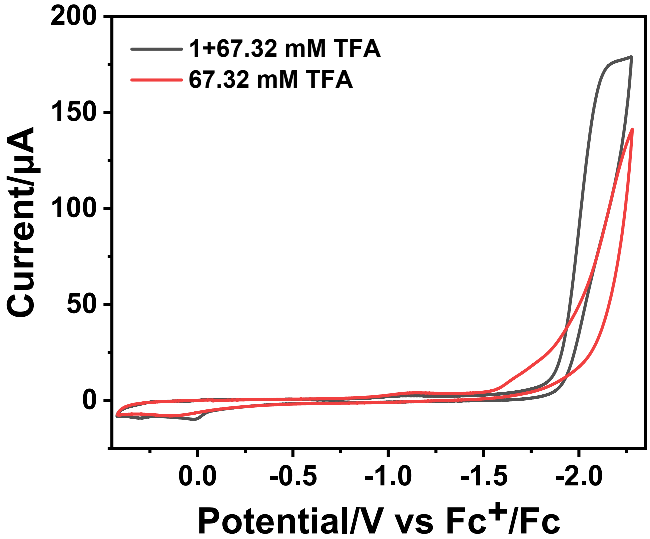


Figure S21. Red: Cyclic voltammogram of 67.32 mM TFA without **1** in DMF. Black: Cyclic voltammogram of 0.25 mM **1** with 67.32 mM TFA in DMF. Conditions: 0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; 100 mV s^{-1} scan rate.

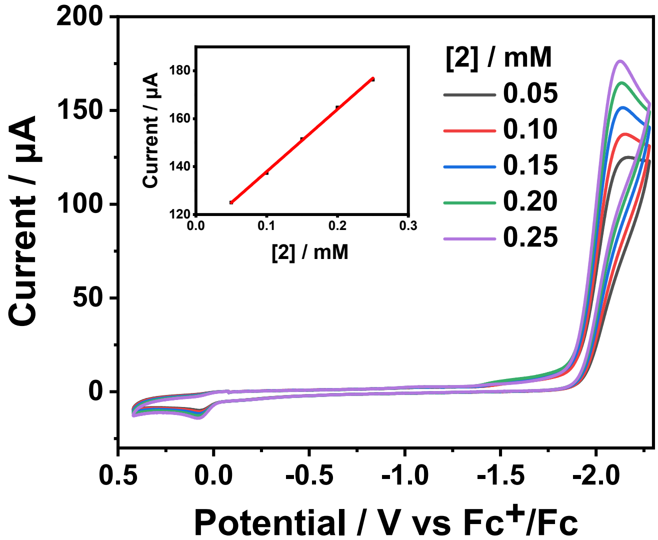
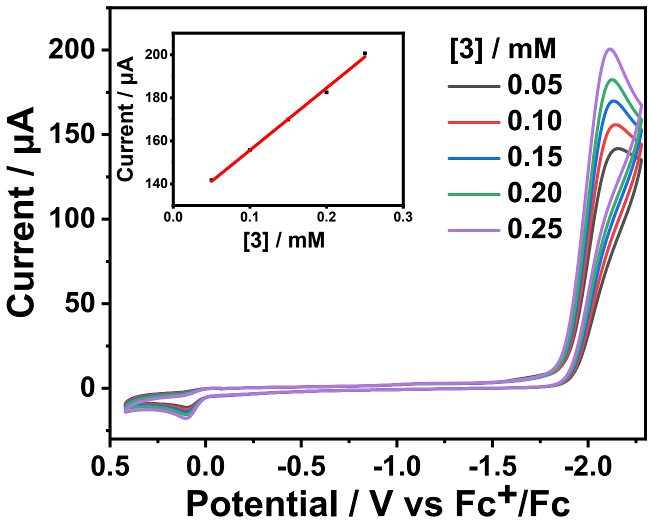


Figure S22. CVs of 0.05-0.25 mM **2** in DMF with 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Insert: Plot of the i_{cat} against the complex **2** concentration.



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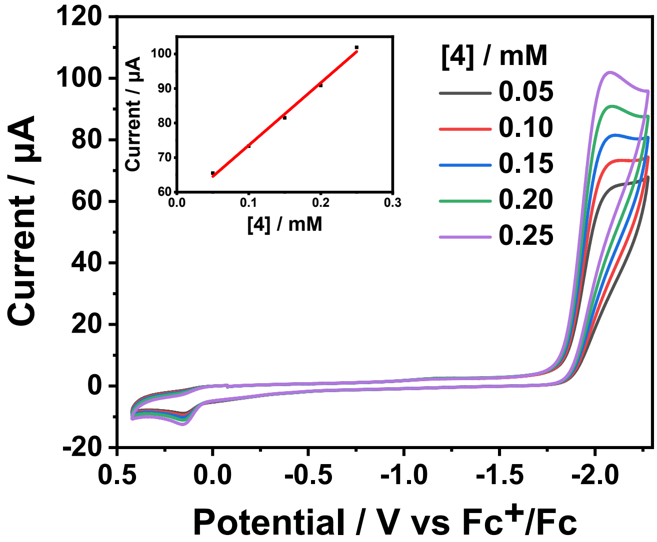

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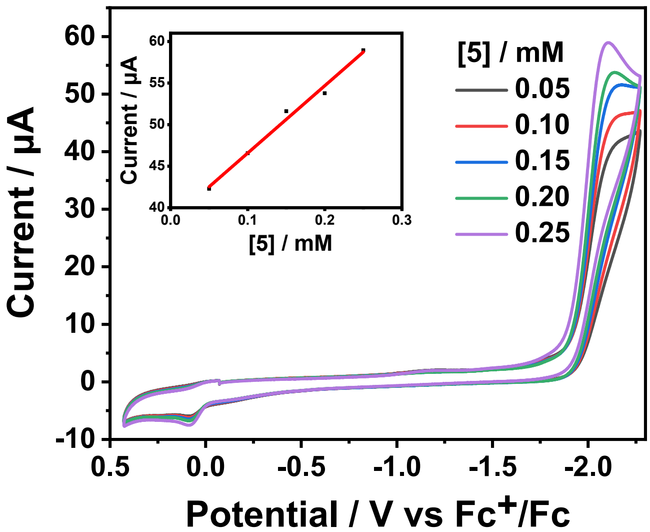

Figure S25. CVs of 0.05-0.25 mM **5** in DMF with 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode). Insert: Plot of the i_{cat} against the complex **5** concentration.

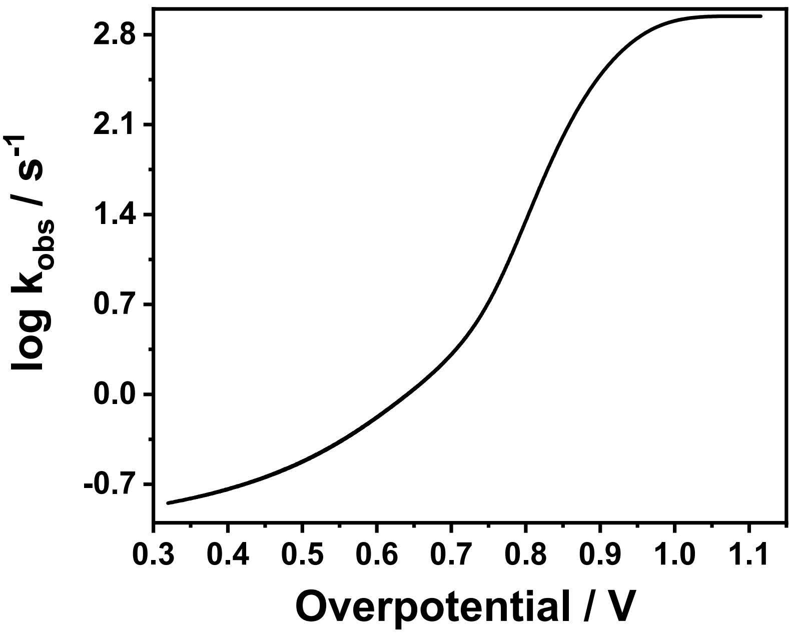

Figure S26. Plot of log k_{obs} versus overpotential of 0.25 mM **2** in DMF in the presence of 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; a glassy carbon working electrode).

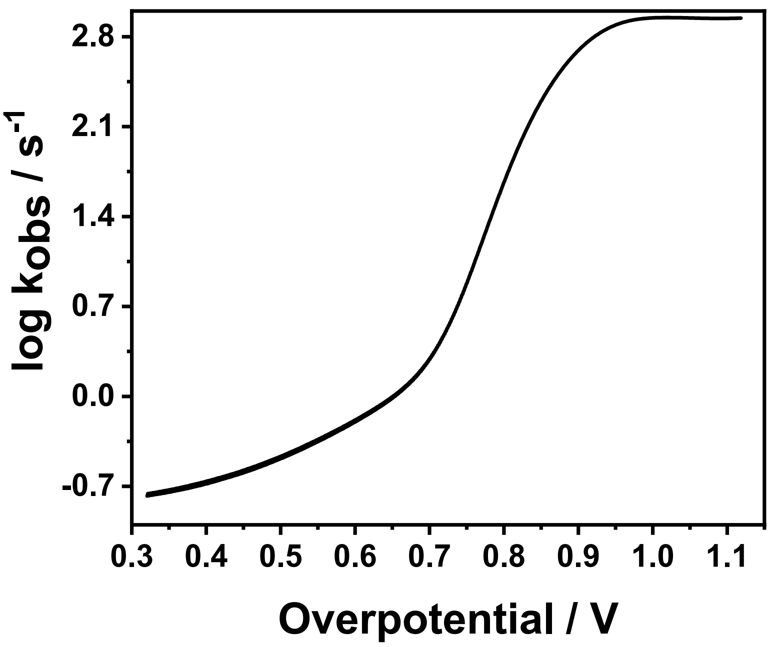

Figure S27. Plot of log k_{obs} versus overpotential of 0.25 mM **3** in DMF in the presence of 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; a glassy carbon working electrode).

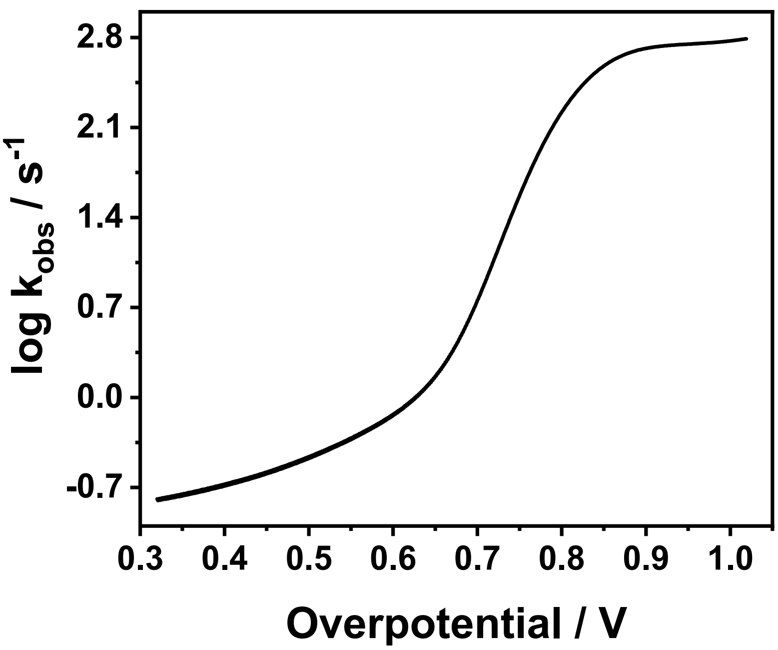

Figure S28. Plot of log k_{obs} versus overpotential of 0.25 mM **4** in DMF in the presence of 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; a glassy carbon working electrode).

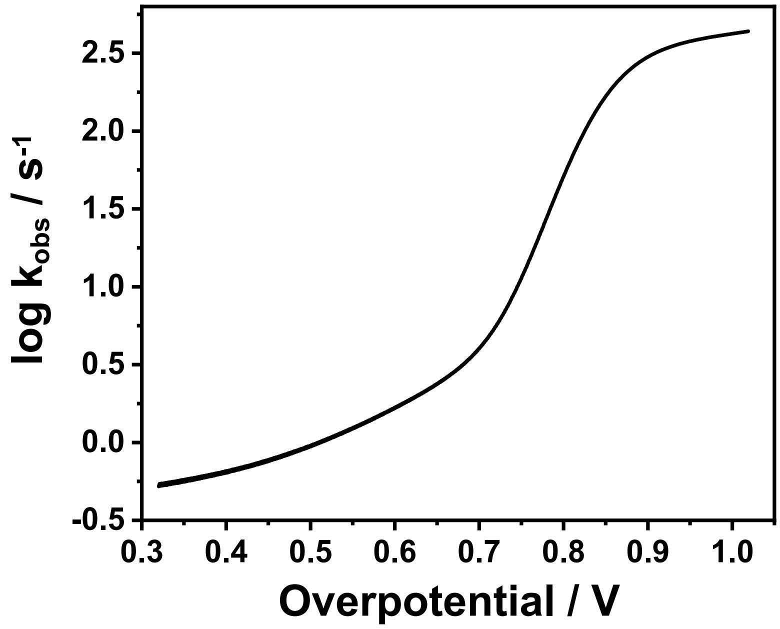

Figure S29. Plot of log k_{obs} versus overpotential of 0.25 mM **5** in DMF in the presence of 67.32 mM TFA at a scan rate of 100 mV s^{-1} (0.1 M n-Bu_4NPF_6 supporting electrolyte; a glassy carbon working electrode).

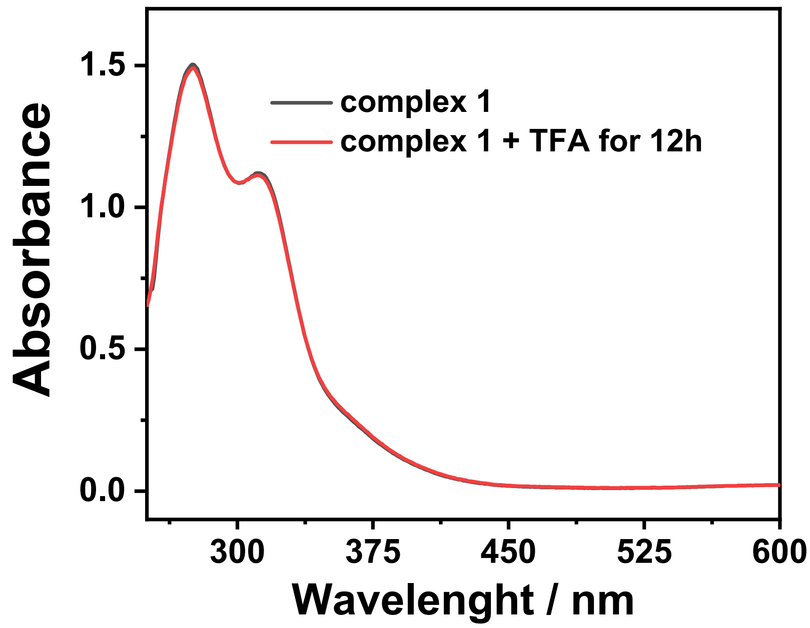

Figure S30. UV-Vis absorption spectra of 0.25 mM **1** in the presence of 5.38 mM TFA in MeCN.

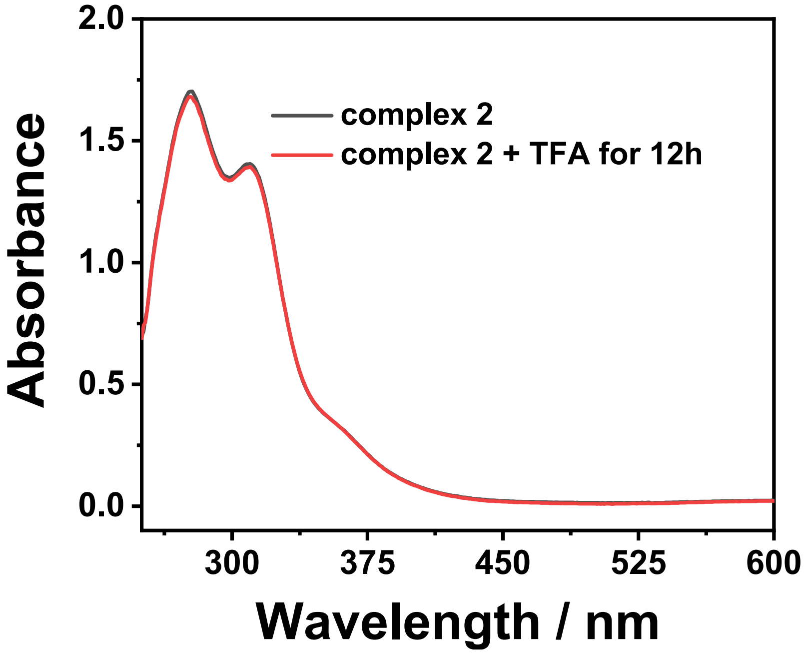

Figure S31. UV-Vis absorption spectra of 0.25 mM **2** in the presence of 5.38 mM TFA in MeCN.

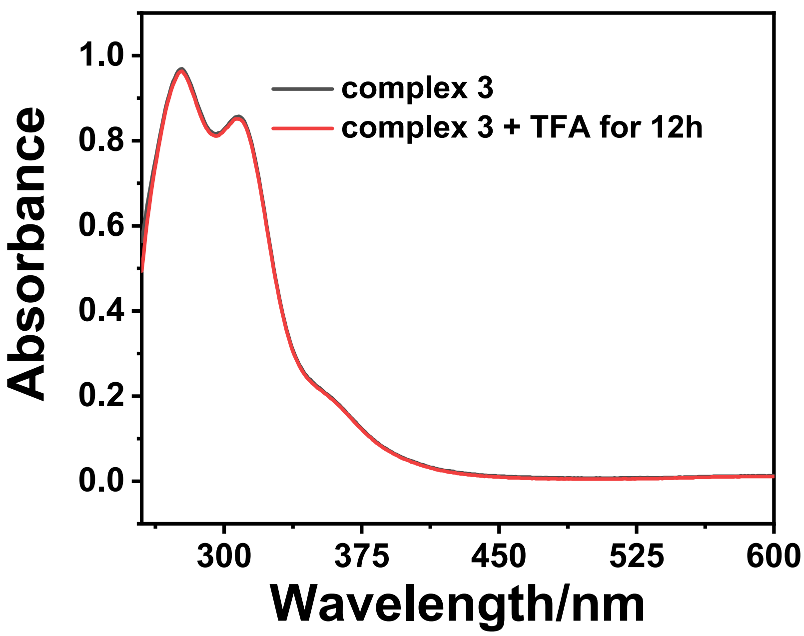

Figure S32. UV-Vis absorption spectra of 0.25 mM **3** in the presence of 5.38 mM TFA in MeCN.

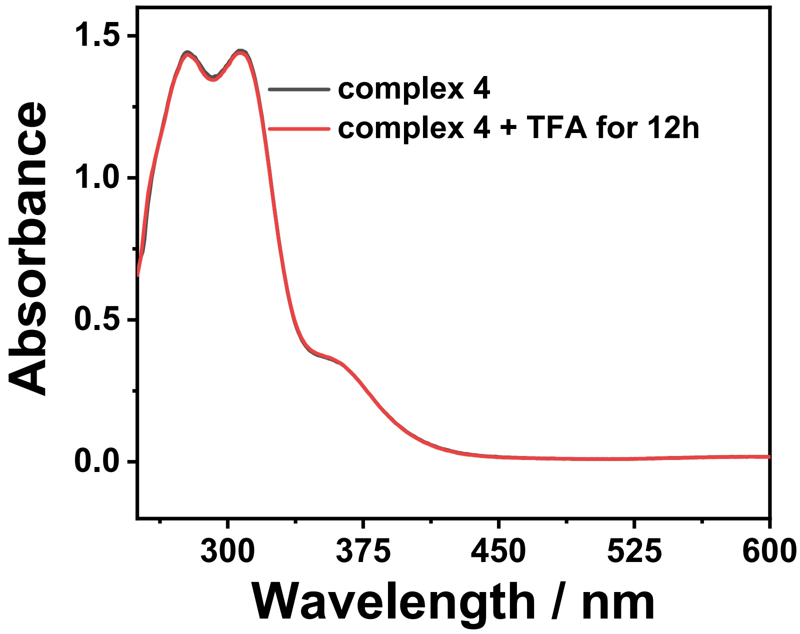

Figure S33. UV-Vis absorption spectra of 0.25 mM **4** in the presence of 5.38 mM TFA in MeCN.

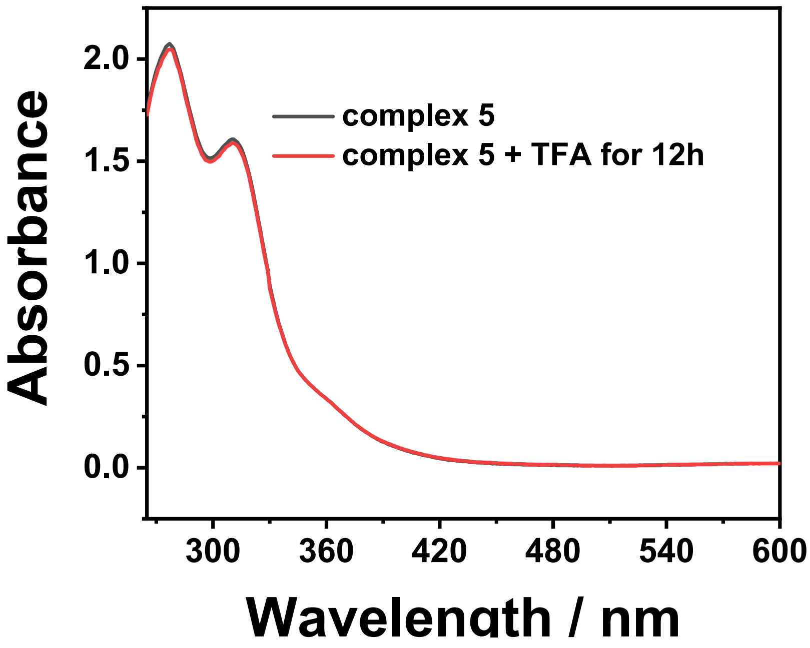

Figure S34. UV-Vis absorption spectra of 0.25 mM **5** in the presence of 5.38 mM TFA in MeCN.

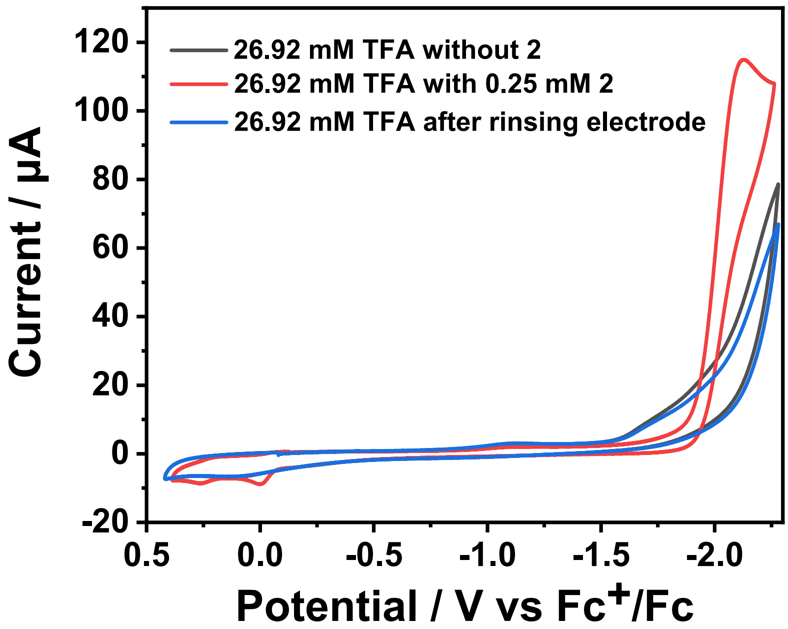

Figure S35. Cyclic voltammograms of **2** (0.25 mM) in DMF with 26.92 mM TFA (red) and a subsequent CV using the same electrode after rinsing and transfer to fresh in DMF of 26.92 mM TFA without adding **2** (blue). For comparison, CV of 26.92 mM TFA without **2** is shown in grey (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

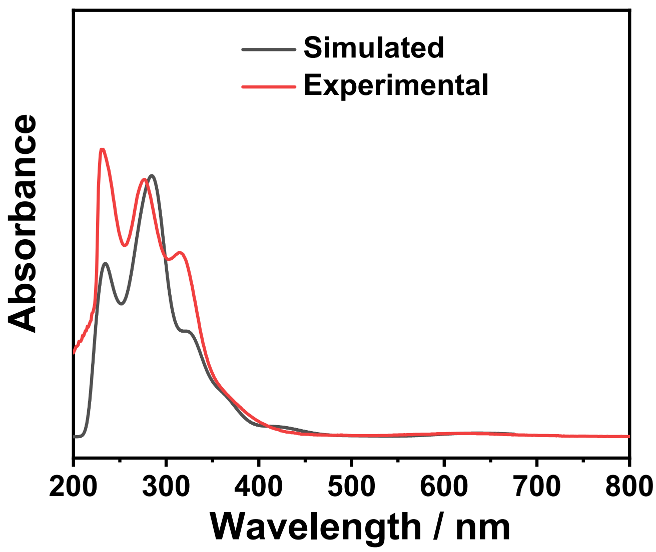

Figure S36. Simulated and experimental UV-vis absorption spectra of complex **1**.

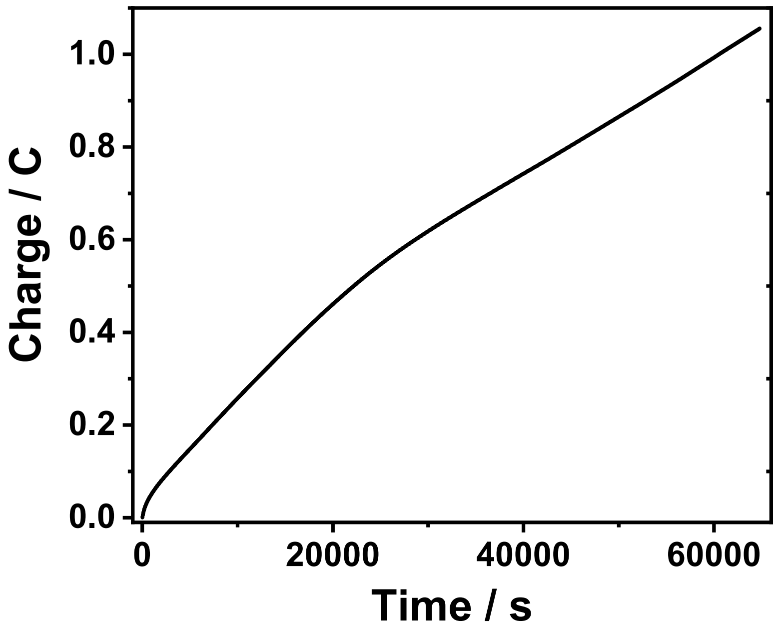

Figure S37. Cumulative coulombs in the presence of 53.8 mM TFA electrolysis for 18 h at a constant potential of -2.00 V (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode).

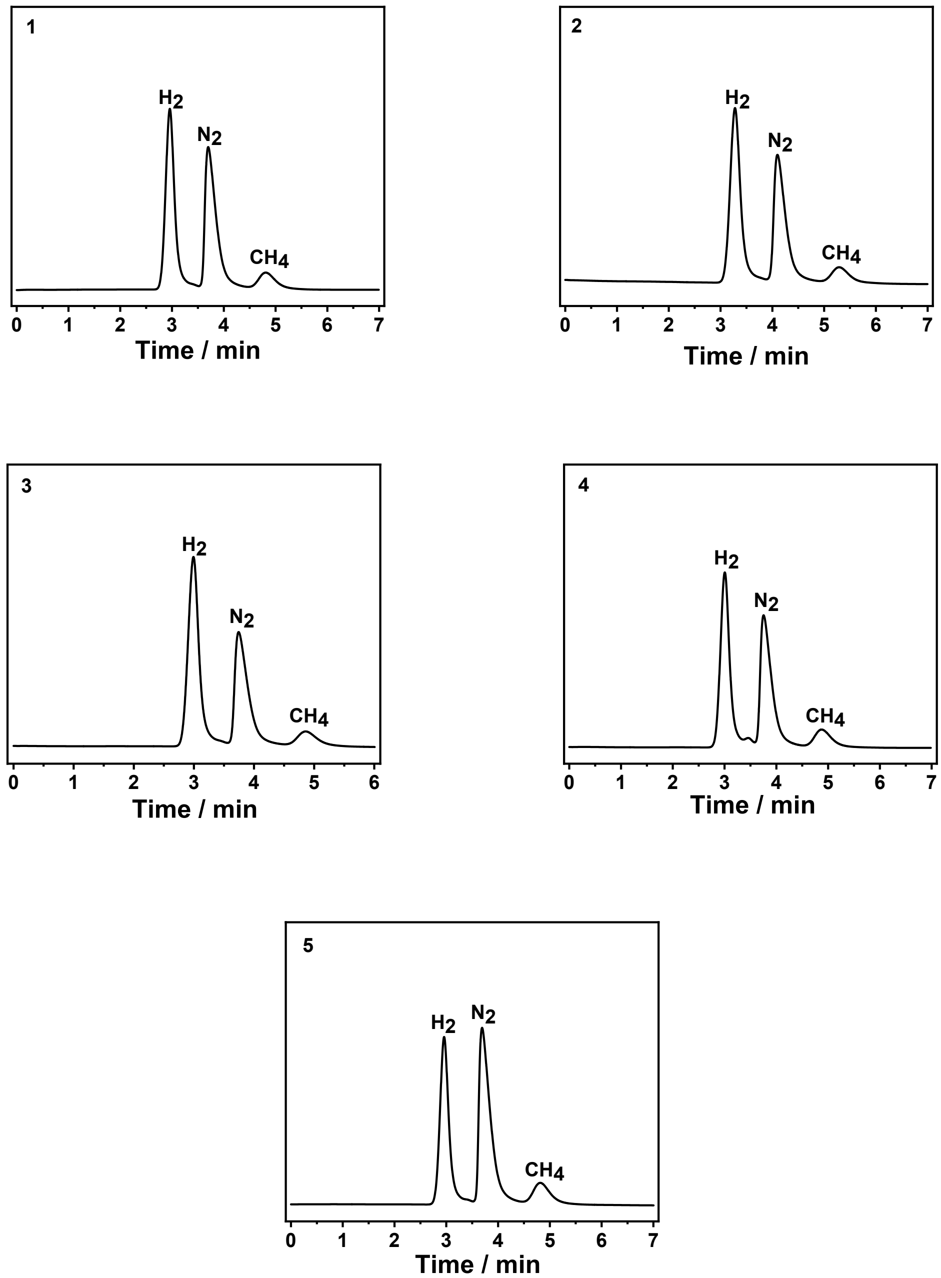

Figure S38. GC-TCD chromatograms of H_2 production of the controlled potential electrolysis of 0.25 mM **1 - 5** with 53.8 mM TFA in DMF over 18 h at a constant potential of -2.00 V, respectively.

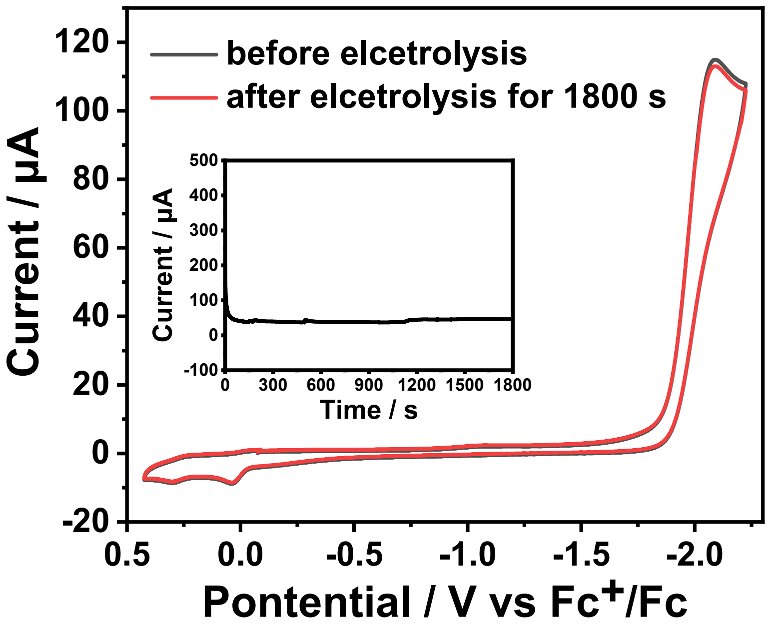

Figure S39. Cyclic voltammograms of 0.25 mM **2** with 26.93 mM TFA before and after electrolysis. Inset: Amperometric i-t curve of the **2** at a constant potential of -2.00 V. (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

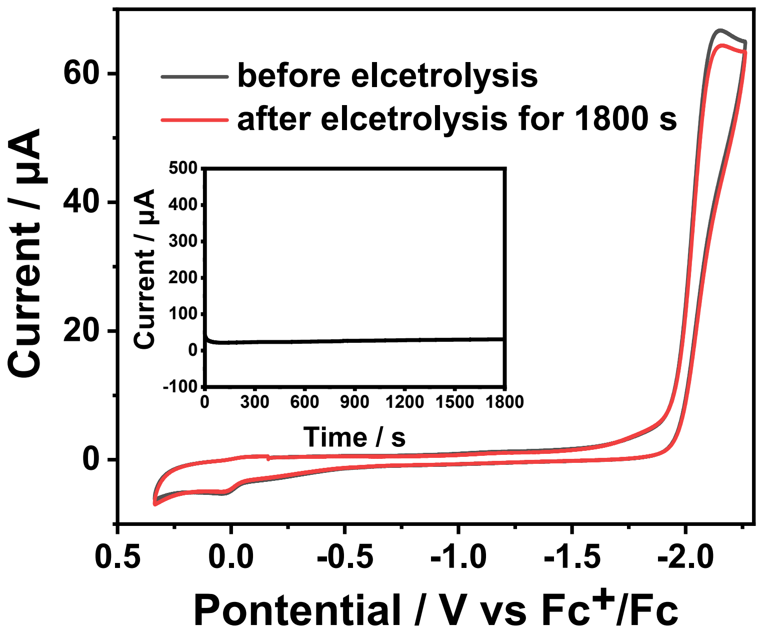

Figure S40. Cyclic voltammograms of 0.25 mM **3** with 26.93 mM TFA before and after electrolysis. Inset: Amperometric i-t curve of **3** at a constant potential of -2.00 V. (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

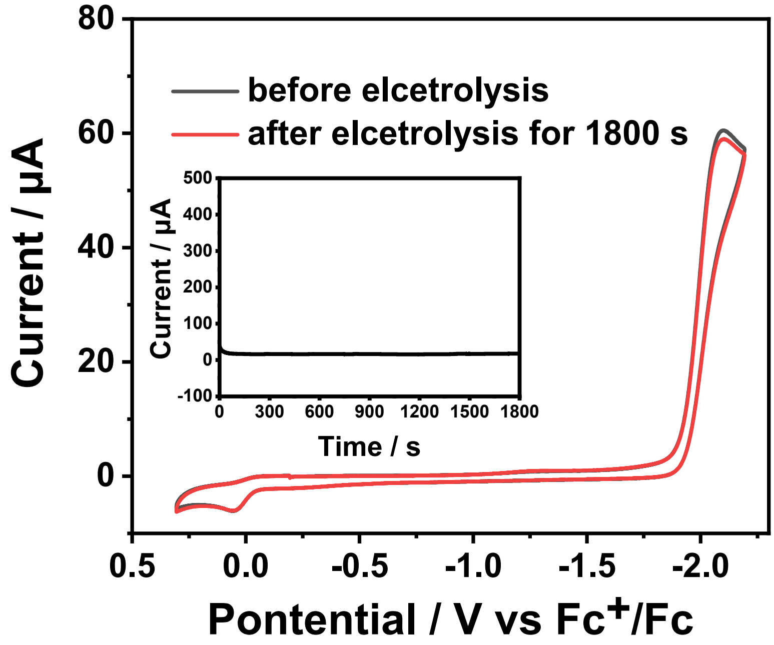

Figure S41. Cyclic voltammograms of 0.25 mM **4** with 26.93 mM TFA before and after electrolysis. Inset: Amperometric i-t curve spectra of **4** at a constant potential of -2.00 V. (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

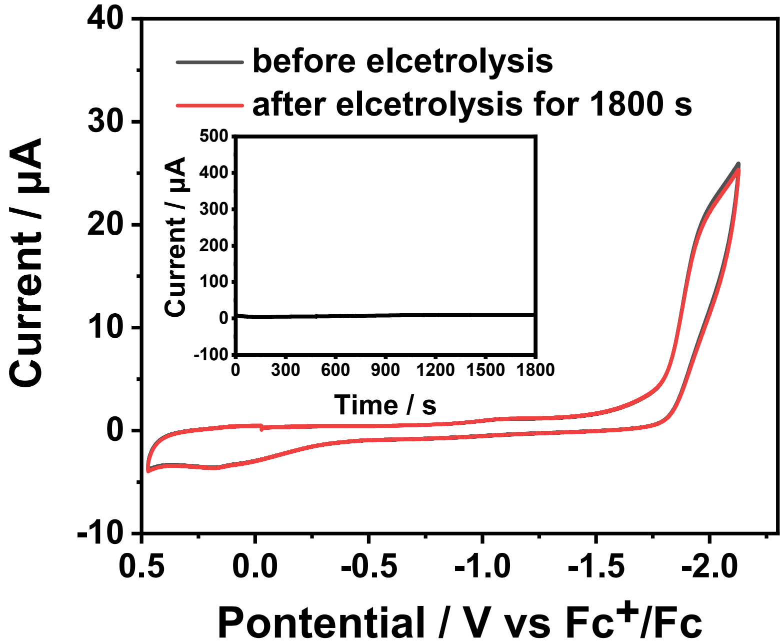

Figure S42. Cyclic voltammograms of 0.25 mM **5** with 26.93 mM TFA before and after electrolysis. Inset: Amperometric i-t curve spectra of **5** at a constant potential of -2.00 V. (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode; scan rate 100 mV s^{-1}).

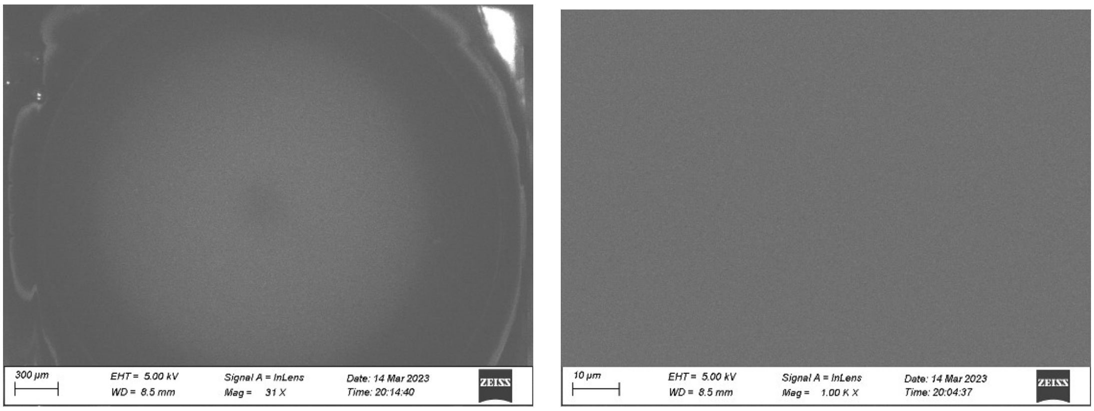

Figure S43. SEM images of the surface of the rinsed glassy carbon electrode after 18 hours of CPE testing at 0.25 mM 1 and 53.8 mM TFA.

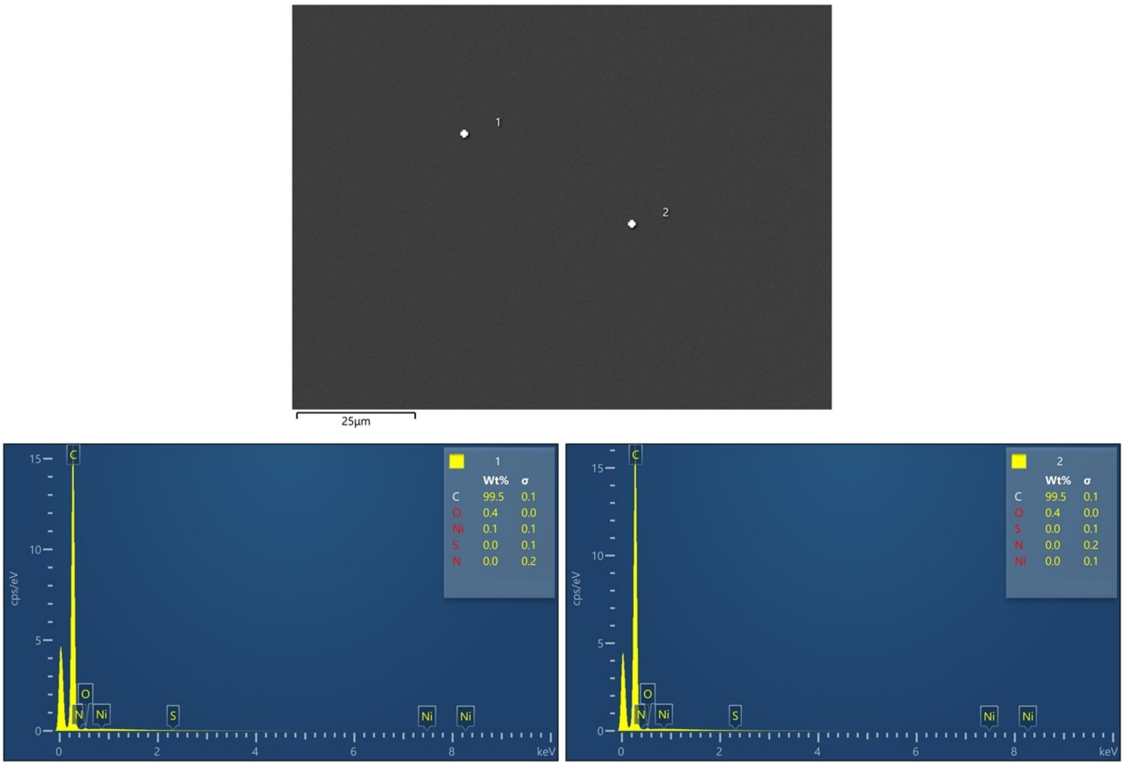

Figure S44. EDS diagrams of the surface of the rinsed glassy carbon electrode after 18 hours of CPE testing at 0.25 mM **1** and 53.8 mM TFA.

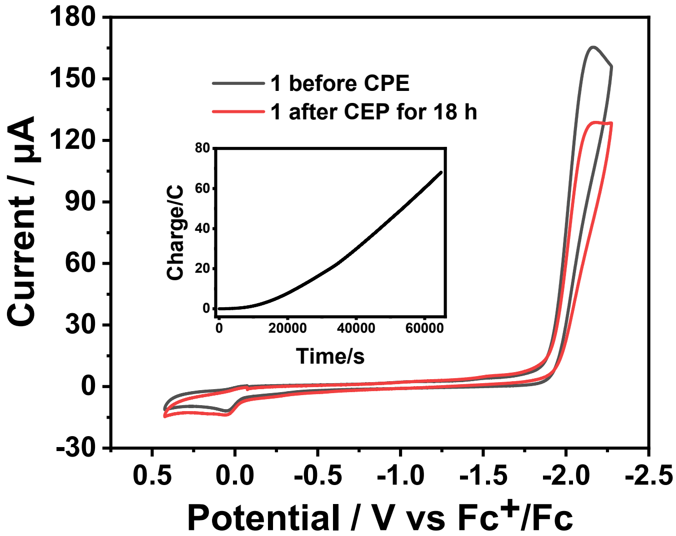

Figure S45. Cyclic voltammograms of 0.25 mM **1** with 53.8 mM TFA before and after CPE for 18 h (0.1 M n-Bu_4NPF_6 supporting electrolyte; glassy carbon working electrode).

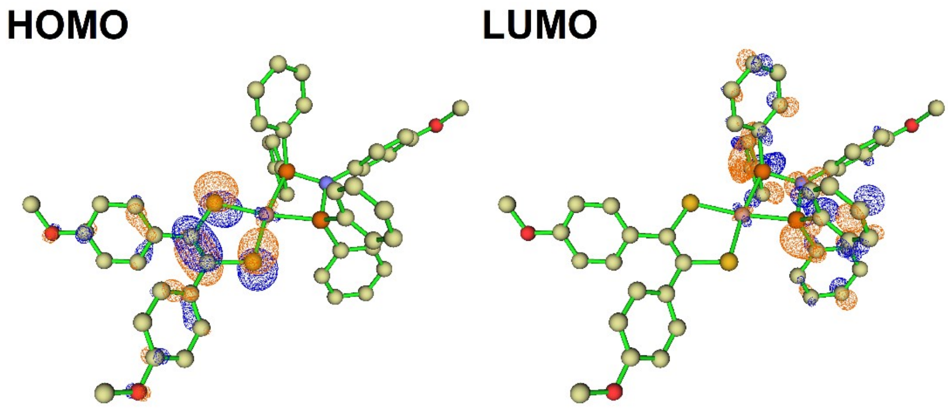

Figure S46. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **1**.

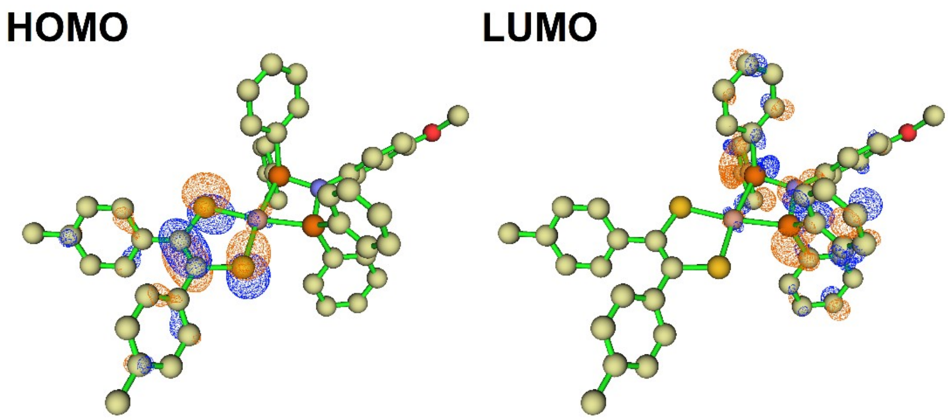

Figure S47. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **2**.

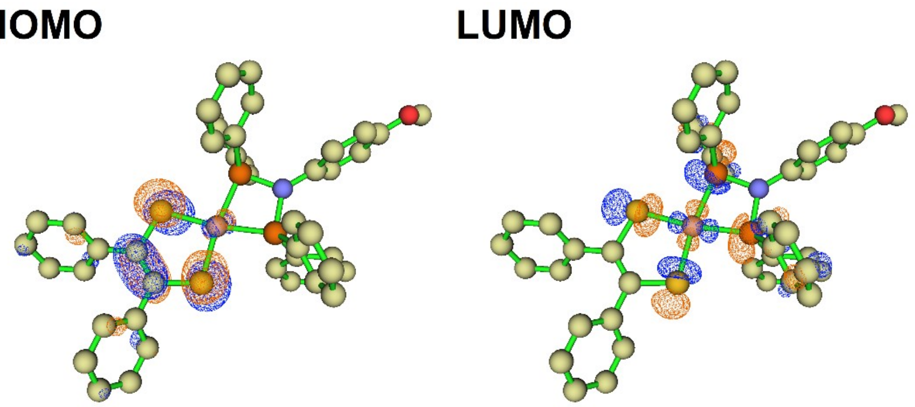

Figure S48. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **3**.

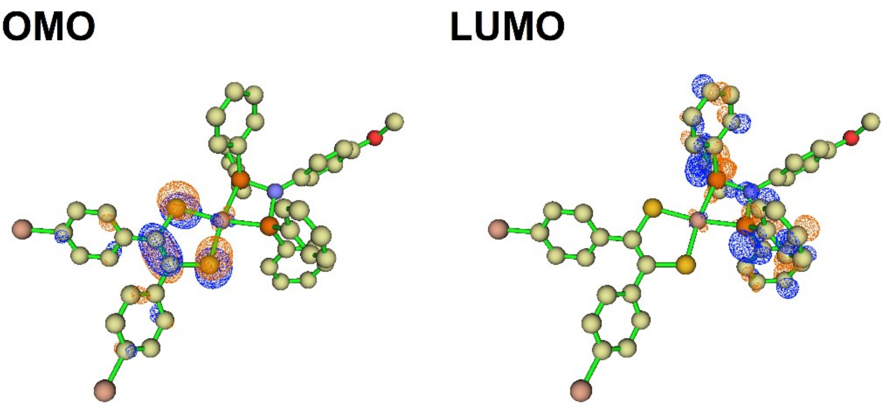

Figure S49. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **4**.

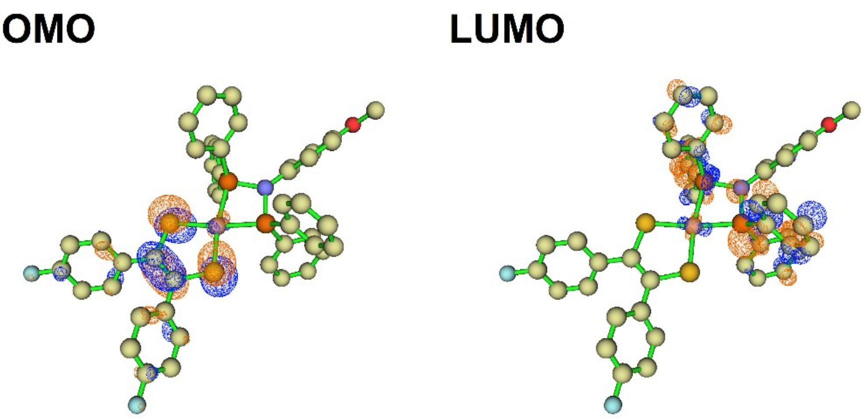

Figure S50. Electron density profiles of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of **5**.

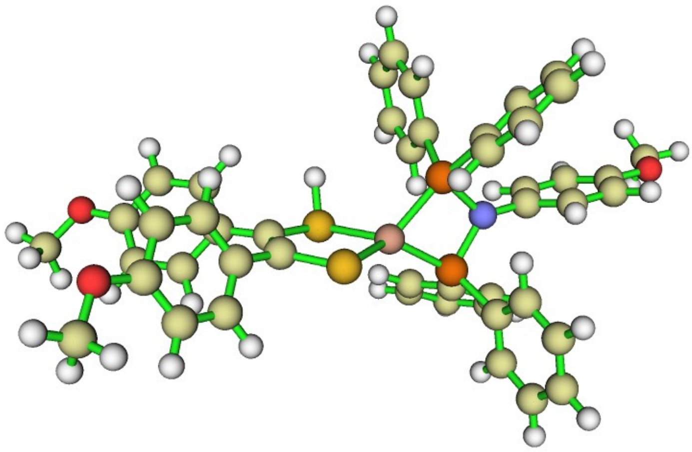

Figure S51. Molecular structure of **[1**(L-H)**]**⁻ after DFT optimization.

```
 Zero-point correction=                           0.767577
(Hartree/Particle)
 Thermal correction to Energy=                    0.820253
 Thermal correction to Enthalpy=                  0.821198
 Thermal correction to Gibbs Free Energy=         0.673390
 Sum of electronic and zero-point Energies=          -5084.544428
 Sum of electronic and thermal Energies=             -5084.491752
 Sum of electronic and thermal Enthalpies=           -5084.490807
 Sum of electronic and thermal Free Energies=        -5084.638615
```

Figure S52. Energy shown in the output file after DFT optimization of [**1**(Ni-H)].

```
 Zero-point correction=                           0.767262
(Hartree/Particle)
 Thermal correction to Energy=                    0.820884
 Thermal correction to Enthalpy=                  0.821828
 Thermal correction to Gibbs Free Energy=         0.669469
 Sum of electronic and zero-point Energies=          -5084.550933
 Sum of electronic and thermal Energies=             -5084.497311
 Sum of electronic and thermal Enthalpies=           -5084.496367
 Sum of electronic and thermal Free Energies=        -5084.648727
```

Figure S53. Energy shown in the output file after DFT optimization of [**1**(L-H)].

Table S1. Crystal data and structure refinements for **2** and **4**·CH_2Cl_2.		
Complex	**2**	**4**·CH_2Cl_2
Empirical formula	$C_{47}H_{41}NNiOP_2S_2$	$C_{46}H_{37}Br_2Cl_2NNiOP_2S_2$
Formula weight	820.58	1035.25
Temperature / K	100.15	100.15
Crystal system	triclinic	triclinic
Space group	P -1	P -1
a / Å	8.8890(18)	8.874(17)
b / Å	14.156(3)	16.683(12)
c / Å	16.604(3)	16.979(12)
α / °	99.930(3)	118.128(4)
β / °	100.826(3)	102.945(4)
Γ / °	95.150(3)	94.354(6)
Volume / Å^3	2005.2(7)	2112(5)
Z	2	2
ρ_{calc} / g cm^{-3}	1.359	1.628
μ / mm^{-1}	0.705	2.691
F(000)	856.0	1044.0
Crystal size / mm^3	0.12 × 0.1 × 0.09	0.18 × 0.12 × 0.11
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2θ range for data collection / °	5.224 to 50.018	4.818 to 50.018
Index ranges	$-10 \leq h \leq 10$	$-9 \leq h \leq 10$
	$-15 \leq k \leq 16$	$-19 \leq k \leq 19$
	$-13 \leq l \leq 19$	$-20 \leq l \leq 11$
Reflections collected	10042	10613
Independent reflections	6981	7306
	R_{int} = 0.0133; R_{sigma} = 0.0283	R_{int} = 0.0479; R_{sigma} = 0.0955
Data / restraints / parameters	6981/0/490	7306/0/533
Goodness-of-fit on F^2	1.037	1.031
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0360; wR_2 = 0.0871	R_1 = 0.0666; wR_2 = 0.1860
Final R indexes [all data]	R_1 = 0.0462; wR_2 = 0.0941	R_1 = 0.0876; wR_2 = 0.1993
Largest diff. peak/hole / e Å^{-3}	1.08 / -0.58	1.20 / -1.78

Table S2. Selected bond lengths (Å) and angles (°) for **2** and **4**·CH_2Cl_2.			
2			
Ni1-S1	2.1322(7)	Ni1-S2	2.1290(8)
Ni1-P2	2.1323(7)	Ni1-P1	2.1425(7)
P2-N1	1.7096(19)	P1-N1	1.718(2)
S2-C9	1.762(2)	S1-C8	1.747(3)
C8-C9	1.381(4)	P2-Ni1-P1	74.38(3)
S1-Ni1-S2	92.42(3)	S1-Ni1-P2	95.19(3)
S2-Ni-P1	98.23(3)	P2-N1-P1	97.84(10)
4·CH_2Cl_2			
Ni1-S1	2.125(2)	Ni1-S2	2.124(2)
Ni1-P2	2.137(2)	Ni1-P1	2.140(2)
P2-N1	1.697(5)	P1-N1	1.706(5)
S1-C7	1.776(7)	S2-C8	1.751(7)
C7-C8	1.344(10)	P2-Ni1-P1	73.63(7)
S1-Ni1-S2	91.76(7)	S1-Ni1-P1	98.34(7)
S2-Ni-P2	97.05(8)	P2-N1-P1	97.7(3)

Diffusion coefficient calculations

The diffusion coefficient (D_0) of the reduction of Ni^{II} to Ni^{I} is calculated by the Randles-Sevcik's equation (Eq. 1). [9]

$$i_{pc} = 0.4463n^{3/2}FAC_{cat}(FvD_0/RT)^{1/2} \tag{1}$$

where, i_{pc} denotes reduction peak current in A, n refers to the number of electron transferred, F is Faraday constant (96500 C mol^{-1}), A expresses the surface area of the glassy carbon working electrode (0.071 cm^2), C_{cat} stands the complex concentration (0.25×10^{-6} mol cm^{-3}), R represents the idea gas constant (8.314 J K^{-1} mol^{-1}), T is the temperature (298 K), D_0 designates the diffusion coefficient for complex in cm^2 s^{-1}, and v is the potential scan rate in V s^{-1}.

Calculation of the diffusion coefficient for complex **1**
Rearranging Eq. 1

$$i_{pc} = 0.4463F^{3/2}AC_{cat}(1/RT)^{1/2}D_0^{1/2}v^{1/2}$$

$$i_{pc} = Sv^{1/2}$$

Where S is obtained using the fitting of the data shown Figure 3 and has a value of 12.45×10^{-6}. Now the derivation of D_0 is possible as follows:

$$D_0 = [S/(0.4463F^{3/2}AC_{cat}(1/RT)^{1/2})^2$$

Using the experimental data, we obtain: $D_0=6.8\times10^{-6}$ cm^2 s^{-1}.

Computational Input Cartesian
[1]
0 1

Ni	3.35370000	4.59560000	12.07100000
S	3.40070000	3.60760000	10.18570000
S	4.25280000	2.93690000	13.06440000
P	3.27960000	5.94530000	13.73330000
P	2.36180000	6.34000000	11.35010000
C	4.14540000	2.06330000	10.52390000
C	4.50160000	1.75640000	11.78040000
N	2.35290000	7.11110000	12.87600000
C	4.84040000	6.73510000	14.21260000
C	2.40730000	5.57020000	15.26560000
C	3.25080000	7.39860000	10.19430000
C	0.67460000	6.18490000	10.71490000
C	4.39180000	1.18840000	9.34900000
C	5.06860000	0.45410000	12.21490000
C	1.88570000	8.40130000	13.25850000
C	5.80210000	6.87240000	13.21630000
C	5.09510000	7.24240000	15.47690000

C	1.06510000	5.90130000	15.41640000
C	3.05940000	4.87330000	16.27890000
C	3.97140000	8.50670000	10.60680000
C	3.33080000	7.00780000	8.85800000
C	0.15430000	6.97900000	9.70100000
C	-0.12340000	5.18350000	11.26580000
C	3.38780000	0.86990000	8.44630000
C	5.64910000	0.63940000	9.14030000
C	4.56160000	-0.75500000	11.75920000
C	6.12340000	0.40390000	13.11470000
C	1.17300000	9.18550000	12.36950000
C	2.13580000	8.89790000	14.53180000
H	5.64650000	6.50770000	12.35300000
C	6.98200000	7.53790000	13.48130000
C	6.27920000	7.90770000	15.73590000
H	4.45320000	7.13260000	16.16860000
H	0.60670000	6.35140000	14.71660000
C	0.39440000	5.57630000	16.58470000
C	2.38150000	4.54630000	17.43930000
H	3.96970000	4.62250000	16.17340000
H	3.95030000	8.77250000	11.51860000
C	4.71860000	9.22470000	9.69980000
C	4.08390000	7.72690000	7.95900000
H	2.85980000	6.23650000	8.56520000
H	0.68710000	7.66190000	9.31090000
C	-1.14360000	6.77370000	9.25890000
C	-1.42200000	4.98920000	10.82440000
H	0.22740000	4.62780000	11.95180000
C	3.62550000	-0.02370000	7.41320000
H	2.52980000	1.26770000	8.53670000
H	6.36150000	0.86710000	9.72620000
C	5.88160000	-0.23220000	8.09540000
H	3.83720000	-0.75410000	11.14460000
C	5.08960000	-1.96020000	12.18180000
C	6.63750000	-0.80470000	13.54340000
H	6.49820000	1.21350000	13.44130000
H	0.99500000	8.85990000	11.49500000
C	0.71510000	10.44080000	12.73890000
C	1.67860000	10.14630000	14.90070000
H	2.62600000	8.37320000	15.15390000
H	7.63540000	7.63470000	12.79840000
C	7.21500000	8.06410000	14.73900000
H	6.44700000	8.25730000	16.60320000
H	-0.52020000	5.81160000	16.68800000

C	1.05260000	4.91240000	17.59670000
H	2.82680000	4.06980000	18.13000000
H	5.19950000	9.99240000	9.98620000
C	4.77250000	8.83530000	8.37830000
H	4.12660000	7.45580000	7.04950000
H	-1.49620000	7.31660000	8.56370000
C	-1.92380000	5.79090000	9.81870000
H	-1.96260000	4.31010000	11.21050000
C	4.86780000	-0.60560000	7.23740000
H	2.92090000	-0.24070000	6.81410000
H	6.75540000	-0.58130000	7.96470000
H	4.72290000	-2.77110000	11.84930000
C	6.14030000	-2.00970000	13.07830000
H	7.34930000	-0.80880000	14.17260000
H	0.22240000	10.96730000	12.12050000
C	0.97500000	10.92620000	14.00540000
H	1.84930000	10.47130000	15.77700000
H	8.02170000	8.53390000	14.91490000
H	0.59590000	4.70510000	18.40350000
H	5.28800000	9.33620000	7.75710000
H	-2.81370000	5.66230000	9.51200000
O	0.56340000	12.14110000	14.47560000
C	0.07330000	13.07820000	13.53050000
H	-0.17570000	13.90670000	13.99090000
H	0.77010000	13.26920000	12.86830000
H	-0.71300000	12.70620000	13.07920000
O	5.11032186	-1.58290140	6.22203548
O	6.68575448	-3.25345085	13.52603120
C	7.80951001	-3.60202516	12.71327695
H	8.28582759	-4.47095476	13.11698837
H	7.47885387	-3.80717063	11.71654135
H	8.50470026	-2.78877128	12.69815661
C	5.05321374	-2.99941471	6.40946204
H	4.92954168	-3.47992662	5.46145701
H	5.96147933	-3.33593737	6.86411149
H	4.22588896	-3.24228824	7.04305982

[1]$^-$

-1 2

Ni	-0.12954080	-0.01660277	-0.07817385
S	-1.62101064	-1.58678479	-0.07696467
S	-1.67054803	1.50533110	-0.08106971
P	1.61051972	1.32461535	-0.03451417
P	1.64714770	-1.30777020	-0.09592553

C	-3.17091865	-0.74209598	-0.07137094
C	-3.19353115	0.61147559	-0.08540777
N	2.73018064	0.02322565	-0.05221881
C	1.99534467	2.30659948	1.44365583
C	2.00294941	2.36533733	-1.47265855
C	2.03000774	-2.33811217	1.35268929
C	2.08802415	-2.28051645	-1.56414640
C	-4.36409146	-1.61294455	0.00635510
C	-4.41560886	1.44211241	-0.16017256
C	4.15345012	0.04499906	-0.01753027
C	0.98840878	2.47885417	2.39617977
C	3.27535199	2.81907615	1.68816441
C	1.91115678	1.75560869	-2.72989665
C	2.31056961	3.72279719	-1.39344353
C	1.83958796	-1.74346074	2.60604725
C	2.43070838	-3.67137308	1.28297081
C	3.39327427	-2.72922341	-1.80066215
C	1.09286226	-2.51627236	-2.51537420
C	-4.53461710	-2.69247170	-0.87215998
C	-5.35457974	-1.40126750	0.96528508
C	-5.41750421	1.17891871	-1.10626782
C	-4.60700700	2.52937914	0.69218617
C	4.83653148	-0.31635521	1.13823020
C	4.88342301	0.43283733	-1.14493852
H	0.00075223	2.07747990	2.20044664
C	1.25729607	3.16219174	3.57713652
C	3.53946748	3.49136019	2.87328099
H	4.06374571	2.69022137	0.95848057
H	1.63570981	0.70993687	-2.80073444
C	2.16092880	2.48358218	-3.88181949
C	2.55118762	4.45372675	-2.55325047
H	2.35895219	4.21586353	-0.43257156
H	1.48962205	-0.71957689	2.66523764
C	2.08391671	-2.46017001	3.76614063
C	2.66532938	-4.39205279	2.45051523
H	2.55467460	-4.15365488	0.32347508
H	4.17310131	-2.54950947	-1.07250617
C	3.69385145	-3.40200973	-2.97676148
C	1.39851852	-3.20110092	-3.68649022
H	0.08625800	-2.16093025	-2.32777723
C	-5.65162942	-3.50531183	-0.80766202
H	-3.77593152	-2.88637704	-1.61932833
H	-5.24384033	-0.58141470	1.66217501
C	-6.48504919	-2.20819539	1.04225763

H	-5.29073934	0.34914090	-1.78819153
C	-6.56068090	1.95159293	-1.17947121
C	-5.75214072	3.31917261	0.62995058
H	-3.84534273	2.76299770	1.42487755
H	4.27621840	-0.60921236	2.01439754
C	6.22731786	-0.30606905	1.17859004
C	6.26482721	0.46271656	-1.10915538
H	4.35737151	0.71113011	-2.04674242
H	0.47065094	3.29872044	4.30825252
C	2.53059428	3.66498873	3.81753823
H	4.53198730	3.88160685	3.06029774
H	2.09023891	2.00191871	-4.84872682
C	2.48456651	3.83640554	-3.79500346
H	2.78965870	5.50736560	-2.48210161
H	1.93552917	-1.99088449	4.73035102
C	2.50054432	-3.78799443	3.68977361
H	2.97494225	-5.42757355	2.38753325
H	4.70578589	-3.74154495	-3.15839184
C	2.69644142	-3.64050157	-3.91908559
H	0.62137791	-3.38697244	-4.41684496
C	-6.63961875	-3.26717019	0.14939101
H	-5.78324348	-4.33267883	-1.49297696
H	-7.22735713	-2.00209586	1.79965497
H	-7.33031417	1.74324188	-1.91134491
C	-6.73957292	3.02873473	-0.30864620
H	-5.85831309	4.14805081	1.31462717
H	6.72856847	-0.59614461	2.09000396
C	6.94911674	0.08876515	0.05164604
H	6.83941872	0.76383246	-1.97492819
H	2.73951387	4.19350547	4.73935691
H	2.67190765	4.40728694	-4.69563055
H	2.68229248	-4.35145566	4.59627489
H	2.93383630	-4.16900005	-4.83396164
O	8.30524986	0.14284969	-0.01734466
C	9.06154586	-0.22376460	1.12675322
H	10.10540878	-0.10716667	0.84518317
H	8.84148564	0.42833167	1.97773297
H	8.87759236	-1.26433652	1.41161599
O	-7.70639753	-4.12096642	0.13370489
O	-7.90162161	3.73256218	-0.45882992
C	-8.12871913	4.84514300	0.38594153
H	-9.09457969	5.25338526	0.09475888
H	-8.16554595	4.55075259	1.44035722
H	-7.35898510	5.61356967	0.25675367

C	-8.74153687	-3.92163052	1.07866552
H	-9.48030699	-4.69689432	0.88499752
H	-8.37493716	-4.02233439	2.10577067
H	-9.21097350	-2.93913202	0.96163012

[1(Ni-H)**]**

0 2

Ni	0.15857236	-0.03281208	0.01678986
S	1.71210079	-1.66155085	0.00204293
S	1.76146226	1.58500959	0.33463165
P	-1.65806498	0.98795414	-0.89339727
P	-1.69535997	-0.97010296	0.94600607
C	3.22178417	-0.73963951	0.10195549
C	3.24288731	0.61428148	0.27581174
N	-2.75216463	0.03089043	0.02770901
C	-2.21724896	0.79760944	-2.62466044
C	-2.03621476	2.72563828	-0.47112158
C	-2.17882633	-2.68943427	0.55906675
C	-2.21172860	-0.72577000	2.68462108
C	4.46543229	-1.53627362	-0.06986607
C	4.50913487	1.36383733	0.49161314
C	-4.17829305	0.06823819	0.03151940
C	-1.45419122	-0.04175640	-3.44055089
C	-3.39192738	1.35909829	-3.13711541
C	-2.21794891	3.05028630	0.87911559
C	-1.96475659	3.76271203	-1.40629834
C	-2.40934756	-3.02160054	-0.78161802
C	-2.14841728	-3.71562431	1.50858986
C	-3.40943137	-1.21023952	3.22117442
C	-1.38581856	0.07300988	3.47974020
C	4.75489797	-2.63526794	0.75298559
C	5.39294606	-1.23218294	-1.06824573
C	5.39893947	1.00479853	1.51550569
C	4.86217324	2.46202007	-0.29528693
C	-4.91022406	-0.60384108	-0.94357276
C	-4.87135664	0.78685521	1.01139550
H	-0.54443052	-0.47990182	-3.04532609
C	-1.85732856	-0.32186016	-4.74221518
C	-3.79453714	1.08000425	-4.43713829
H	-3.99794636	2.00898446	-2.51959640
H	-2.23878495	2.26394326	1.62284550
C	-2.35976421	4.37250158	1.27798342
C	-2.09827505	5.08860993	-1.00417412
H	-1.80284969	3.54191498	-2.45331646

H	-2.39702549	-2.24554857	-1.53621941
C	-2.64237175	-4.33789060	-1.15667005
C	-2.37231153	-5.03617796	1.13005452
H	-1.94922446	-3.49053640	2.54828891
H	-4.06176513	-1.82963328	2.61978300
C	-3.77432969	-0.89364343	4.52370280
C	-1.75038068	0.38959278	4.78448337
H	-0.45781266	0.45140821	3.06573818
C	5.91677386	-3.37252661	0.59989279
H	4.05350920	-2.90789236	1.53167800
H	5.20015130	-0.39582813	-1.72846502
C	6.56633867	-1.96518408	-1.24264134
H	5.15555002	0.16595015	2.15534933
C	6.58358604	1.69120059	1.72773620
C	6.05052420	3.16327267	-0.10099616
H	4.19424867	2.77661705	-1.08761687
H	-4.38985204	-1.15424447	-1.71336276
C	-6.30159112	-0.56686907	-0.95546906
C	-6.25458250	0.82907374	1.01226653
H	-4.31927732	1.30639111	1.78049238
H	-1.25707518	-0.97385735	-5.36493775
C	-3.02887333	0.23837288	-5.24109364
H	-4.70838150	1.51552595	-4.82282568
H	-2.50908801	4.60388490	2.32576769
C	-2.30272111	5.39785999	0.33625957
H	-2.04401385	5.87974482	-1.74237378
H	-2.83007422	-4.57453371	-2.19709006
C	-2.62779019	-5.35108082	-0.20035172
H	-2.34920348	-5.81869296	1.87900164
H	-4.70704113	-1.26835667	4.92768812
C	-2.94628946	-0.09229306	5.30679520
H	-1.10148617	1.00951394	5.39100354
C	6.83702971	-3.04342480	-0.40113505
H	6.13085257	-4.21136246	1.25123948
H	7.24957286	-1.68833913	-2.03283302
H	7.25757962	1.39997971	2.52435534
C	6.92422399	2.77666438	0.91663017
H	6.28195670	3.99924351	-0.74596667
H	-6.83480080	-1.09727845	-1.73058046
C	-6.98283597	0.15294534	0.02758944
H	-6.78976369	1.38287115	1.77341235
H	-3.34502944	0.02213480	-6.25438237
H	-2.41061918	6.42976785	0.64716826
H	-2.80778872	-6.37844517	-0.49233850

H	-3.23304948	0.15336822	6.32213002
O	-8.33499920	0.25427830	0.10898119
C	-9.12745689	-0.42255403	-0.86616125
H	-10.16340857	-0.20813106	-0.61086368
H	-8.92217628	-0.05287900	-1.87487574
H	-8.96364293	-1.50338348	-0.83396261
O	7.94973040	-3.82757712	-0.47556088
O	8.10959998	3.38982582	1.19536890
C	8.50139636	4.49859859	0.39138532
H	9.46669593	4.82273526	0.77659295
H	8.61238938	4.21470021	-0.65935785
H	7.78765547	5.32401554	0.47084952
C	8.89498373	-3.56265229	-1.50838386
H	9.68526180	-4.30220390	-1.39141951
H	8.44542327	-3.67204202	-2.49995574
H	9.32474890	-2.56077185	-1.41397008
H	0.43692150	-0.22292841	-1.39348583

[1(L-H)**]**

0 2

Ni	0.15857236	-0.03281208	0.01678986
S	1.74089553	-1.68121806	-0.14384766
S	1.79025700	1.56534238	0.18874106
P	-1.65806498	0.98795414	-0.89339727
P	-1.69535997	-0.97010296	0.94600607
C	3.25057891	-0.75930672	-0.04393510
C	3.27168205	0.59461427	0.12992115
N	-2.75216463	0.03089043	0.02770901
C	-2.21724896	0.79760944	-2.62466044
C	-2.03621476	2.72563828	-0.47112158
C	-2.17882633	-2.68943427	0.55906675
C	-2.21172860	-0.72577000	2.68462108
C	4.49422703	-1.55594083	-0.21575666
C	4.53792961	1.34417012	0.34572255
C	-4.17829305	0.06823819	0.03151940
C	-1.45419122	-0.04175640	-3.44055089
C	-3.39192738	1.35909829	-3.13711541
C	-2.21794891	3.05028630	0.87911559
C	-1.96475659	3.76271203	-1.40629834
C	-2.40934756	-3.02160054	-0.78161802
C	-2.14841728	-3.71562431	1.50858986
C	-3.40943137	-1.21023952	3.22117442
C	-1.38581856	0.07300988	3.47974020
C	4.78369271	-2.65493515	0.60709500

C	5.42174080	-1.25185015	-1.21413632
C	5.42773421	0.98513132	1.36961510
C	4.89096798	2.44235286	-0.44117752
C	-4.91022406	-0.60384108	-0.94357276
C	-4.87135664	0.78685521	1.01139550
H	-0.54443052	-0.47990182	-3.04532609
C	-1.85732856	-0.32186016	-4.74221518
C	-3.79453714	1.08000425	-4.43713829
H	-3.99794636	2.00898446	-2.51959640
H	-2.23878495	2.26394326	1.62284550
C	-2.35976421	4.37250158	1.27798342
C	-2.09827505	5.08860993	-1.00417412
H	-1.80284969	3.54191498	-2.45331646
H	-2.39702549	-2.24554857	-1.53621941
C	-2.64237175	-4.33789060	-1.15667005
C	-2.37231153	-5.03617796	1.13005452
H	-1.94922446	-3.49053640	2.54828891
H	-4.06176513	-1.82963328	2.61978300
C	-3.77432969	-0.89364343	4.52370280
C	-1.75038068	0.38959278	4.78448337
H	-0.45781266	0.45140821	3.06573818
C	5.94556860	-3.39219382	0.45400220
H	4.08230394	-2.92755957	1.38578741
H	5.22894604	-0.41549534	-1.87435561
C	6.59513341	-1.98485129	-1.38853193
H	5.18434476	0.14628294	2.00945874
C	6.61238078	1.67153338	1.58184561
C	6.07931894	3.14360546	-0.24688675
H	4.22304341	2.75694984	-1.23350746
H	-4.38985204	-1.15424447	-1.71336276
C	-6.30159112	-0.56686907	-0.95546906
C	-6.25458250	0.82907374	1.01226653
H	-4.31927732	1.30639111	1.78049238
H	-1.25707518	-0.97385735	-5.36493775
C	-3.02887333	0.23837288	-5.24109364
H	-4.70838150	1.51552595	-4.82282568
H	-2.50908801	4.60388490	2.32576769
C	-2.30272111	5.39785999	0.33625957
H	-2.04401385	5.87974482	-1.74237378
H	-2.83007422	-4.57453371	-2.19709006
C	-2.62779019	-5.35108082	-0.20035172
H	-2.34920348	-5.81869296	1.87900164
H	-4.70704113	-1.26835667	4.92768812
C	-2.94628946	-0.09229306	5.30679520

H	-1.10148617	1.00951394	5.39100354
C	6.86582445	-3.06309201	-0.54702564
H	6.15964731	-4.23102967	1.10534889
H	7.27836760	-1.70800634	-2.17872361
H	7.28637436	1.38031250	2.37846475
C	6.95301873	2.75699717	0.77073958
H	6.31075144	3.97957630	-0.89185726
H	-6.83480080	-1.09727845	-1.73058046
C	-6.98283597	0.15294534	0.02758944
H	-6.78976369	1.38287115	1.77341235
H	-3.34502944	0.02213480	-6.25438237
H	-2.41061918	6.42976785	0.64716826
H	-2.80778872	-6.37844517	-0.49233850
H	-3.23304948	0.15336822	6.32213002
O	-8.33499920	0.25427830	0.10898119
C	-9.12745689	-0.42255403	-0.86616125
H	-10.16340857	-0.20813106	-0.61086368
H	-8.92217628	-0.05287900	-1.87487574
H	-8.96364293	-1.50338348	-0.83396261
O	7.97852514	-3.84724433	-0.62145147
O	8.13839472	3.37015861	1.04947831
C	8.53019110	4.47893138	0.24549473
H	9.49549067	4.80306805	0.63070236
H	8.64118412	4.19503300	-0.80524844
H	7.81645021	5.30434833	0.32495893
C	8.92377847	-3.58231950	-1.65427445
H	9.71405654	-4.32187111	-1.53731010
H	8.47421801	-3.69170923	-2.64584633
H	9.35354364	-2.58043906	-1.55986067
H	2.01524400	-2.95471116	-0.28186305

[1(L-H)**]**$^-$
-1 1

Ni	0.13423000	0.17494500	-0.08323800
S	1.71863400	-1.44924100	-0.55230100
S	1.81394800	1.70792200	0.02658300
P	-1.78977500	1.10209900	-0.89369000
P	-1.61029400	-0.93236800	0.88258000
C	3.27893600	-0.63360500	-0.19464500
C	3.26714200	0.70794000	0.00926200
N	-2.75590800	0.03493500	0.04992900
C	-2.37470700	0.89635300	-2.60761800
C	-2.28997200	2.78696900	-0.40169900
C	-1.94525200	-2.65934700	0.40540400

C	-2.04830700	-0.80669600	2.64496400
C	4.48868200	-1.48409400	-0.28714500
C	4.53966700	1.43564200	0.27171600
C	-4.18044500	-0.02572900	0.13293000
C	-1.52680100	0.21875200	-3.48738200
C	-3.64269800	1.29205500	-3.04840500
C	-2.35208200	3.06779400	0.96911700
C	-2.45315700	3.83398000	-1.31266100
C	-2.15735100	-2.93401000	-0.95137400
C	-1.82220900	-3.72624300	1.29991000
C	-3.19026000	-1.38794000	3.20635500
C	-1.22880200	-0.00134500	3.44037600
C	4.66660800	-2.57721000	0.57220800
C	5.49057600	-1.22976100	-1.22394900
C	5.35340000	1.08944800	1.35750000
C	4.95647300	2.48585100	-0.54384300
C	-4.91442500	-0.75916800	-0.79401300
C	-4.86232200	0.65276500	1.14772400
H	-0.54593800	-0.09186600	-3.14632800
C	-1.93640400	-0.06354100	-4.78633400
C	-4.05195700	1.00691100	-4.34466200
H	-4.31220800	1.81499600	-2.37838600
H	-2.19832000	2.27395800	1.68966800
C	-2.60407800	4.35744600	1.41580900
C	-2.69806700	5.12820500	-0.86242400
H	-2.38949600	3.64709900	-2.37631500
H	-2.22240500	-2.12015400	-1.66288800
C	-2.27768900	-4.24357400	-1.39593900
C	-1.93518000	-5.03859400	0.85031400
H	-1.63662900	-3.53959900	2.34947700
H	-3.83696400	-2.01080100	2.60237300
C	-3.50412800	-1.16284300	4.54058000
C	-1.54409100	0.22281700	4.77629300
H	-0.34649900	0.45349600	3.00417300
C	5.80065600	-3.36719200	0.50832600
H	3.91061100	-2.80432500	1.31471900
H	5.37817300	-0.39519800	-1.90420700
C	6.63822000	-2.01421200	-1.30354900
H	5.05329000	0.27948900	2.01021400
C	6.53613300	1.76232200	1.61228000
C	6.14938400	3.16448500	-0.31052500
H	4.34327400	2.77854100	-1.38682600
H	-4.39925300	-1.28143100	-1.58673200
C	-6.30308800	-0.81976300	-0.72592100

C	-6.24258300	0.59878500	1.22681800
H	-4.30329000	1.21604400	1.88060900
H	-1.27075300	-0.58788400	-5.46074100
C	-3.20054200	0.32851000	-5.21426300
H	-5.03700400	1.31111100	-4.67693800
H	-2.65756900	4.55653900	2.47923500
C	-2.78016000	5.39278300	0.50017500
H	-2.82677700	5.92896100	-1.58048400
H	-2.45175200	-4.43995300	-2.44683500
C	-2.16919800	-5.30083300	-0.49521900
H	-1.84244300	-5.85560400	1.55545700
H	-4.39192600	-1.61276300	4.96787500
C	-2.68252300	-0.35763500	5.32638300
H	-0.90243600	0.84758300	5.38526200
C	6.80067900	-3.09060200	-0.43002100
H	5.93304200	-4.20357500	1.18331300
H	7.38846300	-1.77890800	-2.04471800
H	7.15591200	1.49193700	2.45822000
C	6.94910400	2.80400000	0.77571000
H	6.43947300	3.96425400	-0.97645700
H	-6.84118300	-1.39503000	-1.46468800
C	-6.97589600	-0.13675200	0.28911800
H	-6.77194500	1.12111700	2.01367900
H	-3.52311400	0.10808200	-6.22455100
H	-2.97490500	6.39970900	0.84824800
H	-2.26126300	-6.32258400	-0.84236500
H	-2.93042700	-0.18429800	6.36647000
O	-8.32401600	-0.12789000	0.44699400
C	-9.12495100	-0.85466600	-0.48524400
H	-10.15540100	-0.71646500	-0.16396200
H	-9.00868100	-0.46449600	-1.50035900
H	-8.88411300	-1.92127200	-0.47312800
O	7.87889300	-3.91716800	-0.41485900
O	8.12745400	3.40075300	1.09704300
C	8.59176500	4.47204100	0.27662900
H	9.53790900	4.79097300	0.70954300
H	8.75955700	4.14347100	-0.75303600
H	7.89092200	5.31161200	0.28240900
C	8.91330500	-3.70405600	-1.37389700
H	9.66029400	-4.47205400	-1.18286600
H	8.53821900	-3.81197100	-2.39565500
H	9.37303300	-2.71856800	-1.25622000
H	1.70606700	-2.34225100	0.45857800

[1(L-H)(Ni-H)]
0 1

Ni	0.20698691	0.51149549	-0.26413565
S	1.65240691	-1.21175751	-0.29899865
S	2.18474844	2.12908314	-0.24259649
P	-1.61948909	0.47434349	-1.42087665
P	-1.38298609	0.28201949	1.22205035
C	3.27035191	-0.43738851	-0.10395265
C	3.33904091	0.92561249	-0.10407565
N	-2.60611109	0.26850349	-0.00506665
C	-2.20364809	-0.89721351	-2.51307365
C	-2.33971609	1.95550749	-2.24928565
C	-1.47286909	-1.36531451	2.03246735
C	-2.14666009	1.38551149	2.49392535
C	4.43451291	-1.35160751	-0.10093865
C	4.65426191	1.59969149	0.09104435
C	-4.01023109	0.08096149	0.12058435
C	-1.32814009	-1.96642551	-2.71693665
C	-3.48573109	-0.96722751	-3.07030465
C	-2.60467309	3.08817349	-1.46754365
C	-2.44508509	2.07579049	-3.64016265
C	-1.53743009	-2.50350051	1.21719335
C	-1.25082809	-1.54700451	3.40253035
C	-3.26038709	1.04320249	3.26967835
C	-1.61549909	2.67150749	2.61962935
C	4.53390891	-2.41093451	0.81493135
C	5.47779191	-1.20925651	-1.01992365
C	5.40544391	1.37532049	1.25170835
C	5.17695491	2.47802049	-0.85628665
C	-4.57582109	-1.18868051	0.02341235
C	-4.86154409	1.16672449	0.35635035
H	-0.33507309	-1.92225451	-2.28615265
C	-1.71908009	-3.08104351	-3.45341465
C	-3.87963709	-2.07810951	-3.80714365
H	-4.18315209	-0.15266151	-2.92505165
H	-2.49800109	3.02951849	-0.39146865
C	-2.99105609	4.28774149	-2.05092765
C	-2.82244809	3.28011049	-4.22734365
H	-2.23185909	1.22536649	-4.27555865
H	-1.67219109	-2.38573751	0.14960035
C	-1.42014209	-3.77845151	1.75582535
C	-1.12335209	-2.82389151	3.94254635
H	-1.17478209	-0.68820551	4.05779835
H	-3.69198209	0.05397149	3.18759135

C	-3.82689109	1.96410649	4.14314435
C	-2.18154809	3.59759949	3.49140935
H	-0.75119309	2.94804849	2.02647935
C	5.62198491	-3.26741251	0.82118935
H	3.74867891	-2.56083651	1.54641235
H	5.43148191	-0.41280551	-1.75137265
C	6.58098891	-2.05844551	-1.02724965
H	5.02535491	0.69732449	2.00568235
C	6.62453391	2.00015049	1.45449435
C	6.40737591	3.10604649	-0.67583565
H	4.61571291	2.67282749	-1.76148365
H	-3.93671709	-2.03872751	-0.16632465
C	-5.94812309	-1.38618651	0.15304035
C	-6.22764109	0.98622549	0.48774135
H	-4.44326409	2.15834249	0.44975935
H	-1.02616509	-3.90069251	-3.60136565
C	-2.99728609	-3.13895451	-3.99962765
H	-4.87743809	-2.11912251	-4.22771665
H	-3.20109409	5.14658249	-1.42414465
C	-3.10342809	4.39015949	-3.43643065
H	-2.90079309	3.34821749	-5.30615365
H	-1.48403309	-4.64342551	1.10608135
C	-1.21433709	-3.94565551	3.12402835
H	-0.95552109	-2.94086151	5.00678335
H	-4.69224609	1.68587449	4.73310435
C	-3.28955509	3.24474049	4.25489735
H	-1.75614209	4.59046949	3.57579535
C	6.65992891	-3.09852551	-0.10064465
H	5.68631191	-4.07524151	1.54001735
H	7.36032591	-1.90307751	-1.75925965
H	7.19304991	1.82592749	2.35983435
C	7.14014291	2.86908849	0.48833535
H	6.77880091	3.77058449	-1.44280765
H	-6.34720709	-2.38648551	0.06716135
C	-6.78382809	-0.29312051	0.38770535
H	-6.88190809	1.82856649	0.67532735
H	-3.30518209	-4.00434351	-4.57411365
H	-3.40224409	5.32577449	-3.89312265
H	-1.11931709	-4.93899951	3.54530235
H	-3.73226609	3.96186749	4.93565635
O	-8.13321709	-0.37199851	0.53407035
C	-8.75219909	-1.65342551	0.43647935
H	-9.81558809	-1.48517651	0.59555635
H	-8.60194909	-2.09585651	-0.55255365

H	-8.37907009	-2.33928251	1.20246235
O	7.68722691	-3.98810051	-0.02132965
O	8.34752791	3.43111549	0.76997035
C	8.90929391	4.33991549	-0.17418765
H	9.85755791	4.66474849	0.25003835
H	9.09402191	3.85515349	-1.13735365
H	8.26469991	5.21091349	-0.32388365
C	8.76127691	-3.86660951	-0.95173565
H	9.45386991	-4.67240551	-0.71576365
H	8.41331491	-3.98234051	-1.98243665
H	9.27632691	-2.90714051	-0.84695265
H	1.56074591	-1.82147451	0.90723335
H	0.70547070	1.28412093	-0.37319512

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