

Supporting Information

Brønsted Acid Scaling Relationships Enable Control Over Product Selectivity from O₂ Reduction with a Mononuclear Cobalt Porphyrin Catalyst

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Table of Contents

I. General considerations	S2
II. OCP measurements of $E_{\text{H}^+/\text{H}_2}$ with different buffered conditions	S2
III. Estimation of pK _a values of DMF-H ⁺ , C ₃ H ₇ SO ₃ H and (CO ₂ H) ₂ using OCP measurements....	S4
IV. Estimation of the reduction potentials of O ₂ /H ₂ O ₂ and O ₂ /H ₂ O	S4
V. Electrochemical experiments	S6
VI. Turnover frequencies of ORR catalyzed by 1.....	S8
VII. Selectivity of ORR catalyzed by 1	S11
VIII. Effective overpotentials of ORR catalyzed by 1	S14
IX. Rate law analysis of O ₂ reduction catalyzed by 1	S15
X. EPR experiments and simulations.....	S22
XI. Considerations for differential pulse voltammetry	S22
XII. Computational details.....	S24
XIII. References.....	S58

I. General considerations

All commercially available reagents and solvents were used as received, except where otherwise noted. Perchloric acid (70%) was obtained from Sigma Aldrich. UV-Vis spectra were recorded on an Agilent Cary 60 spectrometer. EPR spectra were recorded on a Bruker EleXsys E500 spectrometer at 9.3 GHz (X-band) and 100 kHz modulation; microwave power: 10 mW, modulation amplitude: 10 G, T: 110 K.

II. OCP measurements of $E_{\text{H}^+/\text{H}_2}$ with different buffered conditions

A. Open-circuit potential (OCP) measurements for $E_{\text{H}^+/\text{H}_2(\text{DMF})}$ with different buffered conditions.

The H^+/H_2 potential in organic media can be determined through open-circuit potential measurements at a Pt electrode using a recently reported protocol.¹ The H^+/H_2 potentials were measured for DMF with various buffered conditions under 1 atm H_2 (local atmospheric pressure of 752 mm Hg, correction to 1 atm < 1 mV). All DMF solutions were containing 0.1 M $[\text{NBu}_4]\text{[ClO}_4]$ as supporting electrolyte. These conditions were chosen to give media that have stable, well-defined thermodynamics for the H^+/H_2 equilibria. Stable open-circuit potentials of H^+/H_2 ($E_{\text{H}^+/\text{H}_2(\text{DMF})}$) were observed, and $E_{\text{H}^+/\text{H}_2(\text{DMF})}$ were referenced to $\text{Fc}^{*+/0}$ by adding decamethylferrocene and performing CV at a second, glassy carbon working electrode in the same solution (Figure S1). The observed H^+/H_2 potentials under different buffered conditions are listed in Table S1.

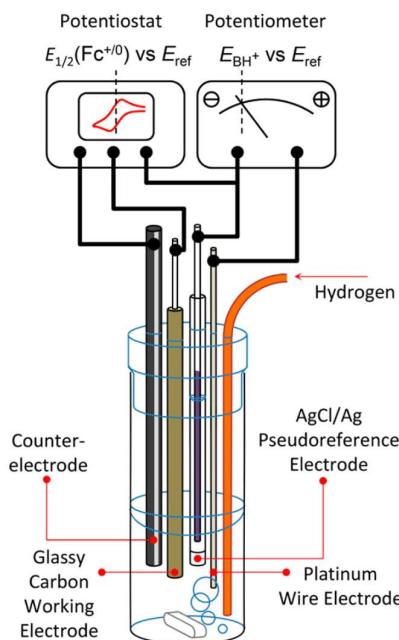


Figure S1. Schematic of the four-electrode cell configuration used for open circuit potential (OCP) measurements.¹ The reduction potential of H^+/H_2 was measured for DMF solutions with various buffered conditions under 1 atm H_2 . All DMF solutions were containing 0.1 M $[\text{NBu}_4]\text{[ClO}_4]$ as supporting electrolyte (Figure S1 is reproduced from ref. 1; copyright 2013 American Chemical Society).

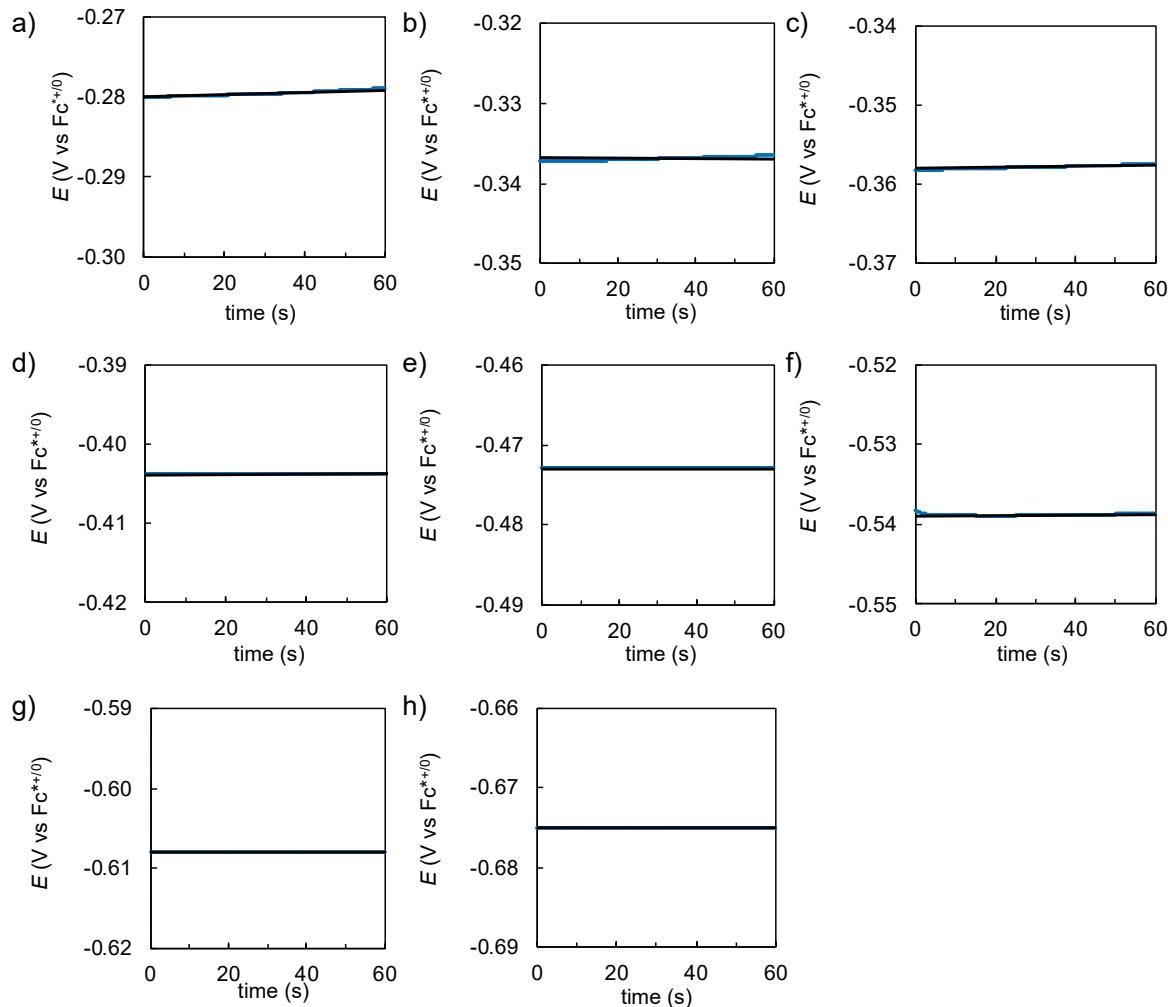


Figure S2. The black traces show the average OCP of $E_{\text{H}^+/\text{H}_2}$ with various buffered conditions in DMF solutions under 1 atm H_2 . (a) 10 mM each of perchloric acid and tetrabutylammonium perchlorate; (b) 10 mM each of *p*-toluenesulfonic acid and sodium *p*-toluenesulfonate; (c) 10 mM each of 1-propanesulfonic acid and sodium 1-propanesulfonate monohydrate; (d) 10 mM each of 2,6-dihydroxybenzoic acid and sodium 2,6-dihydroxybenzoate; (e) 10 mM each of trifluoroacetic acid and sodium trifluoroacetate; (f) 10 mM each of oxalic acid and lithium oxalate; (g) 10 mM each of dichloroacetic acid and sodium dichloroacetate; (h) 10 mM each of maleic acid and sodium maleate. Supporting electrolyte: 0.1 M $[\text{NBu}_4][\text{ClO}_4]$.

Table S1. A summary of $E_{\text{H}^+/\text{H}_2}$ under different buffered conditions in DMF solutions^{a,b}

$E_{\text{H}^+/\text{H}_2}$ (V vs. $\text{Fc}^{**/0}$)	DMF- H^+ /DMF	TsOH/TsONa	$\text{C}_3\text{H}_7\text{SO}_3\text{H}/$ $\text{C}_3\text{H}_7\text{SO}_3\text{Na}$	2,6-(HO) ₂ BA/ 2,6-(NaO) ₂ BA
	-0.28 V	-0.34 V	-0.36 V	-0.40 V
	TFAH/NaTFA	oxalic acid/ lithium oxalate	DCAH/NaDCA	maleic acid/ sodium malonate
	-0.47 V	-0.54 V	-0.61 V	-0.68 V

^aConcentration of each acid and conjugate base is 10 mM; ^bAll potentials are referenced to $\text{Fc}^{**/0}$ in volt, see Figure S2 for the OCP traces; Supporting electrolyte: 0.1 M $[\text{NBu}_4][\text{ClO}_4]$.

III. Estimation of pK_a values of DMF-H^+ , $\text{C}_3\text{H}_7\text{SO}_3\text{H}$ and $(\text{CO}_2\text{H})_2$ using OCP measurements

In Figure S3, the measured OCP values for acids with known pK_{as} in DMF (cf. Figure S2) are plotted with respect to their pK_{as} [2: *p*-toluenesulfonic acid ($pK_a = 2.5$);² 4: 2,6-dihydroxybenzoic acid ($pK_a = 3.6$);^{3,4} 5: trifluoroacetic acid ($pK_a = 4.9$);^{4,5} 7: dichloroacetic acid ($pK_a = 7.5$);^{3,4} 8: maleic acid ($pK_a = 7.9$).^{3,4} The approximately Nernstian slope of $-0.0596 \text{ V}/pK_a$ was then used to determine the pK_a values for the acids with unknown pK_{as} in DMF. From this approach the pK_a values determined for DMF-H^+ , $\text{C}_3\text{H}_7\text{SO}_3\text{H}$, oxalic acid are as follows: DMF-H^+ (1.6), $\text{C}_3\text{H}_7\text{SO}_3\text{H}$ (2.9), and oxalic acid (5.9).

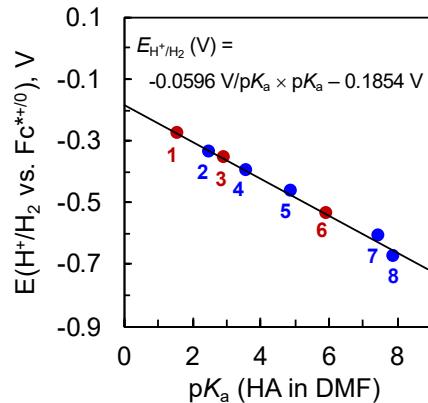
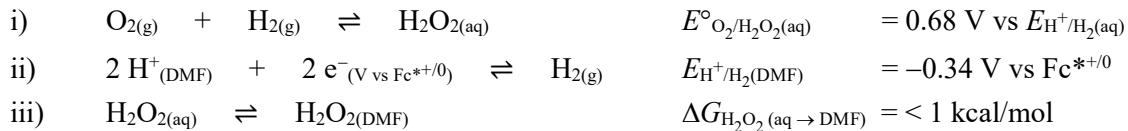


Figure S3. The redox potentials of H^+/H_2 ($E_{\text{H}^+/\text{H}_2}$) vs pK_a for acids with known pK_a in DMF (shown in blue) are plotted to determine the pK_a values of DMF-H^+ (1.6), $\text{C}_3\text{H}_7\text{SO}_3\text{H}$ (2.9) and oxalic acid (5.9) in DMF (shown in red). The redox potentials of H^+/H_2 ($E_{\text{H}^+/\text{H}_2}$) are obtained from the OCP measurements as presented in Section II.

IV. Estimation of the reduction potentials of $\text{O}_2/\text{H}_2\text{O}_2$ and $\text{O}_2/\text{H}_2\text{O}$

A. Estimation of $\text{O}_2/\text{H}_2\text{O}_2$ reduction potential based on OCP measurements of H^+/H_2 .^{2,6}

The reduction potential of $\text{O}_2/\text{H}_2\text{O}_2$ in DMF may be estimated using i) the standard aqueous cell potential for $\text{O}_2 + \text{H}_2 \rightarrow \text{H}_2\text{O}_2$, ii) the measurement of the open circuit potential (OCP) for H^+/H_2 ($E_{\text{H}^+/\text{H}_2}$) with various buffered conditions (Figure S2), and iii) the Gibbs free energy to transfer H_2O_2 from H_2O to DMF.^{7,8} For example, the $\text{O}_2/\text{H}_2\text{O}_2$ couple for the DMF solution in the presence of 10 mM each of *p*-toluenesulfonic acid and sodium *p*-toluenesulfonate is calculated by the following equations:



B. Thermodynamic reduction potentials of $\text{O}_2/\text{H}_2\text{O}_2$ under catalytic conditions.

1. For catalytic O_2 reduction conducted in strong acidic buffers (Table S2, $\text{DMF-H}^+/\text{DMF}$, TsOH/TsONa , $\text{C}_3\text{H}_7\text{SO}_3\text{H/C}_3\text{H}_7\text{SO}_3\text{Na}$, and $2,6-(\text{HO})_2\text{BA}/2,6-(\text{NaO})_2\text{BA}$), each reaction solution contained 100 μM urea- H_2O_2 to provide a stable thermodynamic reference state of $E_{\text{O}_2/\text{H}_2\text{O}_2}$ under non-standard state conditions. For example, the thermodynamic reduction potential of $E_{\text{O}_2/\text{H}_2\text{O}_2}$ for the DMF solution in the presence of 10 mM each of TsOH and TsONa is calculated to be 0.46 V vs $\text{Fc}^{*+/0}$ using the Nernst equation as below:

$$E_{O_2/H_2O_2} = E'_{O_2/H_2O_2} - \frac{0.059}{2} V \times \log\left(\frac{[H_2O_2][A^-]^2}{pO_2[H_A]^2}\right)$$

$$E_{O_2/H_2O_2} = 0.34 \text{ V} (E'_{O_2/H_2O_2}) - 0.030 \text{ V} \times \log([H_2O_2]_{100 \mu\text{M}}/[H_2O_2]_{1 \text{ M}}) = 0.46 \text{ V vs Fc}^{*+/0}$$

Table S2. A summary of thermodynamic reduction potentials of O₂/H₂O₂ under catalytic conditions^{a,b}

Condition	DMF-H ⁺ /DMF	TsOH/TsONa	C ₃ H ₇ SO ₃ H/C ₃ H ₇ SO ₃ Na	2,6-(HO) ₂ BA/2,6-(NaO) ₂ BA
E_{O_2/H_2O_2} (V vs. Fc ^{*+/0})	0.52	0.46	0.44	0.40

^aConcentration of each acid and conjugate base is 10 mM; ^bAll potentials are referenced to Fc^{*+/0} in volt.

2. The thermodynamic reduction potentials of E_{O_2/H_2O_2} for the DMF solution in the presence of strong acidic buffers (Table S2, DMF-H⁺/DMF, TsOH/TsONa, C₃H₇SO₃H/C₃H₇SO₃Na, and 2,6-(HO)₂BA/2,6-(NaO)₂BA) are listed in Table S3. E_{O_2/H_2O} should be +0.55 V relative to E_{O_2/H_2O_2} under the same experimental conditions.

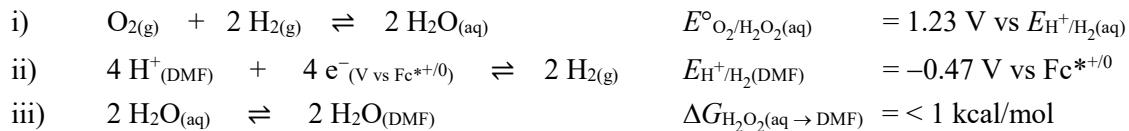
Table S3. A summary of thermodynamic reduction potentials of O₂/H₂O under catalytic conditions^{a,b}

Condition	DMF-H ⁺ /DMF	TsOH/TsONa	C ₃ H ₇ SO ₃ H/C ₃ H ₇ SO ₃ Na	2,6-(HO) ₂ BA/2,6-(NaO) ₂ BA
E_{O_2/H_2O} (V vs. Fc ^{*+/0})	1.07	1.01	0.99	0.95

^aConcentration of each acid and conjugate base is 10 mM; ^bAll potentials are referenced to Fc^{*+/0} in volt.

C. Estimation of O₂/H₂O reduction potential based on OCP measurements of H⁺/H₂.

The reduction potential for O₂/H₂O in DMF may be estimated using i) the standard aqueous cell potential for O₂ + 2 H₂ → 2 H₂O, ii) the measurement of the open circuit potential (OCP) for H⁺/H₂ (E_{H^+/H_2}) with various buffered conditions (Figure S2), and iii) the Gibbs free energy to transfer H₂O from H₂O to DMF.^{2,7} For example, E'_{O_2/H_2O_2} for the DMF solution in the presence of 10 mM each of trifluoroacetic acid and sodium trifluoroacetate is calculated by the following equations:



D. Thermodynamic reduction potentials of O₂/H₂O under catalytic conditions.

For catalytic O₂ reduction conducted in weak acidic buffers (Table S4, TFAH/NaTFA, oxalic acid/lithium oxalate, C₃H₇SO₃H/C₃H₇SO₃Na, and 2,6-(HO)₂BA/2,6-(NaO)₂BA, each reaction solution contained 100 mM deionized H₂O to provide a stable thermodynamic reference state of E_{O_2/H_2O} under non-standard state conditions. For example, the thermodynamic reduction potential of E_{O_2/H_2O} for the DMF solution in the presence of 10 mM each of trifluoroacetic acid and sodium trifluoroacetate is calculated to be 0.79 V vs Fc^{*+/0} using the Nernst equation as below:

$$E_{O_2/H_2O} = E'_{O_2/H_2O} - \frac{0.059}{4} V \times \log\left(\frac{[H_2O]^2[A^-]^4}{pO_2[HA]^4}\right)$$

$$E_{O_2/H_2O} \text{ vs } Fc^{*+/0} (V) = 0.76 V (E'_{O_2/H_2O}) - 0.015 V \times \log([H_2O]^2_{100 \text{ mM}}/[H_2O]^2_{1 \text{ M}}) = 0.79 \text{ V}$$

Table S4. A summary of thermodynamic reduction potentials of O₂/H₂O under catalytic conditions^{a,b}

Condition	TFAH/NaTFA	oxalic acid/ lithium oxalate	DCAH/NaDCA	maleic acid/ sodium malonate
E_{O_2/H_2O} (V vs. Fc ^{*+/0})	0.79	0.72	0.65	0.58

^aConcentration of each acid and conjugate base is 10 mM; ^bAll potentials are referenced to Fc^{*+/0} in volt.

V. Electrochemical experiments

A. General considerations for cyclic voltammetry (CV).

All CV and CPE experiments were performed with a CH Instrument 600E Potentiostat at room temperature. The supporting electrolyte for all electrochemical experiments was 0.1 M tetrabutylammonium perchlorate ([NBu₄][ClO₄]). The three-electrode setup for all cyclic voltammogram (CV) measurements included a glassy carbon (GC) working electrode (3.0 mm diameter), a platinum (Pt) wire counter electrode, and a 0.01 M Ag/AgNO₃ non-aqueous reference electrode.

B. Cyclic Voltammograms of Co complex 1 in DMF.

1. The half-wave potentials of Co complex **1** ($E_{1/2}(Co^{III/II})$) were recorded both in the absence and presence of various acidic buffers (Figure S4). Half-wave potentials were also recorded under buffered conditions because the catalytic rates of O₂ reduction were measured under buffered conditions (*vide infra*). Therefore, the $E_{1/2}(Co^{III/II})$ used to calculate the effective overpotential in the manuscript (cf. eq 3) reflects the actual $E_{1/2}(Co^{III/II})$ under catalytic conditions, which ensures effective overpotential are calculated correctly. The $E_{1/2}(Co^{III/II})$ are only slightly influenced under buffered conditions as shown in Table S5.

2. Buffered conditions are used in the catalytic reaction because protons are consumed in the catalytic reaction, and the presence of "buffer" ensures that there are only negligible changes in the proton concentration (see Section VI for discussion of catalytic O₂ reduction experiments).

Table S5. A summary of half-wave potentials of Co complex **1** in the absence and presence of acid and conjugated base^{a,b}

$E_{1/2}$ (V vs. Fc ^{*+/0})	No acid	^c DMF-H ⁺ /DMF	TsOH/TsONa	C ₃ H ₇ SO ₃ H/ C ₃ H ₇ SO ₃ Na	2,6-(HO) ₂ BA/ 2,6-(NaO) ₂ BA
	0.28 V	0.28 V	0.28 V	0.28 V	0.27 V
TFAH/NaTFA	oxalic acid/ lithium oxalate	DCAH/NaDCA	maleic acid/ sodium malonate		
	0.27 V	0.28 V	0.26 V	0.27 V	

^aConcentration of each acid and conjugate base is 10 mM; ^bAll potentials are referenced to Fc^{*+/0} in volt.

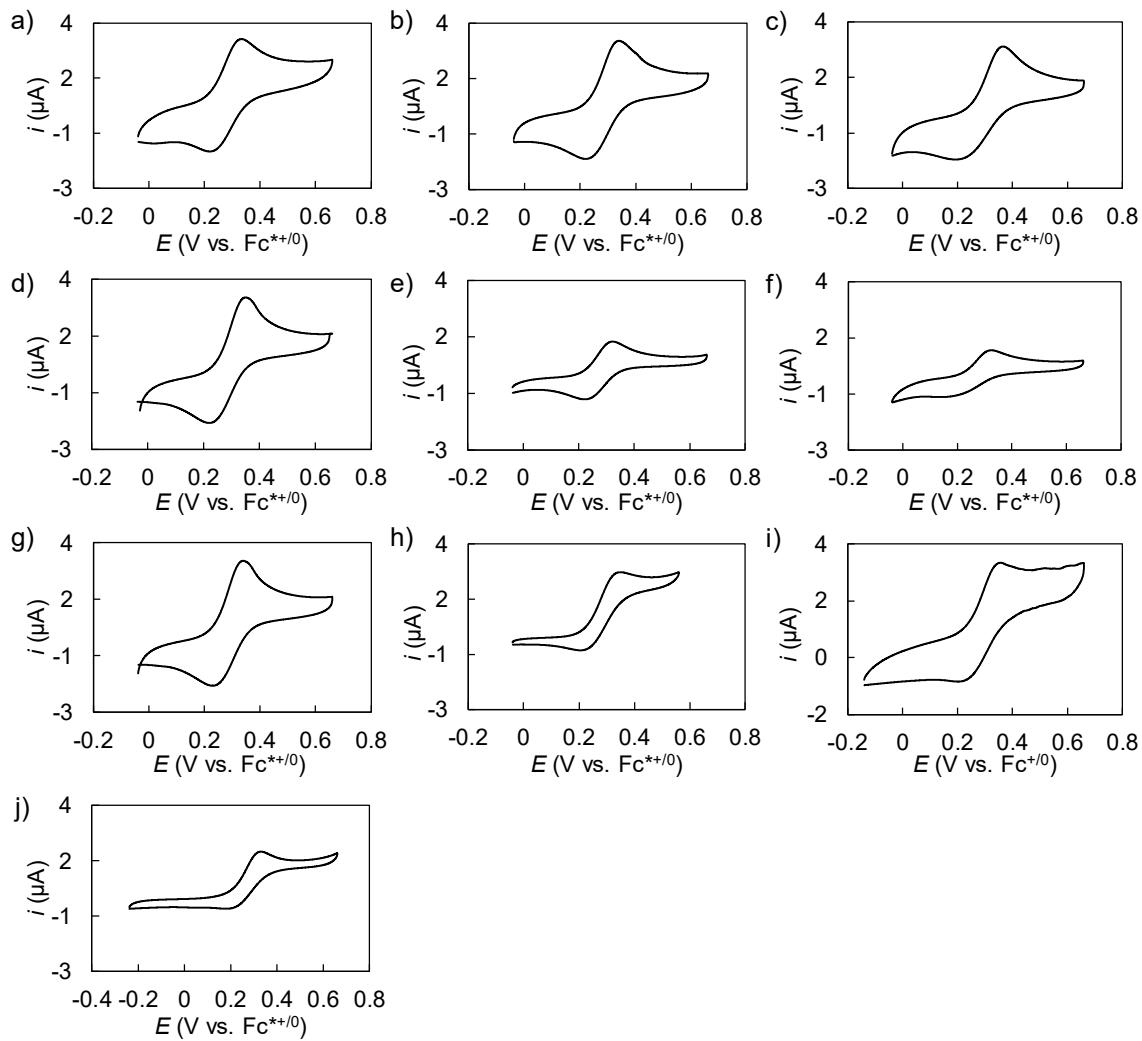


Figure S4. Cyclic voltammograms of 1 mM (a-d, g, i) and 0.5 mM (e, f, h, j) **1** in DMF with various buffered conditions. All CVs were recorded under 1 atm N₂ at the scan rate of 10 mV/s. (a) in the absence of buffered condition; (b) 10 mM each of HClO₄ and [NBu₄][ClO₄]; (c) 10 mM [DMF-H][OTf]; (d) 10 mM each of *p*-toluenesulfonic acid and sodium *p*-toluenesulfonate; (e) 10 mM each of 1-propanesulfonic acid and sodium 1-propanesulfonate monohydrate; (f) 10 mM each of 2,6-dihydroxybenzoic acid and sodium 2,6-dihydroxybenzoate; (g) 10 mM each of trifluoroacetic acid and sodium trifluoroacetate; (h) 10 mM each of oxalic acid and lithium oxalate; (i) 10 mM each of dichloroacetic acid and sodium dichloroacetate; (j) 10 mM each of maleic acid and sodium maleate. See Table S5 for the summary of $E_{1/2}(\text{Co}^{\text{III}/\text{II}})$ under different buffered conditions.

VI. Turnover frequencies of ORR catalyzed by 1

A. General considerations for kinetic studies of O₂ reduction catalyzed by 1.

1. Catalytic O₂ reduction was followed by UV-visible spectroscopy at 780 nm, where an increase in absorption is observed due to the formation of Fc*⁺ (cf. Figure S5).

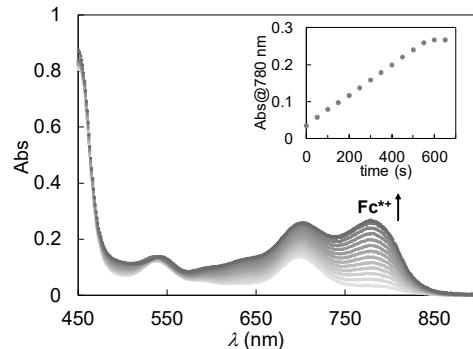


Figure S5. UV-visible spectral changes in the two-electron reduction of O₂ by Fc* (0.5 mM) with **1** (1×10^{-2} mM) in the presence of 10 mM each of HClO₄ and [NBu₄][ClO₄] and 100 μ M H₂O₂ in air-saturated DMF at 298 K. Inset: absorbance changes at 780 nm were due to the formation of Fc*⁺.

2. For the reaction solutions with (1) 10 mM each of HClO₄ and [NBu₄][ClO₄], (2) 10 mM each of *p*-toluenesulfonic acid and sodium *p*-toluenesulfonate, (3) 10 mM each of 1-propanesulfonic acid and sodium 1-propanesulfonate monohydrate, and (4) 10 mM each of 2,6-dihydroxybenzoic acid and sodium 2,6-dihydroxybenzoate as proton sources, a background concentration of 100 μ M urea·H₂O₂ was added to enable estimation of the equilibrium reduction potential of O₂/H₂O₂ under catalytic conditions (cf. Section IV).

3. For the reaction solutions with (5) 10 mM each of trifluoroacetic acid and sodium trifluoroacetate, (6) 10 mM each of oxalic acid and lithium oxalate, (7) 10 mM each of dichloroacetic acid and sodium dichloroacetate, and (8) 10 mM each of maleic acid and sodium maleate as proton sources, a background concentration of 100 mM deionized H₂O was added to enable estimation of the equilibrium reduction potential of O₂/H₂O under catalytic conditions (cf. Section IV).

4. Each catalytic experiment was conducted under buffered conditions. Because protons are consumed in the catalytic reduction of O₂, and the presence of "buffer" ensures that there are not large changes in the proton concentration during the course of the catalytic reaction. In addition, the buffered condition provides the basis for establishing the thermodynamic reduction potential of O₂/H₂O or O₂/H₂O₂ via open-circuit-potential (OCP) measurements. The rate of background oxidation of Fc* by O₂ under each buffered condition is negligible compared to the rate of catalytic ORR.

B. Experimental protocols for initial rate determination for catalytic reduction of O₂ to H₂O₂.

1. A 2.7 mL DMF solution of 1.1 mM Fc*, 110 μ M urea·H₂O₂, and 11 mM each of HA and A⁻ ((a) HClO₄ and [NBu₄][ClO₄], (b) *p*-toluenesulfonic acid and sodium *p*-toluenesulfonate, (c) 1-propanesulfonic acid and sodium 1-propanesulfonate monohydrate, (d) 2,6-dihydroxybenzoic acid and sodium 2,6-dihydroxybenzoate) was vigorously sparged with O₂ for 3 minutes to prepare a O₂-saturated solutions.

2. A 0.3 mL N₂-saturated DMF solution of cobalt complex **1** (50 μ M) was rapidly injected into the O₂-saturated DMF solution containing 1.1 mM Fc*, 110 μ M urea·H₂O₂, and 11 mM each of HA and A⁻. Then the reaction mixture was vigorously shaken for 20 sec and the absorbance was monitored at 780 nm by UV-visible spectroscopy.

3. Final concentrations of each substrate in the reactions:

1 mM Fc*, 5 μ M **1** (Figure S6a and S6b), 10 mM each of HA and A⁻, 100 μ M urea·H₂O₂, and 4.5 mM O₂.⁹

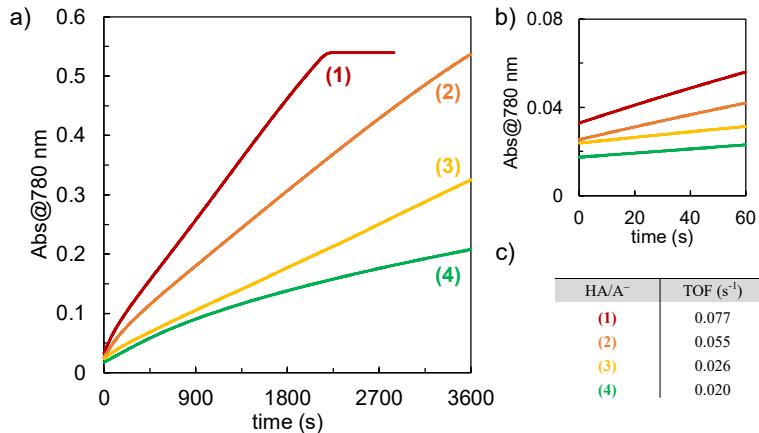


Figure S6. (a) UV-visible time-course raw data for the O₂ reduction catalyzed with **1**. Red trace (1): 10 mM each of HClO₄ and [NBu₄][ClO₄]; orange trace (2): 10 mM each of *p*-toluenesulfonic acid and sodium *p*-toluenesulfonate; yellow trace (3): 10 mM each of 1-propanesulfonic acid and sodium 1-propanesulfonate monohydrate; green trace (4): 10 mM each of 2,6-dihydroxybenzoic acid and sodium 2,6-dihydroxybenzoate; (b) Insets of Figure S6a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) TOF (s⁻¹) of ORR catalyzed with **1** with various buffered conditions.

C. Experimental protocols for initial rate determination for catalytic reduction of O₂ to H₂O.

1. A 2.7 mL DMF solution of 1.1 mM Fc*, 110 mM deionized H₂O, and 11 mM each of HA and A⁻ ((e) trifluoroacetic acid and sodium trifluoroacetate, (f) oxalic acid and lithium oxalate, (g) dichloroacetic acid and sodium dichloroacetate, and (h) maleic acid and sodium maleate as proton sources) was vigorously sparged with O₂ for 3 minutes to prepare a O₂-saturated solution.

2. A 0.3 mL N₂-saturated DMF solution of cobalt complex **1** (50 μ M) was rapidly injected into the O₂-saturated DMF solution containing 1.1 mM Fc*, 110 mM deionized H₂O, and 11 mM each of HA and A⁻ (TFAH/NaTFA, DCAH/NaDCA, and SAH/NaSA). Then the reaction mixture was vigorously shaken for 30 sec and the absorbance was monitored at 780 nm by UV-visible spectroscopy.

3. Final concentrations of each substrate in the reactions:

1 mM Fc*, 5 μ M **1** (Figure S7), 10 mM each of HA and A⁻, 100 mM H₂O, and 4.5 mM O₂.⁹

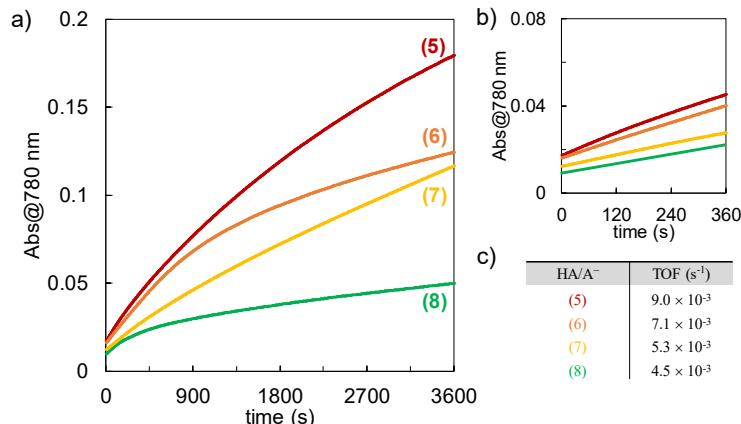


Figure S7. (a) UV-visible time-course raw data for the O_2 reduction catalyzed with **1**. Red trace (5): 10 mM each of trifluoroacetic acid and sodium trifluoroacetate; orange trace (6): 10 mM each of oxalic acid and lithium oxalate; yellow trace (7): 10 mM each of dichloroacetic acid and sodium dichloroacetate; green trace (8): 10 mM each of maleic acid and sodium maleate; (b) Insets of Figure S7a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) TOF (s^{-1}) of ORR catalyzed with **1** with various buffered conditions.

D. Calculations of turnover frequencies (TOFs).

1. Initial rates, in units of $\text{mM}\cdot\text{s}^{-1}$, were obtained by fitting UV-visible time-course data with linear regression during the first ~5-10% of the reaction. The turnover frequencies (TOFs, s^{-1}) were then determined by dividing the number of electron transferred (to account for the conversion of O_2 to H_2O_2 ($n = 2$) or H_2O ($n = 4$) on the basis of consumption of a single-electron reductant, Fc^*) and the catalyst concentration.

2. For $\text{O}_2/\text{H}_2\text{O}_2$, initial rate of O_2 reduction (mM/s) = initial rate of $[\text{Fc}^*]/2$; for $\text{O}_2/\text{H}_2\text{O}$, initial rate of O_2 reduction (mM/s) = initial rate of $[\text{Fc}^*]/4$.

3. Turnover frequency (TOF) for O_2 reduction (s^{-1}) = initial rate of O_2 reduction/[Co] (Figure S6c and S7c).

Table S6. A summary of turnover frequencies (TOFs) of Co complex **1** under different buffered conditions^a

TOF (s^{-1})	DMF-H ⁺ /DMF	TsOH/TsONa	$\text{C}_3\text{H}_5\text{SO}_3\text{H}/\text{C}_3\text{H}_7\text{SO}_3\text{Na}$	$2,6-(\text{HO})_2\text{BA}/2,6-(\text{NaO})_2\text{BA}$
	7.7×10^{-2}	5.5×10^{-2}	2.6×10^{-2}	2.0×10^{-2}
	TFAH/NaTFA	oxalic acid/lithium oxalate	DCAH/NaDCA	maleic acid/sodium malonate
	9.0×10^{-3}	7.1×10^{-3}	5.3×10^{-3}	4.5×10^{-3}

^aConcentration of each acid and conjugate base is 10 mM.

VII. Selectivity of ORR catalyzed by 1

A. $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$ colorimetric assay for H_2O_2 quantification.

1. The first method used for H_2O_2 quantification was a colorimetric assay using aqueous $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$, modified from a literature procedure.^{10,11} A calibration curve was constructed by first preparing a series of 10 mL DMF solutions with various concentrations of urea· H_2O_2 (0.05, 0.10, 0.15, 0.20, and 0.25 mM). A 0.1 mL solution of $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$ was added to the above solutions, respectively. The absorbance at 407 nm was measured by UV-visible spectroscopy to create the calibration curve as shown in Figure S8.

2. To quantify H_2O_2 in the catalytic reaction mixture, a 0.5 mL aliquot of the catalytic reaction was mixed with 2 mL deionized H_2O and 5 mL dichloromethane. The aqueous layer ($\approx 2.1 \text{ mL}$) was collected, and combined with a 20 μL solution of $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$. The absorbance at 407 nm was measured by UV-visible spectroscopy.

3. The absorbance at 407 nm was analyzed with (red trace) and without (black trace) $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$ (cf. Figure S9). The concentrations of H_2O_2 in different catalytic reaction mixtures were calculated from the slope of the calibration curve (cf. Figure S8b, $y = 0.7415x + 0.0044$) as follows:

$$1) \Delta\text{Abs} = \text{Abs}@407 \text{ nm}_{\text{Ti(O)SO}_4} (\text{Fig. S9, red trace}) - \text{Abs}@407 \text{ nm}_{\text{background}} (\text{Fig. S9, black trace})$$

$$2) [\text{H}_2\text{O}_2]_{\text{exp}} (\text{mM}) = (\Delta\text{Abs} - 0.0044)/0.7415$$

3) For a $2\text{e}^-/2\text{H}^+$ catalytic O_2 reduction reaction (Fc^* is 1 mM for all catalytic reactions):

$$[\text{H}_2\text{O}_2] = 0.5 \text{ mM} \times (0.5 \text{ mL (aliquot)}/2.1 \text{ mL (aqueous layer)}) = 0.120 \text{ mM}$$

$$4) \text{Selectivity of H}_2\text{O}_2 (\%) = [\text{H}_2\text{O}_2]_{\text{exp}}/0.120 \text{ mM}$$

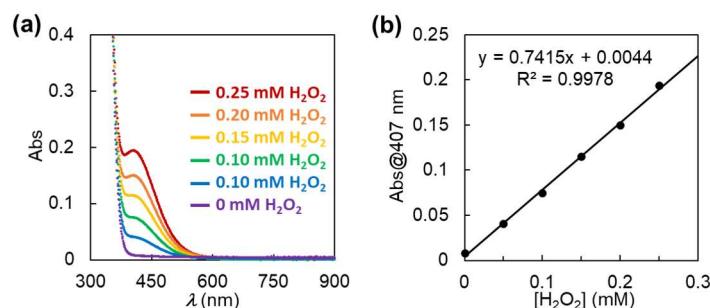


Figure S8. (a) UV-visible spectra for $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$ -based detection of varying (0–0.25 mM) concentrations of H_2O_2 . (b) Calibration curve constructed from data in Figure S8a.

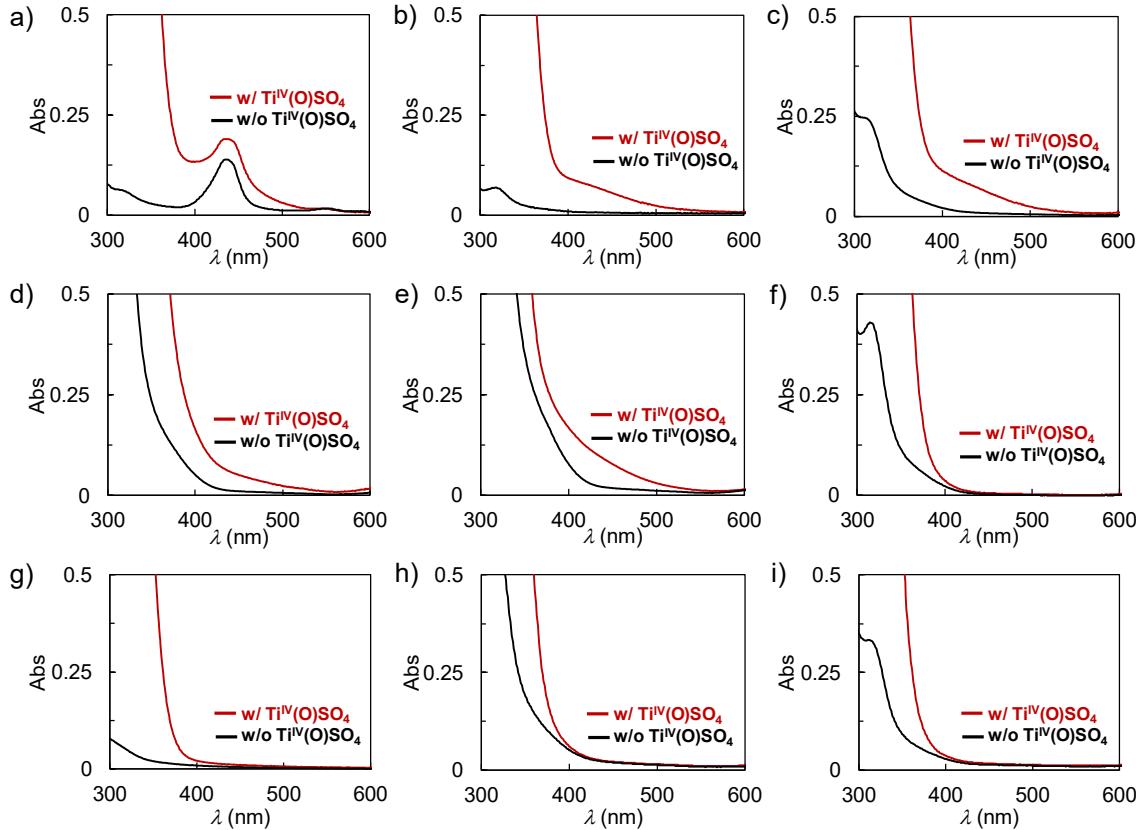


Figure S9. UV-visible spectra for the detection of H_2O_2 from O_2 reduction catalyzed with **1** via treatment with $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$ (red trace) and background spectra without adding $\text{Ti}^{\text{IV}}(\text{O})\text{SO}_4$. (a) 10 mM each of HClO_4 and $[\text{NBu}_4][\text{ClO}_4]$; (b) 10 mM $[\text{DMF-H}][\text{OTf}]$; (c) 10 mM each of *p*-toluenesulfonic acid and sodium *p*-toluenesulfonate; (d) 10 mM each of 1-propanesulfonic acid and sodium 1-propanesulfonate monohydrate; (e) 10 mM each of 2,6-dihydroxybenzoic acid and sodium 2,6-dihydroxybenzoate; (f) 10 mM each of trifluoroacetic acid and sodium trifluoroacetate; (g) 10 mM each of oxalic acid and lithium oxalate; (h) 10 mM each of dichloroacetic acid and sodium dichloroacetate; (i) 10 mM each of maleic acid and sodium maleate. See Table S7 for the summary of selectivity of O_2 reduction under different buffered conditions.

Table S7. A summary of selectivity of O_2 reduction catalyzed with **1** under different buffered conditions^a

Selectivity, $\text{H}_2\text{O}:\text{H}_2\text{O}_2$ (%)	DMF- H^+ /DMF	TsOH/TsONa	$\text{C}_3\text{H}_7\text{SO}_3\text{H}/$ $\text{C}_3\text{H}_7\text{SO}_3\text{Na}$	2,6-(HO) ₂ BA/ 2,6-(NaO) ₂ BA
	5:95	7:93	6:94	1:99
	TFAH/NaTFA	oxalic acid/ lithium oxalate	DCAH/NaDCA	maleic acid/ sodium malonate
	95:5	95:5	98:2	98:2

^aConcentration of each acid and conjugate base is 10 mM.

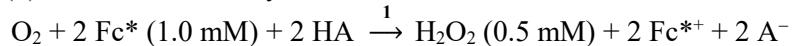
B. Iodometric titration for H_2O_2 quantification

1. The second method used for H_2O_2 quantification was iodometric titration. The amount of H_2O_2 was determined by titration with iodide ion, as described previously in the literature.¹²⁻¹⁴ In an iodometric titration, the formation of I_3^- and the consumption of H_2O_2 follows a one-to-one ratio ($2 \text{NaI} + \text{H}_2\text{O}_2 \rightarrow \text{I}_2 + 2 \text{NaOH}$, $\text{NaI} + \text{I}_2 \rightarrow \text{NaI}_3$). The concentration H_2O_2 can be derived from the concentration of I_3^-

($\text{Abs}@361 \text{ nm} = \epsilon b[\text{I}_3^-]$). All iodometric titrations are conducted anaerobically to avoid the oxidation of I^- to I_3^- by O_2 .

2. A 60 μL aliquot of the 3 mL catalytic reaction mixture was diluted in CH_3CN (2.94 mL), and an excess amount of NaI (0.1 M) was then added. The amount of I_3^- formed was determined by the UV-visible absorption spectroscopy ($\lambda_{\text{max}}@361 \text{ nm}$, $\epsilon = 2.8 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$).¹² The absorbance at 361 nm was compared from aliquots withdrawn and analyzed with and without added NaI (red and black traces, respectively, in Figure S10). The difference in the absorbance at 361 nm was used to quantify the amount of H_2O_2 formed in the catalytic reaction, according to the following considerations:

(1) For a $2\text{e}^-/2\text{H}^+$ catalytic O_2 reduction:



(2) The diluted CH_3CN solution of the product mixture contains the following theoretical amount of hydrogen peroxide: $[\text{H}_2\text{O}_2] (\text{mM}) = (60 \mu\text{L}/3000 \mu\text{L}) \times 0.5 \text{ mM} = 0.01 \text{ mM}$.

(3) $\text{Abs}@361 \text{ nm}$ (red trace, Fig. S11) – $\text{Abs}@361 \text{ nm}$ (black trace, Fig. S10) = $\epsilon b[\text{I}_3^-]$, $[\text{I}_3^-] = [\text{H}_2\text{O}_2]_{\text{exp}}$

(4) Selectivity of H_2O_2 (%) = $[\text{H}_2\text{O}_2]_{\text{exp}}/0.01 \text{ mM}$

3. NaI (0.1 M) and Fc^{*+} (1 mM) were combined in the presence of 10 mM TFAH/NaTFA in DMF anaerobically. The mixture was analyzed by UV-visible spectroscopy (300-900 nm) anaerobically for 60 min. No reaction was observed (i.e., no change in the Fc^{*+} concentration in the absence of **1**).

4. NaI (0.1 M) was combined with catalytic amount of **1** (10 μM) in the presence of 10 mM TFAH/NaTFA in DMF anaerobically. The mixture was analyzed by UV-visible spectroscopy (300-900 nm) anaerobically for 60 min, and no reaction was observed (i.e., no catalytic oxidation of I^- by **1**).

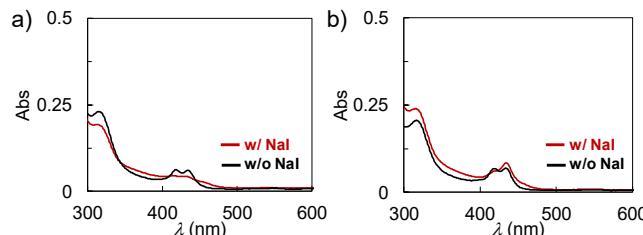


Figure S10. UV-Vis absorption spectral change before (black) and after (red) the addition of NaI (excess, 0.1 M) to a diluted reaction mixture in MeCN. The selectivity for catalytic O_2 reduction to H_2O by **1**: (a) 95% (10 mM each of trifluoroacetic acid and sodium trifluoroacetate); (b) 93% (10 mM each of dichloroacetic acid and sodium dichloroacetate).

VIII. Effective overpotentials of ORR catalyzed by 1

1. The effective overpotentials (η_{eff}) are calculated using the equation: $\eta_{\text{eff}} = E_{\text{O}_2/\text{H}_2\text{O}} - E_{1/2}(\text{Co}^{\text{III}/\text{II}})$.

2. For Figure 4 in the main manuscript, the η_{eff} are not adjusted to account for the background concentration of H₂O or H₂O₂ (Table S8). $E_{\text{O}_2/\text{H}_2\text{O}}$ is supposed to be +1.23 V relative to $E_{\text{H}^+/\text{H}_2}$ under the same experimental conditions, and the $E_{\text{H}^+/\text{H}_2}$ are obtained from the OCP measurement as shown in Section II.

Table S8. The effective overpotentials of O₂ reduction catalyzed by **1** are not adjusted to the account for the background concentration of H₂O or H₂O₂ (cf. Figure 4 in the main manuscript)^{a,b}

Condition	DMF-H ⁺ /DMF	TsOH/TsONa	C ₃ H ₇ SO ₃ H/C ₃ H ₇ SO ₃ Na	2,6-(HO) ₂ BA/2,6-(NaO) ₂ BA	TFAH/NaTFA	oxalic acid/lithium oxalate	DCAH/NaDCA	maleic acid/sodium malonate
$E_{\text{O}_2/\text{H}_2\text{O}}$ (V)	0.95	0.89	0.87	0.53	0.76	0.69	0.62	0.55
$E_{1/2}(\text{Co}^{\text{III}/\text{II}})$ (V)	0.28	0.28	0.28	0.27	0.27	0.28	0.26	0.27
η_{eff} (V)	0.67	0.61	0.59	0.56	0.49	0.41	0.36	0.28

^aConcentration of each acid and conjugate base is 10 mM; ^bAll potentials are referenced to Fc^{*+/0} in volt.

3. For Figure S11, the η_{eff} are adjusted to account for the background concentration of H₂O or H₂O₂ using the Nernst equation as shown in Section IV. The η_{eff} are summarized in the Table S9.

Table S9. The effective overpotentials of O₂ reduction catalyzed by **1** are adjusted to the account for the background concentration of H₂O or H₂O₂ (cf. Figure S11)^{a,b}

Condition	DMF-H ⁺ /DMF	TsOH/TsONa	C ₃ H ₇ SO ₃ H/C ₃ H ₇ SO ₃ Na	2,6-(HO) ₂ BA/2,6-(NaO) ₂ BA	TFAH/NaTFA	oxalic acid/lithium oxalate	DCAH/NaDCA	maleic acid/sodium malonate
$E_{\text{O}_2/\text{H}_2\text{O}}$ (V)	1.07	1.01	0.99	0.95	0.79	0.72	0.65	0.60
$E_{1/2}(\text{Co}^{\text{III}/\text{II}})$ (V)	0.28	0.28	0.28	0.27	0.27	0.28	0.26	0.27
η_{eff} (V)	0.79	0.73	0.71	0.68	0.52	0.44	0.39	0.33

^aConcentration of each acid and conjugate base is 10 mM; ^bAll potentials are referenced to Fc^{*+/0} in volt.

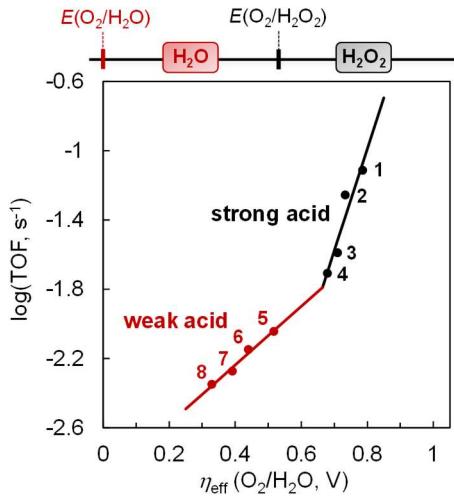


Figure S11. Linear free energy correlations between $\log(\text{TOF} \cdot \text{s}^{-1})$ and the η_{eff} for the O_2 reduction catalyzed by **1**. The η_{eff} values are adjusted to account for the background concentration of H_2O or H_2O_2 (Section IV and Table S9).

IX. Rate law analysis of O_2 reduction catalyzed by **1**

A. ORR rate law and turnover number (TON) determination with $\text{HClO}_4/\text{[NBu}_4\text{][ClO}_4$ (product selectivity: H_2O_2)

1. [Co]-dependence

A 0.3 mL air-saturated DMF solution of **1** (10, 20, 50, 75, and 100 μM) containing 100 mM HClO_4 was rapidly added to a 2.7 mL air-saturated DMF solution containing 1.1 mM Fc^* , 110 μM urea $\cdot\text{H}_2\text{O}_2$, and 11 mM $[\text{NBu}_4\text{ClO}_4]$. The reaction mixture was vigorously shaken for 30 sec, and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature (cf. Figure S5 for a full UV-visible spectrum and a reaction time course). Initial rates of Fc^{*+} formation, in units of mM/s ($R_{\text{init}} = d[\text{Fc}^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first 30 sec of the reaction. These data provide the basis for the plots of R_{init} vs. [**1**] in Figure S12c, which shows first-order kinetics.

The TONs have been determined for the 2 e^- reduction of O_2 (1×10^{-3} M) using 1×10^{-3} M Fc^* with various concentrations of **1** (1 – 10 μM) and 10 mM each of HClO_4 and $[\text{NBu}_4\text{][ClO}_4]$ (see Figure S12 d). TONs were calculated by dividing the number of electrons transferred to account for the conversion of O_2 to H_2O_2 on the basis of consumption of a single-electron reductant (Fc^*) and the catalyst concentration. $\text{TON} = ([\text{Fc}^*]_v/2)/[\text{Co}]$. The reactions using 5 – 10 μM **1** reach completion within 1800 s, so the TONs are at or near the theoretical maximum due to consumption of Fc^* . The reaction using 1 μM **1** has a $\text{TON} = 160$, which is the maximum TON calculated. Additionally, based on the slope of the absorbance vs. time plot for this reaction, the max TON reported is limited by the duration of reaction monitoring, not by catalyst decomposition.

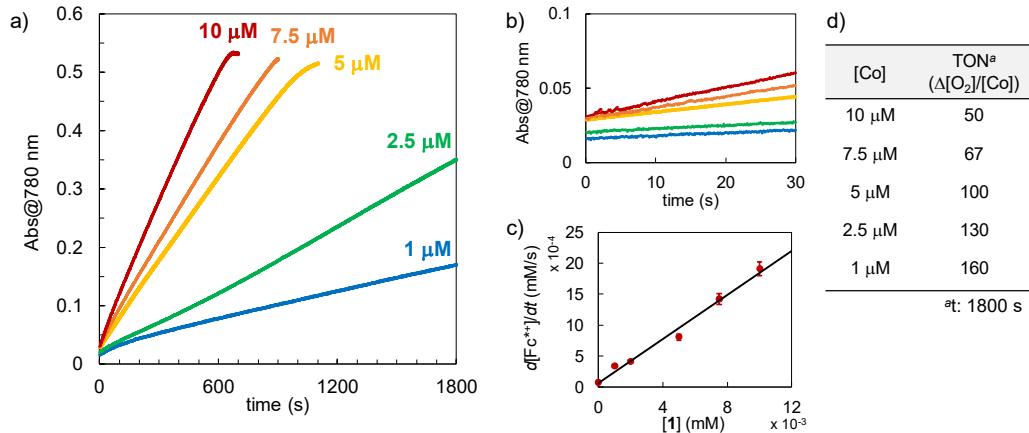


Figure S12. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the two-electron reduction of O_2 (1×10^{-3} M) by Fc^* (1×10^{-3} M) with various concentration of **1** (1, 2.5, 5, 7.5, and 10 μ M) in the presence of 10 mM each of $HClO_4$ and $[NBu_4][ClO_4]$, and 110 μ M urea- H_2O_2 in air-saturated DMF at 298 K; (b) Insets of Figure S12a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. $[1]$ shows a first-order dependence. (d) The turnover number (TON) for ORR with various concentration of **1**.

2. $[HClO_4]$ -dependence

A 0.3 mL air-saturated DMF solution of 75 μ M **1** containing various concentrations of $HClO_4$ (10, 25, 50, and 75 mM) was rapidly added into a 2.7 mL air-saturated DMF solution containing 1.1 mM Fc^* , 110 μ M urea- H_2O_2 , and various concentrations of $[NBu_4ClO_4]$ (1.1, 2.75, 5.5, and 8.25 mM). The reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature (cf. Figure S5 for a full UV-visible spectrum and a reaction time course). Initial rates of Fc^{*+} formation, in units of mM/s ($R_{init} = d[Fc^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first 30 sec of the reaction. These data provide the basis for the plot of R_{init} vs. $[HClO_4]$ in Figure S13c, which shows a first-order dependence.

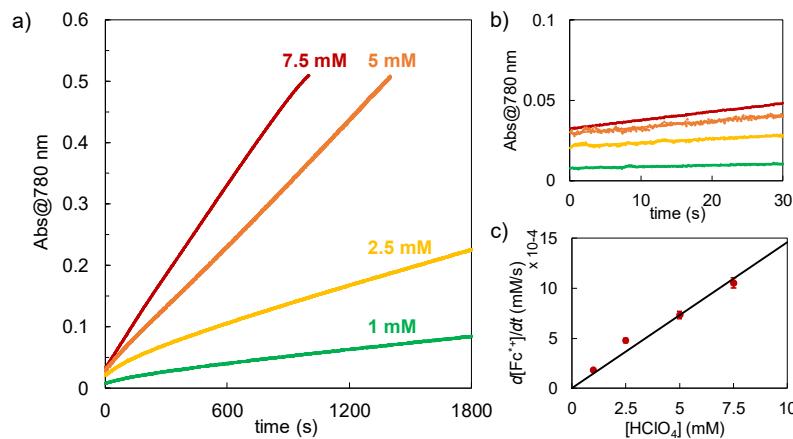


Figure S13. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the two-electron reduction of O_2 (1×10^{-3} M) by Fc^* (1×10^{-3} M) with **1** (7.5×10^{-6} M) in the presence of various concentrations of $HClO_4/[NBu_4][ClO_4]$ (1, 2.5, 5, and 7.5 mM), and 100 μ M urea- H_2O_2 in air-saturated DMF at 298 K; (b) Insets of Figure S13a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. $[HClO_4]$ shows a first-order dependence.

3. $[O_2]$ -dependence

1. A 0.3 mL O_2 -saturated DMF solution of 25 μM **1** containing 100 mM $HClO_4$ was rapidly added into a 2.7 mL O_2 -saturated DMF solution containing 1.1 mM Fc^* , 110 μM urea- H_2O_2 , and 11 mM $[NBu_4ClO_4]$. Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ($[O_2] \approx 5$ mM).⁹

2. A 0.3 mL air-saturated DMF solution of 25 μM **1** containing 100 mM $HClO_4$ was rapidly added into a 2.7 mL air-saturated DMF solution containing 1.1 mM Fc^* , 110 μM urea- H_2O_2 , and 11 mM $[NBu_4ClO_4]$. Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ($[O_2] \approx 1$ mM).

3. A 0.3 mL N_2 -saturated DMF solution of 25 μM **1** containing 100 mM $HClO_4$ was rapidly mixed with 1) an 1.2 mL N_2 -saturated DMF solution containing 1.1 mM Fc^* , 110 μM urea- H_2O_2 , and 11 mM $[NBu_4][ClO_4]$, and 2) an 1.5 mL O_2 -saturated DMF solution of 1.1 mM Fc^* , 110 μM urea- H_2O_2 , and 11 mM $[NBu_4ClO_4]$ (total volume for the reaction solution: 3 mL). Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ($[O_2] \approx 2.5$ mM).

4. Initial rates of Fc^{*+} formation, in units of mM/s ($R_{init} = d[Fc^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first 30 sec of the reaction. These data provide the basis for the plots of R_{init} vs. $[O_2]$ in Figure S14c, which shows a first-order dependence.

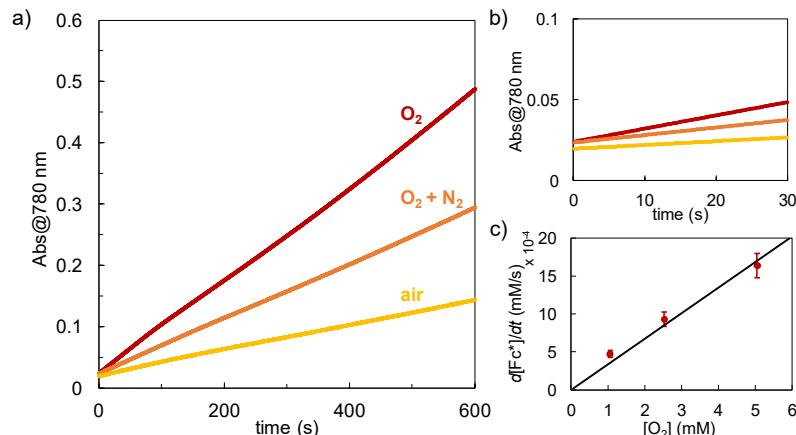


Figure S14. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the two-electron reduction of various concentration of O_2 (1, 3, and 5 mM) by Fc^* (1×10^{-3} M) with **1** (2.5×10^{-6} M) in the presence of 10 mM each of $HClO_4$ and $[NBu_4][ClO_4]$, and 100 μM urea- H_2O_2 in DMF at 298 K; (b) Insets of Figure S14c: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. $[O_2]$ shows a first-order dependence.

4. [Fc^{*}]-dependence

A 0.3 mL air-saturated DMF solution of 75 μ M **1** containing 100 mM HClO₄ was rapidly added to a 2.7 mL air-saturated DMF solution containing various concentration Fc^{*} (0.56, 1.1, 1.65, and 2.75 mM), 110 μ M urea·H₂O₂, and 11 mM [NBu₄]ClO₄. The reaction mixture was vigorously shaken for 30 sec, and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature (cf. Figure S5 for a full UV-visible spectrum and a reaction time course). Initial rates of Fc^{*+} formation, in units of mM/s ($R_{\text{init}} = d[\text{Fc}^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first 30 sec of the reaction. These data provide the basis for the plots of R_{init} vs. [Fc^{*}] in Figure S15c, which shows a zero-order dependence.

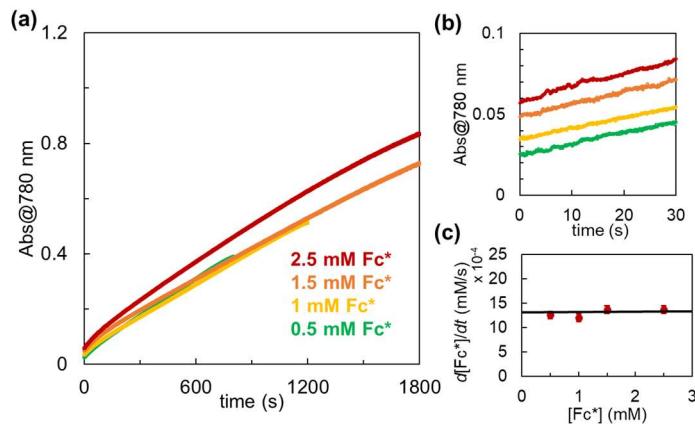


Figure S15. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the two-electron reduction of O₂ (1×10^{-3} M) by various concentrations of Fc^{*} (0.5, 1, 1.5, and 2.5 mM) with **1** (7.5×10^{-6} M) in the presence of 10 mM each of HClO₄ and [NBu₄][ClO₄], and 100 μ M urea·H₂O₂ in air-saturated DMF at 298 K; (b) Insets of Figure S15a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. [Fc^{*}] shows a zero-order dependence.

B. ORR rate law and turnover number (TON) determination with DCAH/NaDCA (product selectivity: H₂O)

1. [Co]-dependence

A 0.3 mL air-saturated DMF solution of **1** (50, 87.5, 125, 187.5, 250, and 300 μ M) containing 100 mM DCAH was rapidly added to a 2.7 mL air-saturated DMF solution containing 1.65 mM Fc^{*}, 110 mM H₂O, and 11 mM NaDCA. The reaction mixture was vigorously shaken for 30 sec, and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature (cf. Figure S5 for a full UV-visible spectrum and a reaction time course). Initial rates of Fc^{*+} formation, in units of mM/s ($R_{\text{init}} = d[\text{Fc}^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first ~5% of the reaction. These data provide the basis for the plots of R_{init} vs. [1] in Figure S16c, which shows first-order kinetics.

The TONs were determined for the 4 e⁻ reduction of O₂ (1×10^{-3} M) using 1.5×10^{-3} M Fc^{*} with various concentrations of **1** (5 – 30 μ M) and 10 mM each of DCAH and NaDCA (see Figure S16 d). TONs were calculated by dividing the number of electrons transferred to account for the conversion of O₂ to H₂O on the basis of consumption of a single-electron reductant (Fc^{*}) and the catalyst concentration. $\text{TON} = ([\text{Fc}^*]/4)/[\text{Co}]$. The TONs for these reactions range from 3.9 – 8.9 (30 and 5 μ M **1**, respectively), which is significantly lower than the theoretical TONs of 12.5 – 75, indicating that catalyst decomposition does occur under these reaction conditions.

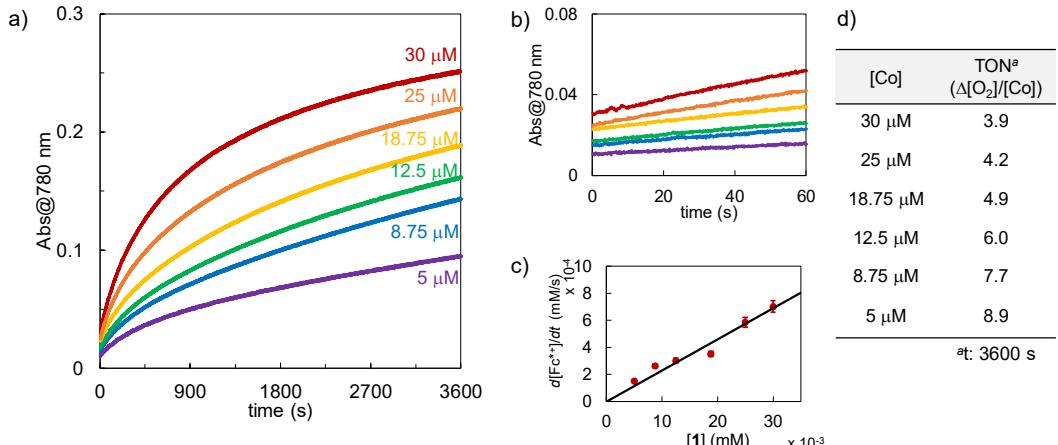


Figure S16. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the four-electron reduction of O_2 (1×10^{-3} M) by Fc^* (1.5×10^{-3} M) with various concentration of **1** (5, 8.75, 12.75, 18.75, 25, and 30 μM) in the presence of 10 mM each of DCAH and NaDCA, and 100 mM H_2O in air-saturated DMF at 298 K; (b) Insets of Figure S16a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. $[\mathbf{1}]$ shows first-order kinetics. (d) The turnover number (TON) for ORR with various concentration of **1**.

2. [DCAH]-dependence

A 0.3 mL air-saturated DMF solution of 600 μM **1** containing various concentrations of DCAH (75, 100, 150, 250, and 300 mM) was rapidly added into a 2.7 mL air-saturated DMF solution containing 0.56 mM Fc^* , 110 mM H_2O , and various amounts of NaDCA (82.5, 110, 165, and 330 mM). The reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature (cf. Figure S5 for a full UV-visible spectrum and a reaction time course). Initial rates of Fc^{*+} formation, in units of mM/s ($R_{\text{init}} = d[\text{Fc}^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first ~5% of the reaction. These data provide the basis for the plot of R_{init} vs. [DCAH] in Figure S17c, which shows first-order kinetics.

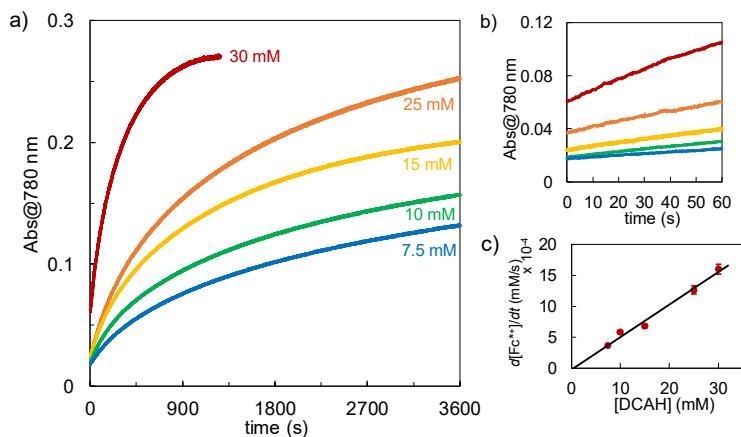


Figure S17. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the four-electron reduction of O_2 (1×10^{-3} M) by Fc^* (5×10^{-4} M) with **1** (6×10^{-5} M) in the presence of various concentrations of DCAH/NaDCA (7.5, 10, 15, 25, and 30 mM) and 100 mM H_2O in air-saturated DMF at 298 K; (b) Insets of Figure S17a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. [DCAH] shows first-order kinetics.

3. [Fc^{*}]-dependence

A 0.3 mL air-saturated DMF solution of 400 μ M **1** containing 100 mM DCAH was rapidly added to a 2.7 mL air-saturated DMF solution containing various concentrations of Fc^{*} (0.55, 0.825, 1.1, 1.65, and 2.2 mM), 110 mM H₂O, and 11 mM NaDCA. The reaction mixture was vigorously shaken for 30 sec, and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature (cf. Figure S5 for a full UV-visible spectrum and a reaction time course). Initial rates of Fc^{*+} formation, in units of mM/s ($R_{\text{init}} = d[\text{Fc}^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first ~5% of the reaction. These data provide the basis for the plots of R_{init} vs. [Fc^{*}] in Figure S18c, which shows first-order kinetics.

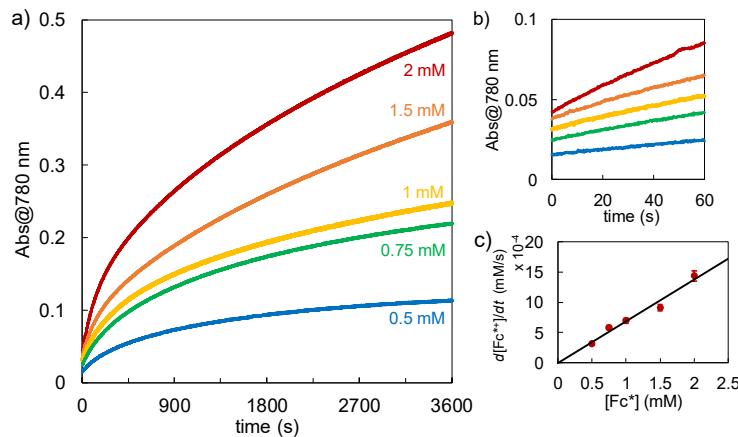


Figure S18. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the four-electron reduction of O₂ (1×10^{-3} M) by various concentrations of Fc^{*} (0.5, 0.75, 1, 1.5, and 2 mM) with **1** (4×10^{-5} M) in the presence of 10 mM each of DCAH and NaDCA, and 100 mM H₂O in air-saturated DMF at 298 K; (b) Insets of Figure S18a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. [Fc^{*}] shows first-order kinetics.

4. [O₂]-dependence

1. A 0.3 mL O₂-saturated DMF solution of 300 μ M **1** containing 100 mM DCAH was rapidly added into a 2.7 mL O₂-saturated DMF solution containing 1.1 mM Fc^{*}, 110 mM H₂O, and 11 mM NaDCA. Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ([O₂] \approx 5 mM, red trace in Figure S19).⁹

2. A 0.3 mL air-saturated DMF solution of 300 μ M **1** containing 100 mM DCAH was rapidly added into a 2.7 mL air-saturated DMF solution containing 1.1 mM Fc^{*}, 110 mM H₂O, and 11 mM NaDCA. Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ([O₂] \approx 1 mM, green trace in Figure S19).

3. A 0.3 mL air-saturated DMF solution of 300 μ M **1** containing 100 mM DCAH was rapidly mixed with 1) an 1.2 mL air-saturated DMF solution containing 1.1 mM Fc^{*}, 110 mM H₂O, and 11 mM NaDCA, and 2) an 1.5 mL O₂-saturated DMF solution containing 1.1 mM Fc^{*}, 110 mM H₂O, and 11 mM NaDCA (total volume of the reaction solution: 3 mL). Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ([O₂] \approx 3 mM, yellow trace in Figure S19).

4. A 0.3 mL N₂-saturated DMF solution of 300 μ M **1** containing 100 mM DCAH was rapidly mixed with 1) an 1.2 mL N₂-saturated DMF solution containing 1.1 mM Fc^{*}, 110 mM H₂O, and 11 mM NaDCA, and 2) an 1.5 mL O₂-saturated DMF solution containing 1.1 mM Fc^{*}, 110 mM H₂O, and 11 mM NaDCA

(total volume of the reaction solution: 3 mL). Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ($[\text{O}_2] \approx 2.5 \text{ mM}$, blue trace in Figure S19).

5. A 0.3 mL N_2 -saturated DMF solution of $300 \mu\text{M}$ **1** containing 100 mM DCAH was rapidly mixed with 1) an 1.2 mL N_2 -saturated DMF solution containing 1.1 mM Fc^* , 110 mM H_2O , and 11 mM NaDCA, and 2) an 1.5 mL air-saturated DMF solution containing 1.1 mM Fc^* , 110 mM H_2O , and 11 mM NaDCA (total volume of the reaction solution: 3 mL). Then the reaction mixture was vigorously shaken for 30 sec and the absorbance of Fc^{*+} was monitored at 780 nm by UV-visible spectroscopy at ambient temperature ($[\text{O}_2] \approx 0.5 \text{ mM}$, orange trace in Figure S19).

6. Initial rates of Fc^{*+} formation, in units of mM/s ($R_{\text{init}} = d[\text{Fc}^*]/dt$), were obtained by fitting UV-visible time-course data with linear regression during the first $\sim 5\%$ of the reaction. These data provide the basis for the plots of R_{init} vs. $[\text{O}_2]$ in Figure S19c, which shows zero-order kinetics.

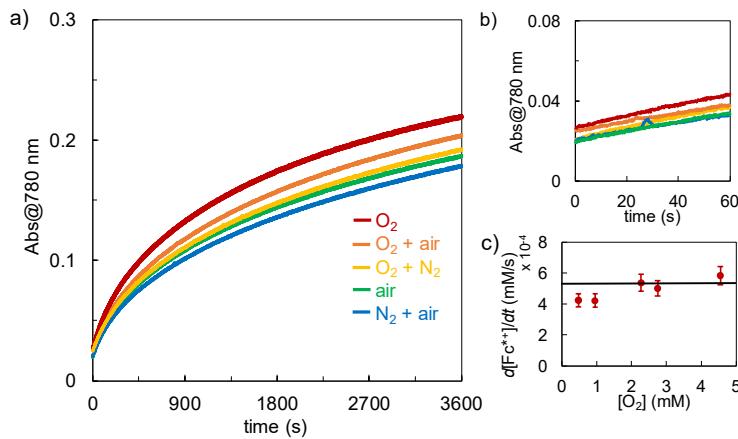


Figure S19. (a) Time profiles of absorbance at 780 nm due to the formation of Fc^{*+} in the four-electron reduction of various concentration of O_2 (0.5, 1, 2.5, 3, and 5 mM) by Fc^* ($1 \times 10^{-3} \text{ M}$) with **1** ($3 \times 10^{-5} \text{ M}$) in the presence of 10 mM each of DCAH and NaDCA, and 100 mM H_2O in DMF at 298 K; (b) Insets of Figure S19a: the data points are fitted with linear regression to calculate the initial rates (mM/s); (c) A plot of R_{init} vs. $[\text{O}_2]$ shows zero-order kinetics.

X. EPR experiments and simulations

EPR parameters for all experiments: X-band, microwave frequency ca. 9.3 GHz, modulation 100 kHz; 10 mW microwave power 10 mW, modulation amplitude 10 G. EPR spectra were simulated using XSophe software from Bruker company.¹⁵

A. EPR spectrum of Co^{II} under N₂

To generate the spectrum for Co complex **1** (Co^{II}) in DMF under N₂, Co complex **1** was dissolved in N₂-saturated DMF in a glove box to prepare a 1 mM solution of DMF. An 0.3 mL N₂-saturated DMF solution of 1 mM **1** was transferred to a quartz EPR tube and the tube capped with a septum. The sample was removed from the glove box and frozen in liquid nitrogen. The experimental EPR spectrum was recorded at 110 K. The simulated EPR spectrum indicates that Co complex **1** exists in the low-spin state by comparing simulated g-factor and hyperfine constants (*A*) to literature values.¹⁶⁻²²

B. EPR spectrum of Co^{II(O₂)} under O₂

To generate the Co^{III}-superoxide species, the above N₂-saturated DMF solution of **1** (Co^{II}) was vigorously sparged with O₂ for 3 min at room temperature. The sample was then quickly capped with a septum and frozen in liquid N₂. The experimental EPR spectrum was recorded at 110 K. The simulated EPR spectrum indicates that Co^{III}-superoxide is generated under aerobic conditions by comparing simulated g-factor and hyperfine constants to literature values.¹⁶

C. Co^{II(O₂)} is unreactive toward DCAH

To investigate whether the Co^{III}-superoxide intermediate can be protonated by trifluoroacetic acid (TFAH) in DMF, the above DMF solution Co^{III}-superoxide was added 10 mM TFAH/NaTFA and vigorously shaken for 3 min at room temperature. The sample was then quickly capped with a septum and frozen in liquid N₂. The experimental EPR spectrum was recorded at 110 K. The identical EPR spectra indicate that Co^{III}-superoxide species is not protonated in the presence of 10 mM DCAH in DMF (cf. Figure 6 in the main manuscript).

D. Reaction of Co^{II(O₂)} with HClO₄

To investigate whether the Co^{III}-superoxide intermediate can be protonated by HClO₄ in DMF, the above DMF solution Co^{III}-superoxide was added 10 mM HClO₄/[NBu₄][ClO₄] and vigorously shaken for 3 min at room temperature. The sample was then quickly capped with a septum and frozen in liquid N₂. The experimental EPR spectrum was recorded at 110 K (cf. Figure 6 in the main manuscript).

XI. Considerations for differential pulse voltammetry²³

1. All DPV were conducted on a Pine WaveNow potentiostat. The three-electrode setup for all cyclic voltammogram (CV) measurements included a glassy carbon (GC) working electrode (3.0 mm diameter), a platinum (Pt) wire counter electrode, and a 0.01 M Ag/AgNO₃ non-aqueous reference electrode. All reported potentials are relative to the Fe^{*+0}.

2. For the DPV studies of **1** under anaerobic conditions, three electrodes were immersed into the electrochemical cell containing 50 µM **1** and 0.1 M [NBu₄][ClO₄] in 10 mL DMF at various buffered conditions. DPV were started by scanning in the positive (anodic) direction under 1 atm N₂ (cf. Figure S20). DPV parameters: pulse amplitude of 50 mV, a pulse width of 50 ms, a pulse period of 500 ms, and a scan rate of 0.5 mV/s.

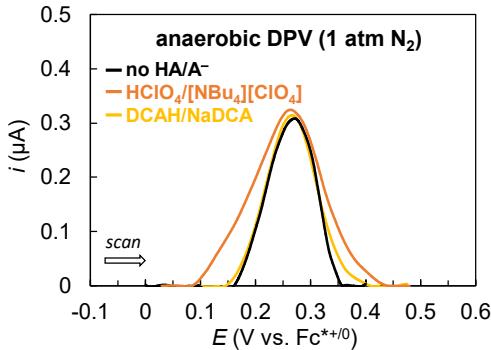


Figure S20. DPV of **1** (50 μM) under anaerobic conditions (1 atm N_2). Peak potentials (vs. $\text{Fc}^{*+/0}$): black trace (without acids) = 0.27 V; orange trace (10 mM HClO_4) = 0.27 V; yellow trace (10 mM DCAH/NaDCA).

3. For the DPV studies of **1** under aerobic conditions in the absence of acids, three electrodes were immersed into the electrochemical cell containing 50 μM **1** and 0.1 M $[\text{NBu}_4][\text{ClO}_4]$ in 10 mL DMF. DPV were started by scanning in the negative (cathodic) direction under 1 atm air (cf. Figure 7 in the main manuscript). DPV parameters: pulse amplitude of 50 mV, a pulse width of 50 ms, a pulse period of 500 ms, and a scan rate of 0.5 mV/s.

4. For the DPV studies of **1** under aerobic conditions with 10 mM HClO_4 , three electrodes were immersed into the electrochemical cell containing 50 μM **1** and 0.1 M $[\text{NBu}_4][\text{ClO}_4]$ in 10 mL DMF. DPV were started by scanning in the negative (cathodic) direction under 1 atm air (cf. Figure 7 in the main manuscript). DPV parameters: pulse amplitude of 50 mV, a pulse width of 50 ms, a pulse period of 500 ms, and a scan rate of 1 mV/s.

5. For the DPV studies of **1** under aerobic conditions with 10 mM each of DCAH and NaDCA, three electrodes were immersed into the electrochemical cell containing 50 μM **1** and 0.1 M $[\text{NBu}_4][\text{ClO}_4]$ in 10 mL DMF. DPV were started by scanning in the negative (cathodic) direction under 1 atm air (cf. Figure 7 in the main manuscript). DPV parameters: pulse amplitude of 50 mV, a pulse width of 50 ms, a pulse period of 500 ms, and a scan rate of 0.5 mV/s.

6. For the DPV studies of **1** under catalytic conditions with 5 mM HClO_4 , three electrodes were immersed into the electrochemical cell containing 25 μM **1**, 6 mM Fc^* , and 0.1 M $[\text{NBu}_4][\text{ClO}_4]$ in 10 mL DMF. DPV were started by scanning in the positive (anodic) direction under 1 atm air (cf. Figure 7 in the main manuscript). DPV parameters: pulse amplitude of 100 mV, a pulse width of 10 ms, a pulse period of 100 ms, and a scan rate of 0.5 mV/s.

7. For the DPV studies of **1** under catalytic conditions with 5 mM each of DCAH and NaDCA, three electrodes were immersed into the electrochemical cell containing 100 μM **1**, 4 mM Fc^* , and 0.1 M $[\text{NBu}_4][\text{ClO}_4]$ in 10 mL DMF. DPV were started by scanning in the negative (cathodic) direction under 1 atm air (cf. Figure 7 in the main manuscript). DPV parameters: pulse amplitude of 50 mV, a pulse width of 50 ms, a pulse period of 500 ms, and a scan rate of 1 mV/s.

XII. Computational details

(a) Density functional theory (DFT) calculations utilizing the BP86 functional^{24,25} were employed to study the thermodynamics of the catalytic pathways. The 6-31G** basis set²⁶ was used for the non-metal atoms except for the O atoms not part of the porphyrin ligand scaffold or the axial solvent ligand (i.e., dioxygen in the adduct and the acids and conjugate bases), which were given diffuse basis functions, corresponding to the 6-31+G** basis set. The LANL2DZ basis set²⁷ was used for the Co center. The geometries for the species in the catalytic pathway were optimized in the gas phase, and subsequently the solvation free energy was calculated via the SMD implicit solvation model.⁷ All computations were performed with Gaussian 09.²⁸

(b) Vibrational frequency calculations at the optimized geometries were performed to account for zero-point energy and entropic contributions, allowing for the calculation of reaction free energies at 298.15 K. Each vibrational analysis also confirmed that the specific optimized geometry corresponds to a minimum by the absence of imaginary frequencies. The rotational entropy for each species, except gas phase O₂, was calculated and removed from the free energy, as prescribed for reactions involving different numbers of reactants and products in solution.²⁹ To account for the experimental partial pressure of 1 atm O₂ and the concentration of N,N-dimethylformamide (DMF) solvent being 12.9 M, standard state corrections were applied as follows

(1) The free energy of gas-phase O₂ was calculated at 1 atm partial pressure. To account for changing the concentration from 1 atm in the gas phase to 1 M in solution, the ideal gas law was applied for a correction: $RT\ln(24.5) = 1.89 \text{ kcal/mol}$.

(2) The free energy of DMF was calculated at 1 atm partial pressure, and an analogous correction to account for the change in concentration from 1 atm to 12.9 M in the gas phase using the ideal gas law, $RT\ln(24.5 \times 12.9) = 3.41 \text{ kcal/mol}$, was applied. Furthermore, the solvation free energy of DMF in DMF was calculated from physical constants of DMF³⁰ to be -6.54 kcal/mol. This value was added to the standard state corrected molar gas-phase free energy to yield the molar solution-phase free energy.

(3) For all other species considered, molar solution phase free energies were calculated in Gaussian 09 from a gas-phase geometry optimization followed by a solvation free energy calculation at the optimized geometry.

(c) Redox potentials of possible mechanistic steps (e.g., electron or concerted electron-proton transfers) were calculated relative to a specified reference reaction. Specifically, the Co^{III/II} redox potential for **1** was calculated, and the value was set equal to the experimental value, with the difference providing a correction for all other calculated redox potentials. Thus, all other calculated redox potentials are reported relative to this reference redox potential to facilitate comparisons to experimental values. As the experimental Co^{III/II} redox potential is referenced to the Fc^{*+/0} couple, all reported calculated redox potentials are also referenced to this couple.

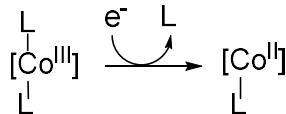


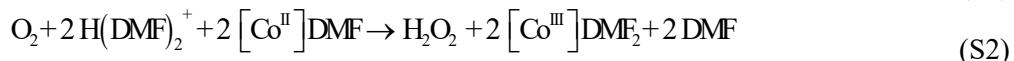
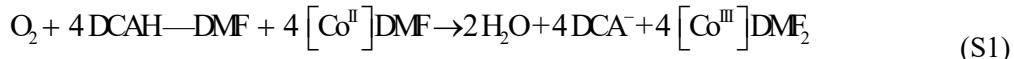
Figure S21. The half-wave potential of **1** is calculated to be 0.28 V, which agrees with the experimental value by construction.

(d) Computed catalytic pathways for the O₂ reduction to H₂O₂/H₂O catalyzed by **1**.

The redox potentials and free energies of individual reactions steps for ORR catalyzed by **1** were computed independently with DMF-H⁺ and DCAH as the acid (Figures S22-S25). DFT calculations for these types of complex reaction mechanisms are associated with certain limitations and errors. In particular, the implicit solvent model neglects hydrogen-bonding interactions between the solvent and the acid as well as between the solvent and the intermediates along the reaction pathway. Discrepancies in the quantitative interpretation of the free energy diagrams in the context of the experimental data can also arise inherent limitations of DFT, especially for reaction intermediates involving O₂, and the differences between the standard states used for the calculations and the experimental conditions. Thus, the quantitative values are not definitive and should be viewed as only a guide to understand trends. Despite these limitations, however, the calculations have played an essential role in the interpretation of the experimental data and in the generation of the qualitative free energy diagrams in Figure 8 of the main paper, which are consistent with the experimental data.

To partially account for the limitations of DFT, the calculations were performed with two different treatments of the acid. In the first treatment, the acid was represented as a single DMF-H⁺ or DCAH molecule. This approach provides free energy diagrams that are in good agreement with the experimental kinetic, spectroscopic and CV data that provide insights into intermediates early in the reaction pathway, and the computational results are presented in Figures S22-S25.

In a second treatment, the acid was represented as a hydrogen-bonded complex with a solvent molecule, corresponding to (DMF)₂H⁺ or DMF-DCAH. Thus, the second treatment includes the free energy associated with breaking the hydrogen-bonding interaction between the acid and the solvent molecule. Given that two or four acid molecules are required for the catalytic cycle to produce H₂O₂ or H₂O, respectively, this difference significantly impacts the overall thermodynamics, and the results aligns better with the experimentally observed overall reaction thermodynamics. The calculation of the effective overpotential defined in Equation 3 of the main manuscript requires the computation of the redox potentials with respect to the Co^{III/II} reference and the inclusion of the free energies associated with breaking the hydrogen-bonding interaction between each equivalent of acid and a solvent DMF molecule. The reactions corresponding to the effective overpotentials for producing H₂O with a weak acid or H₂O₂ with a strong acid are as follows:



Using these equations, we observe agreement within the error of DFT between the experimental and computed effective overpotentials for the reduction of oxygen to H₂O₂ or H₂O under their respective conditions. These results are provided in Table 3 of the main paper.

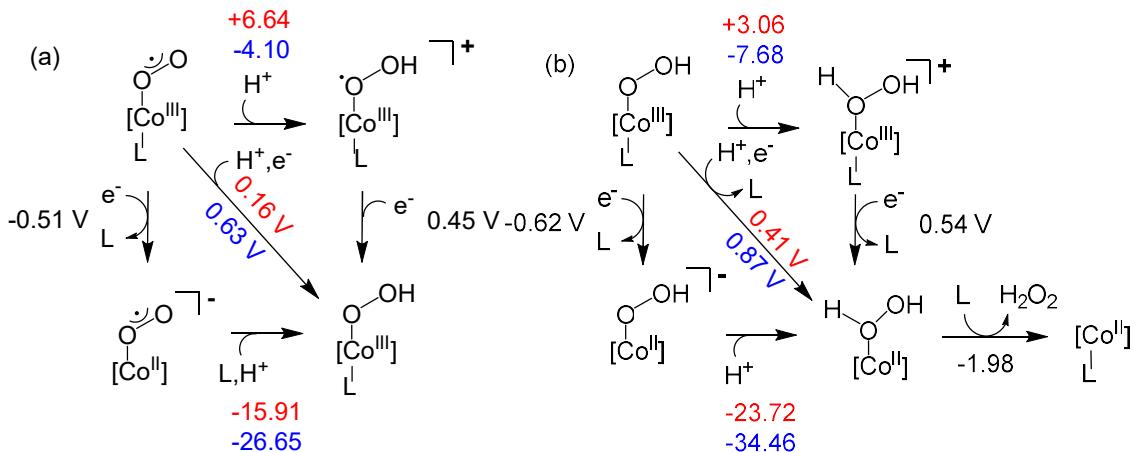


Figure S22. Computed redox potentials and reaction free energies for the (a) first and (b) second proton-coupled electron transfer steps in the mechanistic pathway. The numbers in red correspond to weak acid (DCAH) catalytic conditions, and the numbers in blue correspond to strong acid (DMF- H^+) catalytic conditions. All values in red and blue are in kcal/mol unless otherwise noted, and redox potentials are relative to $\text{Fc}^{*0/+}$.

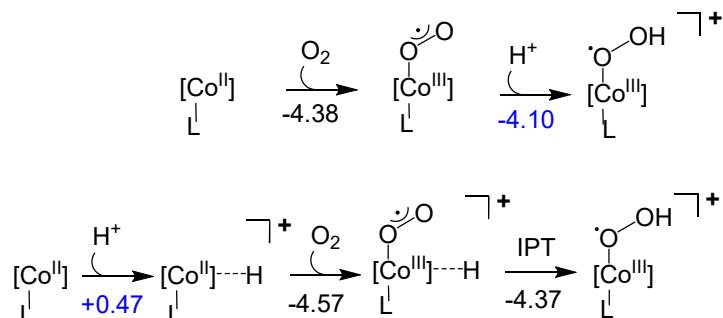


Figure S23. Computed thermodynamics of O_2 binding, pre- O_2 binding protonation of the nitrogen on the porphyrin ancillary ligand of the Co complex, and intramolecular proton transfer (IPT) in strong acid conditions. All values are in kcal/mol. The numbers in blue correspond to strong acid (DMF- H^+) conditions.

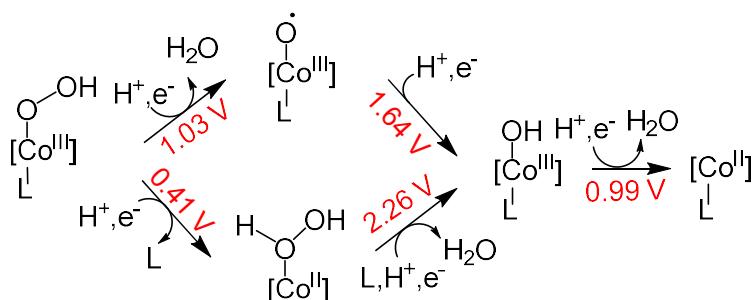


Figure S24. Computed redox pathways for production of water in weak acid catalytic conditions (i.e., with DCAH as the acid source). All redox values are relative to $\text{Fc}^{*0/+}$.

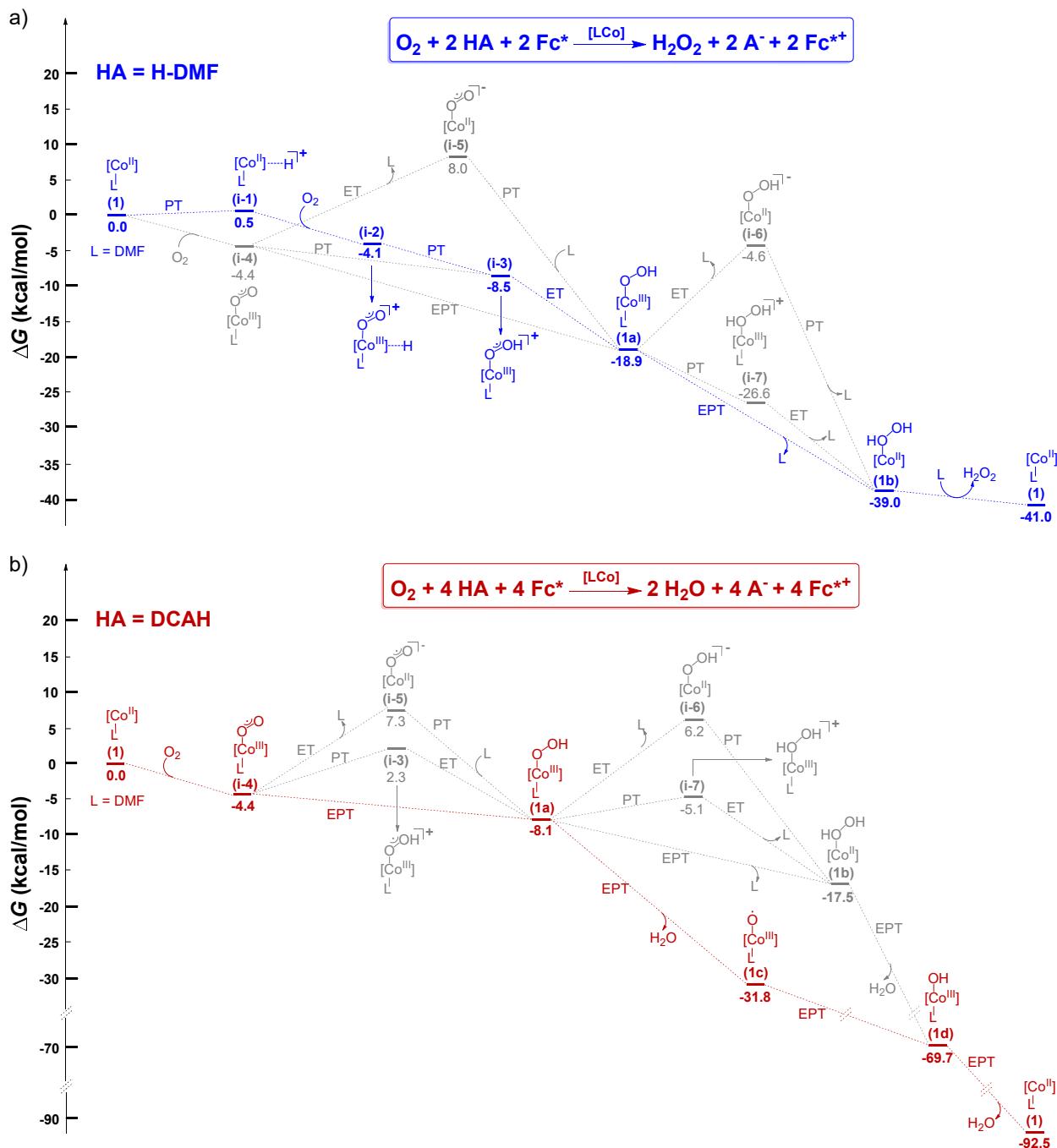


Figure S25. Calculated free energy profiles for $\text{O}_2/\text{H}_2\text{O}$ and $\text{O}_2/\text{H}_2\text{O}_2$ pathways in (a) strong acid (DMF- H^+) and (b) weak acid (DCAH) conditions. All redox potentials are coupled to $\text{Fc}^{*+/0}$.

DMF**-248.4457129**

C	0.748422	-0.329038	-0.001048
O	1.602394	-1.181946	0.240640
N	0.714533	0.940614	0.528290
H	-0.111775	-0.503547	-0.695266
C	-0.334496	1.886264	0.186972
H	-1.034461	1.414694	-0.522097
H	-0.902696	2.196569	1.084371
H	0.082960	2.795046	-0.286632
C	1.752385	1.364216	1.458859
H	2.443388	0.518233	1.586471
H	2.303042	2.237902	1.063839
H	1.316217	1.639010	2.437039

O₂**-150.3524578**

O	-2.333798	0.401575	0.000000
O	-1.102107	0.401575	0.000000

H₂O₂**-151.5678342**

O	-0.46767900	-0.45789900	-0.03837800
H	-0.66743500	0.36804000	0.45167500
O	1.00801800	-0.38955900	-0.03837800
H	1.20777400	-1.21549800	0.45167600

H₂O**-76.434985**

O	-0.40482100	-0.44494000	0.00000000
H	0.56813000	-0.40638500	0.00000000
H	-0.69325500	0.48507400	0.00000000

DCAH**-1148.315705**

C	-0.32022700	0.27968900	0.10939300
O	0.80780000	0.19788200	0.55475800
O	-0.92182200	1.44030500	-0.27797800
C	-1.30933400	-0.88503400	-0.09174500
H	-0.28213600	2.16300500	-0.09111200
Cl	-0.45965900	-2.34857600	-0.65820100
Cl	-2.17514200	-1.14745400	1.47495200
H	-2.07382200	-0.62441900	-0.83470800

DCA⁻**-1147.874328**

C	-0.34526000	0.38726100	0.17296900
O	0.65938000	0.21860500	0.90296500
O	-0.77421700	1.39401800	-0.47165300
C	-1.32568500	-0.84546400	-0.04197100
Cl	-0.50336900	-2.27106500	-0.87651900

Cl -2.10339100 -1.41906800 1.53005000
H -2.16632100 -0.58062900 -0.69465500

HDMF⁺

-248.8699825
C 0.51446100 -0.28979400 -0.09259200
O 1.44589200 -1.20776900 0.08451600
N 0.65131400 0.89683600 0.43555900
H -0.38155800 -0.51466900 -0.68391800
C -0.38885000 1.93022800 0.24152100
H -1.21053000 1.53551200 -0.37209400
H -0.77567500 2.23493400 1.22633000
H 0.06298700 2.79998400 -0.26016700
C 1.82956300 1.27818300 1.24569500
H 1.48267200 1.56859200 2.24983100
H 2.53108400 0.43892900 1.31746100
H 2.31826300 2.14015500 0.76502000
H 1.22255600 -2.05121400 -0.36253200

DCAH-DMF

-1396.77725
C -0.87841600 0.56845500 0.12179300
O -1.48083100 1.35537900 0.84817200
O 0.12568900 0.85663000 -0.70367600
C -1.21355300 -0.93853400 0.03002900
Cl -1.42839700 -1.64862300 1.66310100
Cl -2.69049400 -1.13681800 -0.99688900
H -0.40676700 -1.48845200 -0.46941400
H 0.33060200 1.88240800 -0.67523700
O 0.65894700 3.36731400 -0.66539100
C -0.06039200 4.04799000 0.11089200
N 0.05475200 5.38460700 0.26743000
H -0.84823900 3.56425500 0.72247900
C -0.81478900 6.11258100 1.18757800
C 1.05216500 6.15125000 -0.47808200
H -1.50888800 5.41038600 1.67362600
H -0.21725900 6.61909700 1.96648400
H -1.40176500 6.87490600 0.64479100
H 1.61499000 5.45940400 -1.11911200
H 0.55619500 6.91574400 -1.10173100
H 1.74287000 6.65706900 0.21941500

H(DMF)₂⁺

-497.3340117
H 1.54904800 1.28042000 -0.10147900
N 2.41655500 1.15590300 -2.86191100
C 1.62740500 0.34970700 -2.15664900
C 2.69919600 0.85146900 -4.27647000
C 3.05603200 2.37006000 -2.33230300
O 1.27321100 0.45066800 -0.93213100
H 1.23103100 -0.51693400 -2.70860400

H	2.18014600	-0.06941200	-4.57758700
H	2.35451000	1.68504100	-4.90963000
H	3.78420300	0.71770800	-4.41578700
H	2.79502000	2.52902600	-1.28006300
H	4.15008700	2.27159300	-2.42535400
H	2.72581900	3.23911100	-2.92469900
O	1.82488700	2.11017700	0.72917400
C	1.47069500	2.21114400	1.95369200
N	0.68154400	1.40495200	2.65895800
H	1.86707100	3.07778700	2.50564400
C	0.39890500	1.70939000	4.07351600
C	0.04206600	0.19079400	2.12935400
H	0.91795600	2.63027200	4.37463000
H	-0.68610200	1.84315400	4.21283300
H	0.74359000	0.87582100	4.70667800
H	0.30307800	0.03182600	1.07711400
H	0.37227800	-0.67825600	2.72175100
H	-1.05198900	0.28926300	2.22240500

1

	-2763.78765		
Co	-0.33087900	-0.04010700	0.60951300
N	1.58298100	-0.02495700	0.11090300
C	2.15671700	0.58355400	-0.99719900
C	2.64023800	-0.62185500	0.78562400
C	3.58311700	0.33492600	-1.03279200
C	3.88102300	-0.42256200	0.06619200
H	4.25466900	0.68647900	-1.81388700
H	4.85052200	-0.80056700	0.38538900
N	0.12807100	-0.86486600	2.35423500
C	-0.72455000	-1.06531200	3.43308800
C	1.38285700	-1.25091800	2.80622500
C	0.01824800	-1.52619600	4.58802400
C	1.31559800	-1.68594800	4.18524500
H	-0.41311700	-1.72890000	5.56634700
H	2.16185600	-2.05048600	4.76461100
N	-2.26421500	-0.26651700	1.00733400
C	-3.33449800	-0.16729700	0.12081900
C	-2.82537400	-0.68547600	2.20653100
C	-4.56053900	-0.59787800	0.75752700
C	-4.25006500	-0.88918200	2.05845000
H	-5.52798700	-0.66738700	0.26386800
H	-4.90919800	-1.25227700	2.84505700
N	-0.79570500	0.68478600	-1.18148200
C	-2.06219900	0.84121000	-1.73228000
C	0.06688900	1.32880800	-2.06291200
C	-1.99478200	1.62942300	-2.94364400
C	-0.67787600	1.95406800	-3.13368900
H	-2.85403600	1.91393500	-3.54849400
H	-0.24040500	2.55279700	-3.93048900
C	-2.12615500	-0.96837000	3.39479200

C	-2.92221700	-1.26185100	4.62681900
C	-2.89596100	-2.52824500	5.24629900
C	-3.75382600	-0.26866700	5.19921000
C	-3.65347200	-2.80403200	6.39688900
H	-2.27936400	-3.32112000	4.81067200
C	-4.51220700	-0.52487900	6.34365700
H	-3.79368600	0.72226500	4.73519600
C	-4.46600600	-1.79681200	6.95353700
H	-3.60978700	-3.80219100	6.83982200
H	-5.14728300	0.24620300	6.79015700
C	-3.26773000	0.36554100	-1.17916300
C	-4.51500600	0.47937900	-1.99479100
C	-4.61419800	-0.16657000	-3.25227800
C	-5.62494500	1.23296500	-1.56012400
C	-5.76882900	-0.06986800	-4.03117800
H	-3.76830400	-0.76158900	-3.61124500
C	-6.79424800	1.34206200	-2.33117600
H	-5.57082200	1.75464700	-0.59892400
C	-6.87055900	0.68565300	-3.57530900
H	-5.84695400	-0.57809800	-4.99693200
H	-7.62806300	1.94243600	-1.95857700
C	1.47124600	1.30569400	-1.99058900
C	2.27159600	2.00765000	-3.04080000
C	3.15385200	3.05145700	-2.69394300
C	2.18881400	1.64485100	-4.40756000
C	3.92210700	3.72275600	-3.65970400
H	3.23648100	3.34881600	-1.64330400
C	2.94612500	2.30090000	-5.38057500
H	1.52744500	0.82360200	-4.70178100
C	3.81842000	3.34812700	-5.01369500
H	4.58820700	4.53112100	-3.34767400
H	2.88849600	2.01354000	-6.43475300
C	2.57076400	-1.21781200	2.05608400
C	3.82480100	-1.78370500	2.64881600
C	4.46440200	-1.17178600	3.75326300
C	4.41363900	-2.94463100	2.10987700
C	5.63617000	-1.70258000	4.29855500
H	4.03429700	-0.26003200	4.18062100
C	5.59295200	-3.49076300	2.64448600
H	3.93590100	-3.43609500	1.25576700
C	6.20936500	-2.86864600	3.74759600
H	6.13379000	-1.22695400	5.14909200
H	6.01346000	-4.39618900	2.19974000
O	7.36036300	-3.30961100	4.35502800
C	7.97145400	-4.48518900	3.82326900
H	8.27828000	-4.34685600	2.76853700
H	8.86442800	-4.66523100	4.43951500
H	7.29977500	-5.36275100	3.88981400
O	4.51693400	3.92858200	-6.04430400
C	5.41999300	4.98307000	-5.71148300
H	6.21610800	4.63926000	-5.02328800

H	5.87442700	5.30100200	-6.66116900
H	4.89521400	5.84331100	-5.25278500
O	-5.24676500	-1.94810000	8.07354000
C	-5.22543700	-3.22135900	8.71962200
H	-4.21070200	-3.48296300	9.07653300
H	-5.90130900	-3.13210400	9.58259400
H	-5.59051700	-4.02593900	8.05259600
O	-7.95762700	0.71732900	-4.41375600
C	-9.09672500	1.46259600	-3.98296900
H	-8.85884700	2.53576200	-3.85055200
H	-9.84628800	1.35402600	-4.78031500
H	-9.51140100	1.06651300	-3.03602700
C	-1.11152200	2.84120200	1.20786500
O	-0.22302700	2.02274700	1.50808800
N	-1.16451700	4.11887300	1.67905800
H	-1.94261500	2.58338800	0.51916800
C	-2.22618700	5.03217900	1.27983900
H	-2.91045900	4.51940300	0.58601000
H	-2.80401100	5.37431200	2.15849300
H	-1.81050700	5.92105700	0.77004700
C	-0.14149600	4.61294200	2.59556200
H	0.56927500	3.79559500	2.78092900
H	0.39040000	5.47517200	2.15392800
H	-0.59811600	4.93190900	3.54999700

[Co^{III}](DMF)₂

-3012.071928

Co	-0.34254700	-0.14015000	0.51141900
N	1.57430700	-0.03897400	0.04426400
C	2.14174600	0.66864000	-1.00577400
C	2.61702900	-0.69986400	0.67748300
C	3.56562900	0.41823900	-1.04926600
C	3.85596000	-0.44148300	-0.02181600
H	4.24368100	0.83945100	-1.78910300
H	4.82420400	-0.84427400	0.26930900
N	0.12337100	-0.90023500	2.28350800
C	-0.70772900	-0.99161100	3.38892500
C	1.36721000	-1.35033300	2.69312900
C	0.05005300	-1.45455500	4.53283600
C	1.31353800	-1.73673900	4.08718200
H	-0.35193300	-1.57938900	5.53608000
H	2.15145500	-2.14113400	4.65145600
N	-2.27216600	-0.25551000	0.95352000
C	-3.32483500	-0.27345100	0.04270900
C	-2.81454300	-0.60819600	2.17819200
C	-4.53587200	-0.69802500	0.70671900
C	-4.22988700	-0.86210900	2.03337100
H	-5.49662000	-0.84197100	0.21651000
H	-4.88546600	-1.17742200	2.84295400
N	-0.79764800	0.63715800	-1.25542700
C	-2.06516000	0.73333800	-1.81655500

C	0.04364200	1.40199500	-2.06164300
C	-2.02058900	1.59017900	-2.97740400
C	-0.72720800	2.03331200	-3.10558900
H	-2.88463000	1.84919800	-3.58674400
H	-0.32385800	2.71869300	-3.84856700
C	-2.10688100	-0.83033200	3.37923100
C	-2.89479300	-1.00744100	4.63382100
C	-2.86226500	-2.20518700	5.38003200
C	-3.73673100	0.03449800	5.09804200
C	-3.61899900	-2.36435400	6.55098300
H	-2.25162900	-3.04156900	5.02488500
C	-4.49046800	-0.10524900	6.26325300
H	-3.78449500	0.97277000	4.53542300
C	-4.43624200	-1.30764000	7.00412100
H	-3.57511400	-3.31257400	7.09195500
H	-5.12939200	0.70397100	6.62849600
C	-3.25781600	0.19072100	-1.28647600
C	-4.47905800	0.20908100	-2.14107300
C	-4.46960300	-0.42113100	-3.41186500
C	-5.66697800	0.86147900	-1.74492200
C	-5.59528000	-0.41607000	-4.23470100
H	-3.56159700	-0.93392300	-3.74571400
C	-6.80691600	0.88069800	-2.56265900
H	-5.69603400	1.38573100	-0.78417000
C	-6.77855700	0.23420300	-3.81621400
H	-5.59058000	-0.91406700	-5.20855900
H	-7.70149100	1.40772300	-2.22253300
C	1.44944900	1.44894600	-1.95641800
C	2.24250300	2.26889900	-2.91770700
C	3.12920600	3.26164200	-2.44718000
C	2.15705000	2.07497300	-4.31973500
C	3.89261100	4.04634700	-3.32473000
H	3.21519000	3.43140900	-1.36871600
C	2.91258100	2.84322500	-5.20557400
H	1.50114600	1.29257700	-4.71506900
C	3.78608200	3.84097500	-4.71621200
H	4.55837000	4.81165500	-2.91877500
H	2.85553300	2.68469700	-6.28634700
C	2.54161000	-1.36604300	1.91619900
C	3.78341800	-1.99860700	2.46021000
C	4.45154200	-1.46923100	3.59163400
C	4.33980300	-3.13499800	1.83926900
C	5.61571600	-2.05944900	4.08543000
H	4.05646000	-0.57087200	4.07711600
C	5.50932000	-3.74221000	2.32454200
H	3.84267000	-3.56237900	0.96179000
C	6.15415100	-3.20536600	3.45777800
H	6.13713400	-1.64684800	4.95396700
H	5.90315200	-4.62797300	1.82047600
O	7.29357600	-3.70645000	4.02116700
C	7.88032100	-4.86533500	3.41887000

H	8.18531400	-4.66967000	2.37365900
H	8.77083200	-5.09511300	4.02038400
H	7.18975700	-5.72921300	3.44275400
O	4.47645900	4.53792400	-5.66548500
C	5.38524900	5.55193700	-5.22000400
H	6.18622900	5.12831600	-4.58582700
H	5.82842300	5.97547600	-6.13194300
H	4.86049800	6.35050500	-4.66297900
O	-5.21056100	-1.34396100	8.12804400
C	-5.18760800	-2.54056300	8.91563500
H	-4.17204600	-2.75508000	9.29745100
H	-5.86278500	-2.35249200	9.76195700
H	-5.55465700	-3.41150700	8.34114400
O	-7.82273700	0.18192400	-4.69337700
C	-9.04720500	0.82189900	-4.31342600
H	-8.90810500	1.90948000	-4.16830100
H	-9.74239000	0.65228500	-5.14728000
H	-9.46631200	0.37924800	-3.39067500
C	-1.06748200	2.51077200	1.11732400
O	-0.18673100	1.62168900	1.31720200
N	-0.99954700	3.72716300	1.67827100
H	-1.93831300	2.32466400	0.46892800
C	-2.02347600	4.73943000	1.41398400
H	-2.78568500	4.33177600	0.73378400
H	-2.50960600	5.04456800	2.35655900
H	-1.56768300	5.62915600	0.94649400
C	0.10527100	4.09766100	2.56901800
H	0.77759600	3.23723700	2.67812100
H	0.65887700	4.95201000	2.14376800
H	-0.29295000	4.38680000	3.55627400
C	0.04491700	-2.28069900	-1.27574700
O	-0.47554000	-1.95801900	-0.16647700
N	-0.04576700	-3.52156100	-1.77724000
H	0.60117200	-1.55086100	-1.88501100
C	0.57143400	-3.86558700	-3.05925300
H	1.07572900	-2.98352500	-3.48067600
H	1.31476600	-4.66944100	-2.92070900
H	-0.19674800	-4.21372500	-3.77105400
C	-0.76300500	-4.58368400	-1.06356600
H	-1.17244800	-4.17218600	-0.13231300
H	-1.58307100	-4.96844300	-1.69314500
H	-0.07184900	-5.41200000	-0.83263400

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	-2914.147082		
Co	-0.35537200	-0.14987300	0.52297300
N	1.57851700	-0.04984400	0.05850300
C	2.14996300	0.62724400	-1.00823000
C	2.63209200	-0.64282600	0.73724700
C	3.58429200	0.43179100	-1.01287800
C	3.88096400	-0.36817900	0.05856400

H	4.26368300	0.84692500	-1.75520600
H	4.85602500	-0.72200000	0.38877400
N	0.11187200	-0.92319700	2.30153400
C	-0.73516100	-1.08750300	3.38496400
C	1.36101400	-1.33625300	2.73294300
C	0.00704100	-1.57212900	4.53102200
C	1.29352300	-1.77603600	4.11193200
H	-0.41751800	-1.75535800	5.51609500
H	2.13480600	-2.16344300	4.68356500
N	-2.27961300	-0.32582900	0.95009800
C	-3.33973600	-0.23748400	0.06202000
C	-2.83508000	-0.66558800	2.16911300
C	-4.57680000	-0.59580900	0.72624100
C	-4.26907400	-0.82524200	2.03968100
H	-5.54995600	-0.65201100	0.24237600
H	-4.93509200	-1.11736200	2.84959000
N	-0.79849400	0.58584300	-1.27178600
C	-2.06229900	0.70270100	-1.82566700
C	0.05140900	1.28323100	-2.12054900
C	-2.00637600	1.49178200	-3.03734500
C	-0.70292100	1.87888700	-3.20184100
H	-2.86912700	1.75070100	-3.64847400
H	-0.28180200	2.51208500	-3.98048800
C	-2.13350200	-0.93608600	3.36024100
C	-2.92513900	-1.14444300	4.61138200
C	-2.95256800	-2.38442000	5.28164600
C	-3.69771000	-0.08661800	5.15070300
C	-3.70648500	-2.57427200	6.45193500
H	-2.38373900	-3.22527400	4.87138600
C	-4.45099900	-0.25821600	6.31390200
H	-3.69161400	0.88574000	4.64765200
C	-4.45937800	-1.50489700	6.97565300
H	-3.70665900	-3.55417600	6.93591000
H	-5.03906300	0.56219300	6.73597800
C	-3.26456300	0.23077700	-1.26279700
C	-4.51119200	0.32954300	-2.08125000
C	-4.62858300	-0.37455200	-3.30462400
C	-5.59762700	1.13685400	-1.68469800
C	-5.78204100	-0.28752900	-4.08697100
H	-3.79754900	-1.00571100	-3.63640000
C	-6.76430600	1.23732800	-2.46028400
H	-5.52104400	1.71306600	-0.75710700
C	-6.86198400	0.51930400	-3.66856100
H	-5.87528100	-0.83918700	-5.02727900
H	-7.57833300	1.88254700	-2.12060500
C	1.45372100	1.33768000	-2.00692400
C	2.24608400	2.11996800	-3.00382700
C	3.05775700	3.19454500	-2.58425000
C	2.22666500	1.81280400	-4.38631100
C	3.81778200	3.94601700	-3.49518100
H	3.08447800	3.45510900	-1.52122500

C	2.97752100	2.54890100	-5.30560700
H	1.61735000	0.97412900	-4.73890200
C	3.77884900	3.62470200	-4.86634700
H	4.42439500	4.77741100	-3.12768900
H	2.96722700	2.30633900	-6.37250100
C	2.55136900	-1.29027600	1.98418000
C	3.80660300	-1.86151800	2.56845200
C	4.43006700	-1.27935600	3.69858900
C	4.41800700	-2.99267700	1.99284000
C	5.60517800	-1.81242200	4.23362500
H	3.98558400	-0.38773400	4.15254800
C	5.60105300	-3.54117800	2.51693700
H	3.95487500	-3.45959700	1.11702500
C	6.19944600	-2.95027900	3.64685400
H	6.09007000	-1.35895800	5.10331600
H	6.03909300	-4.42356800	2.04363100
O	7.35149000	-3.39591500	4.24776100
C	7.98577800	-4.54164700	3.67955100
H	8.29943700	-4.36025500	2.63335300
H	8.87618400	-4.72982800	4.29696600
H	7.32765500	-5.43150800	3.70848200
O	4.47631800	4.28514700	-5.84730900
C	5.29645600	5.38252200	-5.44270900
H	6.09087600	5.06340300	-4.74096700
H	5.75906500	5.76717100	-6.36324300
H	4.70046900	6.18672600	-4.97032400
O	-5.23028200	-1.57060300	8.11041700
C	-5.25906200	-2.81348600	8.81236000
H	-4.25218900	-3.10781200	9.16615400
H	-5.91565900	-2.65376400	9.68001900
H	-5.67306200	-3.62827100	8.18744100
O	-7.94971500	0.53742400	-4.50634100
C	-9.06292100	1.34377400	-4.11807300
H	-8.78828000	2.41357500	-4.04467300
H	-9.81633400	1.21675000	-4.90903400
H	-9.48973400	1.01453500	-3.15123200
O	-0.23172200	1.58967800	1.30382400
C	0.08117100	-2.43750900	-1.34363900
O	-0.44976900	-2.17618100	-0.24380100
N	0.04949400	-3.66507400	-1.92393300
H	0.62316500	-1.66918600	-1.92849700
C	0.69151700	-3.91258500	-3.20890000
H	1.16361600	-2.98598300	-3.57010200
H	1.47018000	-4.69151500	-3.11444100
H	-0.04805500	-4.24866600	-3.95860200
C	-0.63414400	-4.78067600	-1.27359700
H	-1.06190000	-4.41673200	-0.32950900
H	-1.44065200	-5.16727400	-1.92197600
H	0.07725400	-5.60044600	-1.06749700
O	-1.14870400	2.44679000	1.04570100

1-H⁺**-2764.211166**

Co	-0.40554100	-0.12146700	0.62418600
N	1.62094600	-0.30737000	0.03460800
C	2.17647300	0.57976500	-0.97246700
C	2.67218500	-0.46972600	1.02235800
C	3.46476200	0.97369300	-0.55653600
C	3.76664000	0.33477400	0.64516000
H	4.08322800	1.69260100	-1.09183000
H	4.66793300	0.45314800	1.24468400
N	0.03526300	-1.15298600	2.25942400
C	-0.86398100	-1.60980500	3.21443700
C	1.27083200	-1.67530400	2.64908800
C	-0.20191300	-2.47824800	4.16513500
C	1.11160800	-2.54913000	3.79205900
H	-0.69051900	-2.96644100	5.00567700
H	1.91442200	-3.11878000	4.25573000
N	-2.29973600	-0.13445800	1.07202400
C	-3.35867300	0.30566800	0.28599000
C	-2.86483800	-0.50614400	2.28496000
C	-4.59328600	0.25548500	1.03845100
C	-4.28637400	-0.23766200	2.27762000
H	-5.57134400	0.51965300	0.64175300
H	-4.96194700	-0.45998100	3.10111000
N	-0.80755800	0.49190300	-1.22280000
C	-2.06932300	0.62386500	-1.79480600
C	0.08844700	0.74459600	-2.26487900
C	-1.96026200	0.89294000	-3.21219100
C	-0.62507700	0.94521000	-3.50657500
H	-2.80396600	1.02669400	-3.88612900
H	-0.15343900	1.11253400	-4.47287100
C	-2.21777200	-1.23622700	3.30289700
C	-3.01900400	-1.66471300	4.48997700
C	-3.30916500	-3.02387100	4.72823600
C	-3.52279300	-0.70603700	5.40269900
C	-4.06941900	-3.42769700	5.83685300
H	-2.95172800	-3.78180100	4.02313700
C	-4.27581000	-1.09289500	6.51179100
H	-3.30530200	0.35515800	5.24224900
C	-4.55637200	-2.45946100	6.73982800
H	-4.28356000	-4.48926800	5.98076600
H	-4.65643500	-0.35615700	7.22499800
C	-3.28785600	0.60985700	-1.08948300
C	-4.55484200	0.90123900	-1.82798000
C	-5.02408500	0.02369800	-2.83661200
C	-5.32223000	2.04822600	-1.54040200
C	-6.20809200	0.28547000	-3.52632300
H	-4.45697400	-0.88450800	-3.06564200
C	-6.51359900	2.32759000	-2.22837400
H	-4.97750100	2.74641600	-0.77001100
C	-6.96441100	1.44232200	-3.22979500

H	-6.57838400	-0.39681600	-4.29678700
H	-7.07501100	3.23222800	-1.98339100
C	1.48745800	0.92985500	-2.14016400
C	2.26199000	1.55802300	-3.24344000
C	1.85108800	2.77470200	-3.83398600
C	3.45494400	0.95934000	-3.72687000
C	2.58638700	3.37752100	-4.86346700
H	0.94707400	3.26978100	-3.46526400
C	4.19229800	1.54218000	-4.75524900
H	3.78799400	0.00691700	-3.30182500
C	3.76544000	2.75998700	-5.33467600
H	2.24267200	4.32544500	-5.28390100
H	5.10040400	1.07097800	-5.14176200
C	2.53833600	-1.28065800	2.15672200
C	3.77915200	-1.63437800	2.89736800
C	3.91506600	-1.37576100	4.28666800
C	4.87656800	-2.21891900	2.22570500
C	5.08784300	-1.69429400	4.96788800
H	3.09199100	-0.89730400	4.82645800
C	6.05857000	-2.55493100	2.89961200
H	4.79399900	-2.44044400	1.15640400
C	6.17094500	-2.29324800	4.28225600
H	5.19991400	-1.48273400	6.03505200
H	6.87583100	-3.02545400	2.34821300
O	7.26611100	-2.57144700	5.04252400
C	8.39492100	-3.17902200	4.39889600
H	8.80450900	-2.52912300	3.60369600
H	9.14910200	-3.31118300	5.18670400
H	8.13364200	-4.16468700	3.97172100
O	4.55739600	3.24681300	-6.32997400
C	4.16300300	4.47037900	-6.96615700
H	4.14123600	5.31052900	-6.24766200
H	4.92638400	4.66532000	-7.73175600
H	3.17376600	4.37293800	-7.45003900
O	-5.30140600	-2.73092300	7.85055800
C	-5.61382600	-4.10204800	8.12646600
H	-4.69849900	-4.70207400	8.28531800
H	-6.20721500	-4.09117900	9.05118500
H	-6.21172800	-4.55315700	7.31276200
O	-8.10388900	1.60542900	-3.96259600
C	-8.91259500	2.75717900	-3.69381200
H	-8.36022400	3.69520200	-3.88977200
H	-9.76667600	2.68756400	-4.38155200
H	-9.28105300	2.75915300	-2.65102000
C	-0.63058600	2.79998100	1.29449600
O	0.11637700	1.80771300	1.45706500
N	-0.41312600	4.01365900	1.85191600
H	-1.54410600	2.74652300	0.66824200
C	-1.32175100	5.13341100	1.61901200
H	-2.14126800	4.81483700	0.95677000
H	-1.75289600	5.48759800	2.57204600

H	-0.78747900	5.97434800	1.14249700
C	0.74435000	4.24585700	2.71667000
H	1.30581200	3.30610300	2.80190500
H	1.39207500	5.02938700	2.28612000
H	0.41134200	4.57267800	3.71704000
H	1.38897400	-1.22222700	-0.38838000

1a-H⁺

-2914.570907

Co	-0.31451500	-0.04380100	0.48022800
N	1.75968500	0.40024800	0.19140900
C	2.28825400	0.57405200	-1.14647600
C	2.77865700	-0.32269500	0.92308600
C	3.53532700	-0.08569200	-1.21803500
C	3.83386400	-0.62204100	0.03314200
H	4.12200400	-0.18044500	-2.13076200
H	4.70187000	-1.22327900	0.30040100
N	0.15595600	-0.81887300	2.26205600
C	-0.76188300	-1.17156200	3.23639300
C	1.38280800	-0.74514000	2.91143000
C	-0.12115000	-1.23027800	4.53251300
C	1.20707700	-0.95799700	4.33180600
H	-0.63417800	-1.42981400	5.47128800
H	2.00191500	-0.89336700	5.07256300
N	-2.21360700	-0.37951300	0.77639100
C	-3.23480100	-0.15014400	-0.13180900
C	-2.75118300	-1.17747800	1.77288100
C	-4.40874800	-0.90044600	0.25353200
C	-4.10693800	-1.54176200	1.42931200
H	-5.33822400	-0.93238200	-0.31199300
H	-4.74108100	-2.20267900	2.01719200
N	-0.69338500	0.86146000	-1.25920200
C	-1.94857500	1.29259300	-1.66815100
C	0.21510300	1.54691500	-2.05947700
C	-1.82175500	2.32214300	-2.67434000
C	-0.48139500	2.47552100	-2.92019300
H	-2.65369400	2.86508600	-3.11861000
H	0.00311200	3.16858900	-3.60564000
C	-2.11940200	-1.48097900	3.00171500
C	-2.91055900	-2.11285600	4.08743600
C	-2.45190300	-3.28294300	4.73525200
C	-4.14606500	-1.55985800	4.51766800
C	-3.18816600	-3.89369500	5.75941600
H	-1.51123900	-3.73904200	4.41008500
C	-4.88145700	-2.14801200	5.54418200
H	-4.50894400	-0.63593100	4.05680100
C	-4.41232800	-3.32521800	6.17310400
H	-2.80946900	-4.80886000	6.22043400
H	-5.82160100	-1.71058900	5.89189000
C	-3.17215500	0.74341000	-1.22863700
C	-4.42888400	1.11332800	-1.92688300

C	-4.54974300	1.00851200	-3.33780300
C	-5.54663100	1.59299700	-1.20498100
C	-5.72952500	1.35854600	-3.99107000
H	-3.70715500	0.62368100	-3.92134200
C	-6.73433600	1.96243600	-1.84963400
H	-5.46993500	1.71129500	-0.11959200
C	-6.83458600	1.84375100	-3.25294700
H	-5.82950200	1.26178000	-5.07588500
H	-7.56606600	2.35142100	-1.25779800
C	1.61250900	1.29693700	-2.13872200
C	2.38119100	1.74940500	-3.32451700
C	3.62565900	2.40517900	-3.17634600
C	1.90357800	1.53123300	-4.64446100
C	4.36655300	2.83849700	-4.28326400
H	4.00697000	2.60859600	-2.17037600
C	2.63383500	1.94708400	-5.75488900
H	0.95395700	1.00727900	-4.79095300
C	3.87291900	2.60960600	-5.58626100
H	5.31216600	3.36189900	-4.12450200
H	2.27450800	1.76633200	-6.77192400
C	2.65199000	-0.65970100	2.27860200
C	3.88558000	-1.02710900	3.01731200
C	5.04088100	-0.20335200	2.94904800
C	3.96581600	-2.20899300	3.79017600
C	6.20887600	-0.53645900	3.63031100
H	5.00223200	0.72718000	2.37364100
C	5.13686300	-2.56207100	4.47298500
H	3.10072900	-2.87787900	3.83607200
C	6.26947500	-1.72161600	4.40068500
H	7.09107000	0.10898700	3.59629400
H	5.16375700	-3.49194900	5.04573600
O	7.45642900	-1.95704600	5.02441000
C	7.56920300	-3.13472700	5.83588800
H	7.43267500	-4.05319500	5.23572000
H	8.58833400	-3.11509500	6.24556300
H	6.83901800	-3.12382700	6.66580200
O	4.50183000	2.98021400	-6.73504900
C	5.76217900	3.65741400	-6.62485300
H	6.51675500	3.02568200	-6.12114200
H	6.08220400	3.85614000	-7.65677600
H	5.65924500	4.61453200	-6.08145400
O	-5.21052400	-3.82303100	7.15839100
C	-4.77607900	-5.00612600	7.84241700
H	-3.81011200	-4.84424900	8.35535600
H	-5.55407200	-5.21963600	8.58816100
H	-4.68661800	-5.86346500	7.14986800
O	-7.93596500	2.16507900	-3.98662200
C	-9.08592700	2.66520800	-3.28946900
H	-8.85801600	3.60874000	-2.76045100
H	-9.84206900	2.85429000	-4.06368000
H	-9.47545300	1.92280800	-2.56879300

O	-0.33300900	1.64508400	1.37744900
C	-0.73899600	-2.34516400	-1.30054000
O	0.01860800	-1.89290400	-0.40329800
N	-0.57580000	-3.55236600	-1.87749700
H	-1.60384100	-1.76651000	-1.67456300
C	-1.48894300	-4.02693800	-2.91670200
H	-2.26468000	-3.26970400	-3.10525900
H	-0.93955200	-4.21656900	-3.85535300
H	-1.97763000	-4.96451700	-2.59930300
C	0.52061600	-4.43931600	-1.48257500
H	1.09843800	-3.94947500	-0.68813400
H	0.11560400	-5.39677000	-1.11230900
H	1.17453600	-4.64205000	-2.34826800
O	-1.28366800	2.48275600	1.17009100
H	1.56422300	1.31507500	0.63448500

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-2665.833911

Co	-0.39689300	-0.05720200	0.57285100
N	1.54009400	-0.02845600	0.13191500
C	2.13003700	0.24096400	-1.09952000
C	2.60657900	-0.28867000	0.98591900
C	3.56845700	0.08936800	-1.02469500
C	3.86688500	-0.19728000	0.27974400
H	4.254444000	0.21265100	-1.86121200
H	4.84685200	-0.34885600	0.72954900
N	0.02297100	-0.84186400	2.33805300
C	-0.86144800	-1.37478000	3.26857100
C	1.26507400	-0.88851000	2.96187000
C	-0.17158200	-1.72560400	4.49283100
C	1.14740200	-1.41340100	4.30635000
H	-0.64850300	-2.14310000	5.37827900
H	1.97832800	-1.54648800	4.99762200
N	-2.32548400	-0.30428900	0.92881300
C	-3.38574700	0.13714000	0.14915600
C	-2.92007500	-1.01398700	1.96735600
C	-4.64735600	-0.34292500	0.67325000
C	-4.35590400	-1.08168700	1.78775200
H	-5.61957700	-0.16025200	0.21779600
H	-5.04258200	-1.62233900	2.43734000
N	-0.81739100	0.64181000	-1.22662400
C	-2.04864000	1.11027200	-1.67213600
C	0.07039400	0.95024700	-2.24951800
C	-1.91400800	1.77516700	-2.95157100
C	-0.60357800	1.65030600	-3.32377400
H	-2.72348300	2.26810000	-3.48745000
H	-0.11742600	2.02799400	-4.22204900
C	-2.24654700	-1.52980400	3.08665100
C	-3.03204000	-2.22512700	4.15275100
C	-2.78887100	-3.57826700	4.46565500
C	-4.03654300	-1.55539900	4.89355800

C	-3.50998300	-4.25100400	5.46782100
H	-2.01740000	-4.11772100	3.90648200
C	-4.76529200	-2.20872800	5.89183500
H	-4.23472400	-0.50033000	4.67987300
C	-4.50651600	-3.56325500	6.18498300
H	-3.29073500	-5.30269300	5.67135100
H	-5.53596800	-1.68614700	6.46735500
C	-3.27798600	0.89147500	-1.03146300
C	-4.53247200	1.42782300	-1.64242400
C	-4.98450600	1.01726000	-2.91982200
C	-5.32116800	2.36379600	-0.94186600
C	-6.16480000	1.52316300	-3.47340200
H	-4.39715100	0.28115200	-3.47816900
C	-6.51050800	2.88204800	-1.48277800
H	-4.98484900	2.69851900	0.04450200
C	-6.93546400	2.46125300	-2.75686700
H	-6.51598800	1.19945600	-4.45841400
H	-7.08541000	3.61302200	-0.90778900
C	1.45295000	0.69802200	-2.24224100
C	2.23197500	0.99464000	-3.48455200
C	3.22667900	1.99355200	-3.51615500
C	1.98108300	0.28688100	-4.68528100
C	3.95593700	2.27813200	-4.68412900
H	3.42667600	2.56784200	-2.60594400
C	2.69465100	0.55749800	-5.85667000
H	1.21093200	-0.49129000	-4.68714800
C	3.69024900	1.55555200	-5.86226200
H	4.71321800	3.06653700	-4.66319400
H	2.50229800	0.00385600	-6.78120200
C	2.49764500	-0.61444400	2.34790700
C	3.74286600	-0.74233600	3.17017600
C	4.02131500	0.18244900	4.20526800
C	4.66948900	-1.78281700	2.96010500
C	5.17401100	0.07405600	4.98926000
H	3.31518200	0.99933400	4.38587900
C	5.83711700	-1.90452100	3.73497900
H	4.46947700	-2.51858200	2.17414100
C	6.09154700	-0.97058300	4.75636100
H	5.38963500	0.79318700	5.78584200
H	6.52708900	-2.72981200	3.53890400
O	7.20049400	-0.98915600	5.58123300
C	8.14566400	-2.03095900	5.36646100
H	8.58023900	-1.99282100	4.34768400
H	8.94582800	-1.87332600	6.10590200
H	7.70030600	-3.03376100	5.52250300
O	4.34070300	1.74646300	-7.06648900
C	5.34833500	2.75118900	-7.10212100
H	6.17366400	2.53556000	-6.39474000
H	5.74394600	2.74901500	-8.12941900
H	4.94030100	3.75553900	-6.87263800
O	-5.27925200	-4.11761500	7.18767000

C	-5.03361100	-5.48174200	7.51059800
H	-3.99571300	-5.64355900	7.86366700
H	-5.73387400	-5.73330600	8.32189500
H	-5.22156100	-6.15221100	6.64845400
O	-8.08339700	2.90076300	-3.38889600
C	-8.88073300	3.84941800	-2.68851100
H	-8.32630300	4.78699600	-2.48524700
H	-9.73622800	4.07141700	-3.34488200
H	-9.25595000	3.44604800	-1.72700000
O	-0.30453400	1.99365100	1.44346400
O	-1.28057400	2.82681200	1.25338600

1b

-2914.577878

Co	-0.32401900	-0.15029400	0.45855600
N	1.56929300	-0.10313800	-0.01995300
C	2.14142600	0.65181600	-1.02172600
C	2.60944600	-0.78732900	0.58843100
C	3.56385700	0.40131400	-1.08426900
C	3.85196700	-0.50799200	-0.09821100
H	4.24459500	0.85167000	-1.80399600
H	4.82237400	-0.91473800	0.17887600
N	0.14936700	-0.87817800	2.25140600
C	-0.66590300	-0.91820700	3.37001700
C	1.37898400	-1.35193300	2.65986300
C	0.09280200	-1.36075900	4.52039700
C	1.33904100	-1.70078600	4.06383200
H	-0.28579000	-1.43064700	5.53734300
H	2.16322400	-2.12503200	4.63234900
N	-2.25100100	-0.26327300	0.91494400
C	-3.30138400	-0.33109400	0.01156600
C	-2.79033500	-0.55137900	2.14945000
C	-4.50927000	-0.74337800	0.68927800
C	-4.20283500	-0.83465400	2.02448900
H	-5.46606100	-0.93863400	0.21009800
H	-4.85567400	-1.12579300	2.84493100
N	-0.77535600	0.55638000	-1.32161300
C	-2.03320900	0.62596700	-1.88588200
C	0.03720700	1.36949800	-2.09749300
C	-2.01636900	1.50505800	-3.03353300
C	-0.74215100	2.00365700	-3.13469200
H	-2.88526100	1.75875800	-3.63746100
H	-0.36870900	2.73902500	-3.84367000
C	-2.06571200	-0.72775700	3.36039300
C	-2.84870500	-0.81842800	4.61698500
C	-2.77430800	-1.93566800	5.48216700
C	-3.74133400	0.23051800	4.96802100
C	-3.53592600	-2.00786300	6.65519000
H	-2.14132400	-2.78510000	5.20831300
C	-4.48867000	0.18218100	6.14151100
H	-3.81796400	1.10713900	4.31727200

C	-4.39255400	-0.93890600	7.00021600
H	-3.46925600	-2.89923300	7.28318600
H	-5.15402800	1.00203600	6.42618300
C	-3.22409500	0.07837200	-1.34095400
C	-4.43024400	0.05615100	-2.20143400
C	-4.37051800	-0.53590400	-3.49237300
C	-5.65665500	0.64036700	-1.80376800
C	-5.48581100	-0.57392700	-4.32447200
H	-3.43348500	-0.99261800	-3.82615100
C	-6.78133900	0.62755900	-2.63768800
H	-5.71721800	1.15556400	-0.84050000
C	-6.70622400	0.00785700	-3.90487700
H	-5.44684200	-1.05036200	-5.30811100
H	-7.70083800	1.11396500	-2.30415000
C	1.43853700	1.47082600	-1.94544100
C	2.22671500	2.37778700	-2.81075000
C	3.12093100	3.30419100	-2.22059300
C	2.13320100	2.35781900	-4.22822200
C	3.86809300	4.19843300	-2.99569400
H	3.19870400	3.34644700	-1.12973600
C	2.88828200	3.22586300	-5.01234500
H	1.48759400	1.62095200	-4.71549000
C	3.75609500	4.16456300	-4.40353000
H	4.52298100	4.91895700	-2.50056000
H	2.83692900	3.19622800	-6.10437100
C	2.53676400	-1.43285100	1.84387400
C	3.75897500	-2.10925100	2.35224900
C	4.41121200	-1.69715100	3.54397100
C	4.32806100	-3.17912200	1.62464800
C	5.56565800	-2.33632300	3.99054900
H	4.02574100	-0.83655500	4.09897100
C	5.47836700	-3.84348500	2.07112700
H	3.84407300	-3.51251100	0.70081800
C	6.10601800	-3.42407700	3.26427200
H	6.08270100	-2.00594500	4.89585900
H	5.87398200	-4.68132300	1.49237300
O	7.22770800	-3.98448100	3.79478900
C	7.82719100	-5.08448100	3.09592400
H	8.15555000	-4.78765900	2.08287700
H	8.70252100	-5.37299500	3.69368900
H	7.13316200	-5.94199800	3.02299400
O	4.43483900	4.97512500	-5.25894700
C	5.33068300	5.94868700	-4.70065000
H	6.14229500	5.46567700	-4.12662500
H	5.75784600	6.48328100	-5.55989400
H	4.79291700	6.66383800	-4.05200400
O	-5.16793400	-0.89110200	8.11684900
C	-5.10517500	-1.99562700	9.03141200
H	-4.08361000	-2.12842800	9.43181000
H	-5.78950900	-1.73910700	9.85147300
H	-5.44038600	-2.93407900	8.55294700

O	-7.73241800	-0.07600000	-4.79356400
C	-8.99501100	0.49955400	-4.42458800
H	-8.90760700	1.58906900	-4.26045500
H	-9.66501200	0.31057300	-5.27426900
H	-9.40579300	0.01991500	-3.51753400
O	-0.14081500	1.55862000	1.19838700
H	-1.87833800	2.30094700	1.36349400
C	-0.02674500	-2.50758700	-1.29739100
O	-0.50002000	-2.13662900	-0.19459600
N	-0.13655900	-3.76619400	-1.77322200
H	0.51954100	-1.80879100	-1.95861900
C	0.43524300	-4.14313000	-3.06444900
H	0.92959800	-3.27251700	-3.52158000
H	1.18029900	-4.94803500	-2.93687100
H	-0.35485600	-4.50281900	-3.74683100
C	-0.83771900	-4.80284800	-1.01258000
H	-1.20685600	-4.36073900	-0.07796500
H	-1.68635800	-5.19453300	-1.59957900
H	-0.15048600	-5.63590600	-0.78448200
O	-1.13077600	2.48956700	0.75216100

1c

-2914.74559

Co	-0.34124000	-0.13804400	0.50459200
N	1.57685500	-0.06869600	0.03109800
C	2.14837100	0.63973400	-1.01229000
C	2.62648900	-0.68319500	0.69407600
C	3.58245000	0.43945300	-1.02354200
C	3.87645900	-0.39687000	0.02078000
H	4.26280400	0.87491600	-1.75332900
H	4.85027200	-0.76443400	0.33959000
N	0.12038500	-0.91745200	2.27819700
C	-0.71615000	-1.04000500	3.37378000
C	1.36125300	-1.36375000	2.69628000
C	0.02663100	-1.53663200	4.51565500
C	1.29882300	-1.78999800	4.08047100
H	-0.38846300	-1.69458400	5.50913500
H	2.13449100	-2.19927700	4.64507200
N	-2.27305100	-0.27284000	0.94803500
C	-3.33383500	-0.22896100	0.05401100
C	-2.82333400	-0.58872300	2.17761200
C	-4.56594000	-0.57584400	0.73130200
C	-4.25601100	-0.75901300	2.05342400
H	-5.53946800	-0.65843900	0.25165200
H	-4.92050900	-1.03248600	2.87125400
N	-0.78868900	0.57581400	-1.29001000
C	-2.04995300	0.67106900	-1.85034000
C	0.05243000	1.29898600	-2.12195400
C	-1.99941500	1.46525000	-3.06028600
C	-0.70428800	1.88618700	-3.20678400
H	-2.86156800	1.70816100	-3.67895600

H	-0.29027400	2.53457000	-3.97673200
C	-2.11081400	-0.85087200	3.36588200
C	-2.89441100	-1.03234500	4.62626800
C	-2.93567800	-2.26438900	5.31092500
C	-3.64958600	0.04084700	5.15952100
C	-3.68395900	-2.43066900	6.48827000
H	-2.38209100	-3.11781900	4.90602300
C	-4.39758100	-0.10663100	6.32943100
H	-3.63420600	1.00825200	4.64712900
C	-4.41848400	-1.34541300	7.00540900
H	-3.69443400	-3.40517500	6.98292700
H	-4.97121800	0.72664100	6.74611300
C	-3.25238800	0.19635600	-1.28633400
C	-4.48942900	0.24783000	-2.12240700
C	-4.56529700	-0.47731200	-3.33719800
C	-5.60754600	1.02656000	-1.75747700
C	-5.70758500	-0.43881100	-4.13925000
H	-3.70914800	-1.08609900	-3.64594000
C	-6.76405500	1.07824500	-2.55281600
H	-5.56556600	1.62098200	-0.83921800
C	-6.81950700	0.33911400	-3.75093200
H	-5.76740800	-1.00688200	-5.07248000
H	-7.60306700	1.70320600	-2.23686100
C	1.45227800	1.37263200	-1.99473600
C	2.24398400	2.19329400	-2.95981800
C	3.03631400	3.26412500	-2.49575400
C	2.24504100	1.92939400	-4.35123200
C	3.79636100	4.05416000	-3.37331600
H	3.04503900	3.49071700	-1.42475700
C	2.99685800	2.70428500	-5.23742300
H	1.65287700	1.09329100	-4.73757900
C	3.77780800	3.77620000	-4.75434600
H	4.38716000	4.88146500	-2.97232300
H	3.00313200	2.49536800	-6.31145500
C	2.54391600	-1.34618000	1.93338500
C	3.79308500	-1.94794400	2.49845700
C	4.43605200	-1.39543400	3.63274300
C	4.38194400	-3.07784400	1.89731400
C	5.60672000	-1.95679800	4.14804500
H	4.01135500	-0.50343800	4.10441700
C	5.56010800	-3.65472800	2.40157800
H	3.90458500	-3.52101700	1.01679700
C	6.17718000	-3.09388900	3.53670700
H	6.10687000	-1.52588000	5.02056200
H	5.98007400	-4.53521900	1.90873400
O	7.32665900	-3.56882300	4.12007700
C	7.93799300	-4.71377900	3.52596600
H	8.24624300	-4.51831500	2.48068100
H	8.83015500	-4.92738100	4.13250200
H	7.26599800	-5.59353900	3.54405400
O	4.47782300	4.47697600	-5.70545600

C	5.27777000	5.57162200	-5.25595600
H	6.06814500	5.24096100	-4.55495600
H	5.74598200	5.99188600	-6.15794600
H	4.66525400	6.35220000	-4.76538400
O	-5.18226200	-1.38772100	8.14594300
C	-5.22191600	-2.62176300	8.86303000
H	-4.21623900	-2.92508600	9.21248400
H	-5.86948900	-2.44294000	9.73371900
H	-5.65159100	-3.43829900	8.25115000
O	-7.89333600	0.30993800	-4.60601000
C	-9.03731500	1.08699000	-4.24869200
H	-8.79717900	2.16585800	-4.18824000
H	-9.77326700	0.92410900	-5.04943500
H	-9.46957400	0.75967200	-3.28360500
O	-0.18333300	1.55802600	1.28113400
H	-1.96246700	2.19723100	1.39732400
C	0.05472300	-2.42421100	-1.32268900
O	-0.48076400	-2.13456400	-0.23095000
N	-0.00287200	-3.65874100	-1.88342300
H	0.62046400	-1.67700400	-1.91112900
C	0.64410000	-3.94193600	-3.15869600
H	1.14249500	-3.03327800	-3.52983600
H	1.40180100	-4.73865200	-3.04484000
H	-0.09731100	-4.27106600	-3.90958400
C	-0.71986000	-4.74729000	-1.22272000
H	-1.14635700	-4.35955500	-0.28767300
H	-1.53017200	-5.12292700	-1.87272200
H	-0.03067300	-5.58119100	-0.99893500
O	-1.19620600	2.48000900	0.84841200

1c

-2666.428214			
Co	-0.22667500	0.09858400	0.46329700
N	1.64514500	0.14776900	-0.13528100
C	2.13640200	0.83227500	-1.23324700
C	2.74088300	-0.52113700	0.40284500
C	3.54356400	0.54901800	-1.42103600
C	3.90986700	-0.32067700	-0.42565100
H	4.15181000	0.93462000	-2.23813200
H	4.88344100	-0.77884300	-0.25767800
N	0.32991600	-0.84385000	2.11585600
C	-0.43872000	-1.01585800	3.25722700
C	1.61015200	-1.24791000	2.46934800
C	0.38707000	-1.46615600	4.35938500
C	1.65067200	-1.64588100	3.86024400
H	0.03839300	-1.62897500	5.37789700
H	2.54516000	-1.96998200	4.39026700
N	-2.14326600	-0.21022400	0.94086400
C	-3.24905800	-0.21299300	0.08844500
C	-2.62256600	-0.64805400	2.16801800
C	-4.41321100	-0.71522800	0.78054600

C	-4.03488900	-0.94767600	2.08012600
H	-5.39414200	-0.86292200	0.33081300
H	-4.63877800	-1.33927100	2.89771300
N	-0.80989500	0.81875300	-1.28246500
C	-2.09851000	0.88935300	-1.79412900
C	-0.02868600	1.57075800	-2.14820800
C	-2.12951100	1.73046300	-2.97203800
C	-0.85261500	2.18592800	-3.16902800
H	-3.02675900	1.97463300	-3.53917400
H	-0.49289300	2.86779000	-3.93768100
C	-1.84137600	-0.89453900	3.31697800
C	-2.55905300	-1.15136800	4.60084600
C	-2.46188800	-2.38361400	5.29407400
C	-3.39659900	-0.16100600	5.15689100
C	-3.15429800	-2.60791600	6.48767300
H	-1.83845500	-3.17932200	4.87406800
C	-4.10169200	-0.36971100	6.35450500
H	-3.48678300	0.80020700	4.64085800
C	-3.97836500	-1.59952800	7.02772100
H	-3.08188400	-3.56398700	7.01603200
H	-4.73029700	0.43188000	6.75173300
C	-3.24866600	0.31544600	-1.21670000
C	-4.52072900	0.34226200	-1.99828400
C	-4.60268600	-0.28189700	-3.26800600
C	-5.67716500	0.99564800	-1.52273900
C	-5.78157500	-0.26258900	-4.01850000
H	-3.71822100	-0.79390600	-3.66046700
C	-6.87194800	1.02360800	-2.26287600
H	-5.63509600	1.50677700	-0.55583100
C	-6.92703800	0.38953300	-3.51818100
H	-5.84239000	-0.75321900	-4.99514400
H	-7.73992700	1.55060700	-1.85743500
C	1.37607000	1.62193800	-2.12141900
C	2.11265600	2.44489400	-3.12670800
C	2.99631500	3.46749100	-2.69988800
C	1.98721700	2.23380000	-4.51549100
C	3.70796200	4.24663200	-3.61593400
H	3.10736500	3.65032500	-1.62646000
C	2.69387400	3.00982800	-5.45142900
H	1.32901900	1.43510400	-4.87232600
C	3.55880400	4.02393300	-5.00024600
H	4.38135700	5.04258500	-3.28255900
H	2.56974300	2.80613800	-6.51857200
C	2.74486600	-1.19386600	1.63852300
C	4.01217200	-1.81086900	2.13430000
C	5.18504100	-1.04538800	2.34799500
C	4.07428000	-3.18888900	2.42809900
C	6.36242200	-1.63140900	2.82165700
H	5.15732000	0.03030600	2.14834000
C	5.24922100	-3.79490800	2.90637300
H	3.17961400	-3.80075100	2.27341700

C	6.40246300	-3.01258600	3.10232700
H	7.26412100	-1.03536800	2.99443500
H	5.25229400	-4.86847600	3.11358400
O	-0.13650600	1.92849700	1.39725400
H	-2.02573400	2.00316500	1.23907900
O	-1.34656300	2.71086200	1.14312900
O	7.61165600	-3.49507500	3.56494400
O	-4.61907700	-1.91837400	8.21010800
O	-8.04262700	0.35080600	-4.33242000
O	4.30292600	4.84763900	-5.82377200
C	7.67751800	-4.88403100	3.86884000
H	6.96163600	-5.16799400	4.66560500
H	7.48161300	-5.51298700	2.97770500
H	8.70329500	-5.06980100	4.22246700
C	4.16473300	4.65109300	-7.22621300
H	4.48581100	3.63672100	-7.53670300
H	3.12200700	4.81026000	-7.56613500
H	4.81789000	5.39733800	-7.70417300
C	-9.21387900	1.00177100	-3.85210700
H	-9.57125400	0.56169000	-2.89996100
H	-9.05181900	2.08739800	-3.70038000
H	-9.98195900	0.85696800	-4.62727200
C	-5.45846900	-0.91840300	8.77724600
H	-4.89415100	0.00048900	9.03209800
H	-6.29191000	-0.64410900	8.10030800
H	-5.87172800	-1.35517800	9.69940400

1c-H⁺

-2915.182089

Co	-0.23997500	-0.08262900	0.40022800
N	1.68808300	0.13458100	-0.06465600
C	2.19216400	0.31994100	-1.35100800
C	2.75872300	-0.30752600	0.70361000
C	3.57617600	-0.08243200	-1.39851600
C	3.93253100	-0.44880900	-0.12328500
H	4.19587200	-0.07507600	-2.29337800
H	4.89926800	-0.80216000	0.23142000
N	0.24703000	-0.85734700	2.16150800
C	-0.63036300	-1.26712900	3.15630500
C	1.49850100	-0.77699300	2.76824800
C	0.06711200	-1.37871600	4.41470200
C	1.37891400	-1.05406300	4.17939900
H	-0.40450200	-1.63616900	5.36104500
H	2.19688000	-0.99944800	4.89487200
N	-2.19914500	-0.17610400	0.92446600
C	-3.26350300	0.10153200	0.05718300
C	-2.70864200	-1.09881700	1.85374400
C	-4.42329600	-0.65279000	0.44271400
C	-4.07460100	-1.40998400	1.53822700
H	-5.37843000	-0.62546500	-0.07908200
H	-4.69282000	-2.11905700	2.08617400

N	-0.73402600	0.86435800	-1.27821800
C	-1.98321200	1.39162100	-1.60359900
C	0.13469500	1.30745300	-2.26987500
C	-1.85820900	2.28035600	-2.73427400
C	-0.55563300	2.20959600	-3.16019500
H	-2.66935700	2.87681200	-3.14708600
H	-0.08663700	2.74136700	-3.98580300
C	-2.00756400	-1.54552700	2.98946300
C	-2.72635600	-2.28742400	4.05614700
C	-2.22201300	-3.50847200	4.55936900
C	-3.93479900	-1.79360800	4.61532100
C	-2.88765600	-4.22337800	5.56430800
H	-1.29743000	-3.91767700	4.13909000
C	-4.60245400	-2.48730400	5.62217700
H	-4.33177300	-0.83339300	4.27147400
C	-4.08797400	-3.71347100	6.10472000
H	-2.47294800	-5.17189100	5.91342200
H	-5.52181800	-2.09661600	6.06743800
C	-3.21254400	0.99225900	-1.03488700
C	-4.49254400	1.44325100	-1.64122500
C	-4.76376700	1.28248500	-3.02526600
C	-5.49392000	2.03698600	-0.83933400
C	-5.97250300	1.70125800	-3.57789500
H	-4.02070900	0.79573500	-3.66478600
C	-6.70902600	2.47498700	-1.38306100
H	-5.30566100	2.18345400	0.22926500
C	-6.95632900	2.30857800	-2.76279900
H	-6.18984900	1.56247600	-4.64078200
H	-7.44747800	2.94925500	-0.73258400
C	1.49325100	0.94524000	-2.40392300
C	2.20136200	1.28315900	-3.66645000
C	3.41098900	2.02639000	-3.66452700
C	1.67814500	0.88319500	-4.91707300
C	4.06351300	2.34803200	-4.85309500
H	3.82237000	2.37990300	-2.71384600
C	2.32882300	1.18964000	-6.12026100
H	0.75122000	0.30102900	-4.94607100
C	3.53145900	1.92811600	-6.09460500
H	4.98468400	2.93763500	-4.85353700
H	1.89984900	0.84698000	-7.06476900
C	2.72019400	-0.59063600	2.08829300
C	4.00630100	-0.74261800	2.81741400
C	4.99108900	0.26969000	2.74982600
C	4.29749100	-1.89462700	3.59390100
C	6.20875100	0.15938000	3.43446400
H	4.78542700	1.17575300	2.17085600
C	5.50908100	-2.02452000	4.27008700
H	3.56541300	-2.70698200	3.64546000
C	6.47650300	-0.99470500	4.20199000
H	6.93322800	0.97477100	3.37402700
H	5.74041700	-2.91858100	4.85608300

O	-0.06494000	1.74519100	1.27944700
H	-1.86016800	1.37184200	1.75085700
C	0.46735400	-2.69169500	-0.28882800
O	-0.39910900	-1.78022700	-0.47052000
N	0.37862900	-3.88939700	-0.88083100
H	1.33904700	-2.53651700	0.36693000
C	1.40224400	-4.91506200	-0.66567900
H	2.17648700	-4.53443300	0.01640500
H	0.94726000	-5.81877800	-0.22565500
H	1.87391700	-5.18642200	-1.62546000
C	-0.73488400	-4.22221400	-1.77688000
H	-1.42044600	-3.36708900	-1.82835600
H	-0.34721800	-4.45043800	-2.78407400
H	-1.27009300	-5.10619600	-1.39146100
O	-1.29720300	2.18450000	1.97000900
H	-0.06526600	2.34371200	0.49293400
O	7.62204800	-1.21661300	4.90495400
O	4.24989600	2.28905400	-7.19478100
O	-8.09724800	2.68899400	-3.40290700
O	-4.81977900	-4.31351000	7.08467400
C	8.63710500	-0.20342400	4.87226900
H	9.00684500	-0.03524900	3.84396100
H	8.26867600	0.75049900	5.29234100
H	9.45636500	-0.58497300	5.49691900
C	-4.33419900	-5.54987500	7.62485400
H	-4.28119900	-6.33656900	6.84957400
H	-3.33951200	-5.42400100	8.09090800
H	-5.06253100	-5.84387900	8.39302200
C	-9.13051500	3.30711300	-2.62340100
H	-9.50295200	2.62747500	-1.83483400
H	-8.78005900	4.24910100	-2.16279300
H	-9.94298400	3.52659600	-3.32960900
C	3.74614400	1.90555900	-8.48133900
H	3.68808800	0.80583800	-8.58139900
H	2.75021600	2.34592500	-8.67286600
H	4.46616500	2.30035400	-9.21121900

1d

-2666.907392			
Co	-0.25069000	0.04830700	0.44650200
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O	-4.89679900	-3.73753000	7.38585900
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C	-4.47415600	-2.77528000	5.57049200
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H	-6.88302400	3.92649000	-0.35244800
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C	3.26371100	1.84961700	-3.89023900
C	1.76975300	0.27809700	-4.96036000
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C	2.41466800	0.48527800	-6.18128600

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C	4.67870100	0.77812700	3.00860000
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C	5.59361600	-1.52341700	4.32898800
H	3.83663100	-2.48941900	3.52609100
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H	6.45320000	1.74553900	3.81271300
H	5.93861800	-2.43372700	4.82579500
O	-0.29313100	1.57798000	1.19887800
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H	-1.27064600	-3.65301100	-1.89963400
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O	4.06732200	1.51609000	-7.50910100
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H	-6.60214000	-4.10817100	6.85420200
H	-6.07829600	-5.25116700	8.14131300

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