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Supporting Information

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Supplementary Materials for

Photocatalytic Hydrogen Evolution by a Synthetic [FeFe]hydrogenase Mimic Encapsulated in a Porphyrin Cage

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1. Materials and methods

All reactions were carried out under an atmosphere of N_2 using standard Schlenk techniques unless otherwise noted. All solvents were distilled prior to use by conventional methods. Complex **1** and cage **$Fe_4(Zn\text{-}L)_6$** (see Chapter 4) were prepared according to literature procedures.[1,2] The supporting electrolyte *n*Bu_4NPF_6 was prepared from saturated solution of KPF_6 and *n*Bu_4NBr in water and recrystallized from hot methanol and dried under vacuum at 80 °C overnight. The acid $HNEt_3PF_6$ was prepared following a literature procedure.[3] All other reagents were purchased from commercial suppliers and used without further purification.

NMR spectroscopy

^1H NMR spectra were recorded on a Bruker AV300 and AV400 spectrometer and they are referenced to the solvent residual signal (5.32 ppm for CD_2Cl_2 and 1.32 ppm for CD_3CN). 2D ^1H-DOSY spectral data were acquired with temperature and magnetic gradient calibration prior to the measurements, and the temperature was kept at 298 K during the measurements.

Mass spectrometry

High resolution mass spectra were collected on a HR-ToF Bruker Daltonik GmbH (Bremen, Germany) Impact II, an ESI-ToF MS capable of resolution of at least 40000 FWHM, which was coupled to a Bruker cryospray unit. Detection was in positive-ion mode and the source voltage was between 4 and 6 kV. The flow rates were 18 uL/hr. The drying gas (N_2) was held at -35 °C and the spray gas was held at – 40 °C. The machine was calibrated prior to every experiment via direct infusion of a TFA-Na solution, which provided a m/z range of singly charged peaks up to 3500 Da in both ion modes.

Steady state UV-vis and IR spectroscopy

Steady state UV-Vis spectra were acquired on a single beam Hewlett Packard 8453 spectrometer in a quartz cuvette with a path length of 10 mm using the solvent as a background. For the determination of the binding constant, a solution of **$Fe_4(Zn\text{-}L)_6$** kept at a constant concentration of 7.7 µM was titrated with an increasing concentration of **1**. The obtained titration curves were then fitted to a 1:2 host-guest model using a Matlab script.[4] Steady state IR measurements were conducted on a Thermo Nicolet Nexus FT-IR spectrometer in a CaF_2 IR cell.

Steady state fluorescence spectroscopy

Steady state fluorescence spectra were recorded on a Spex Fluorolog 3 spectrofluorimeter, equipped with double grating monochromators in the excitation and emission channels. The excitation light source was a 450 W Xe lamp and the detector a Peltier cooled R636-10 photomultiplier tube. In a fluorescence quenching titration, a solution of **$Fe_4(Zn\text{-}L)_6$** kept at a constant concentration of 0.8 µM was titrated with an increasing concentration of **1**. Inner and outer filter corrections were applied for each titration point on the excitation wavelength (550 nm) and the emission wavelength (640 nm) with b = 0.5 cm:

$$I_{corrected} = I_{measured} \cdot 10^{b\cdot((\epsilon_{1@550nm}+\epsilon_{1@640nm})[1]+(\epsilon_{Fe4(Zn-L)6@550nm}+\epsilon_{Fe4(Zn-L)6@640nm})[Fe4(Zn-L)6]}$$

The obtained titration curves were then fitted to a 1:2 host-guest model using a Matlab script.[4]

Time-resolved fluorescence spectroscopy

Time-resolved fluorescence was measured with a time-correlated single-photon counting (TCSPS) setup. A cavity dumped DCM dye laser (Coherent model 700) is pumped by a mode-locked Ar^+ laser (Coherent 486 AS Mode Locker, Coherent Innova 200 laser). A microchannel plate (Hamamatsu R3809) was used as the detector. The overall response function (IRF) was measured from the Rayleigh scattering of colloidal silicon dioxide. The fluorescence decay times were obtained by fitting the fluorescence decays with mono- or biexponentials by numerical iterative reconvolution with the software Igor Pro 5.

Time-resolved IR spectroscopy

Time-resolved IR spectroscopy was measured as previously described.[1] Two commercial beta barium borate (BBO)-based optical parametric amplifiers (OPAs; Spectra-Physics OPA-800C) were pumped by a Ti:sapphire laser (Spectra-Physics Hurricane, 600 µJ) at a repetition rate of 1 kHz. IR probe pulses were generated by difference-frequency mixing signal and idler from one of the OPAs in a $AgGaS_2$ crystal. The visible pump pulses (585 nm; pulse energy, 2.2 µJ) were generated by doubling the signal of the other OPA. The delay positions were scanned by mechanically adjusting the beam path of the UV pump using a Newport ESP300 translation stage. The sample cell with CaF_2 windows spaced 500 µm apart was placed in the IR focus. From the full width at half-maximum of the pump probe cross-correlation function, a temporal resolution of 200 fs was obtained. A custom-built 30-pixel mercury cadmium telluride (MCT) detector coupled to an Oriel MS260i spectrograph was used to record the transient spectra by subtracting nonpumped absorption spectra from the pumped absorption spectra. The sample was pumped at 3 µL/min through the cell during the measurements to ensure fresh solution at all times.

Time-resolved UV-vis spectroscopy

Femtosecond visible transient absorption experiments were performed with a commercially available Ti:sapphire lasers (Spectra-Physics Hurricane, 600 J, 100 fs FWHM). 2.5% of the 800 nm fundamental light was used to generate a white-light continuum from 350 to 850 nm by focusing on a CaF_2 plate. The fundamental light used for the white-light generation was passed twice over a delay stage, providing up to 3.6 ns time delay. The sample cell was a 1 mm quartz cuvette. A commercially available beta barium borate (BBO)-based optical parametric amplifier (OPAs; Spectra-Physics OPA-800C) was pumped with the fundamental 800 nm light to generate a signal which was doubled to create 585 nm pump light (2.2 µJ). The pump light ran at 500 Hz, using a mechanical chopper to produce a non-pumped signal acting as a reference measurement. The spectra were measured using a spectrograph (Shamrock 193i with a 150 lines/mm grating) and a 6 single diode-array (Hamamatsu NMOS S3901-512Q) detector. The readout was done using fast electronics (TEC5).

Electrochemistry

Cyclic voltammetry was acquired of deaerated solutions in freshly distilled acetonitrile. The voltammograms were recorded in a gas-tight single compartment 3-electrode cell with a glassy carbon working electrode, a platinum wire as auxiliary electrode and a leakless Ag/AgCl (3 M KCl) reference electrode (Metrohm 6.0750.100). A 663-VA stand was used along with a PGSTAT302N potentiostat (Metrohm/Autolab). All redox potentials are reported against the ferrocene/ferrocenium (Fc/Fc^+) redox couple used as internal standard. In electrocatalytic studies different amounts of the acid $HNEt_3PF_6$ were added with a microsyringe into the solution in the CV cell.

Hydrogen evolution

In photocatalytic experiments **1** (0.08 mM), **Fe_4(Zn-L)$_6$** (0.08 mM), the proton source and the sacrificial electron donor were transferred into a 5 mL Schlenk flask and dissolved in 5 mL degassed (freeze-pump-thaw) and dry acetonitrile. The solution was continuously stirred at 1000 rpm and subjected to irradiation by LED lights (17.5 V) at 590 nm for 2 h at 298 K. Gas chromatographic analysis of the headspace was performed by direct injection into an Interscience CompactGC, separating H_2, CO, CH_4, O_2 and N_2 on a 5 Å molsieve column, by using argon carrier gas and a TCD detector. As direct injection was used, quantification of the formed hydrogen was not possible.

2. CSI-MS analysis of 1•Fe_4(Zn-L)$_6$

Table S 1. Different charged species observed in the CSI mass spectrum of **1·Fe_4(Zn-L)$_6$** and the corresponding found and calculated [m/z].

Species	Charge	Found [m/z]	Calculated [m/z]
Fe_4(Zn-L)$_6$(**1**)$_1$(OTf)$_0$	8+	799.7373	799.7334
Fe_4(Zn-L)$_6$(**1**)$_1$(OTf)$_1$	7+	935.2636	935.2599
Fe_4(Zn-L)$_6$(**1**)$_1$(OTf)$_2$	6+	1116.1331	1116.1286
Fe_4(Zn-L)$_6$(**1**)$_1$(OTf)$_3$	5+	1369.1499	1369.1448
Fe_4(Zn-L)$_6$(**1**)$_1$(OTf)$_4$	4+	1748.6746	1748.6691

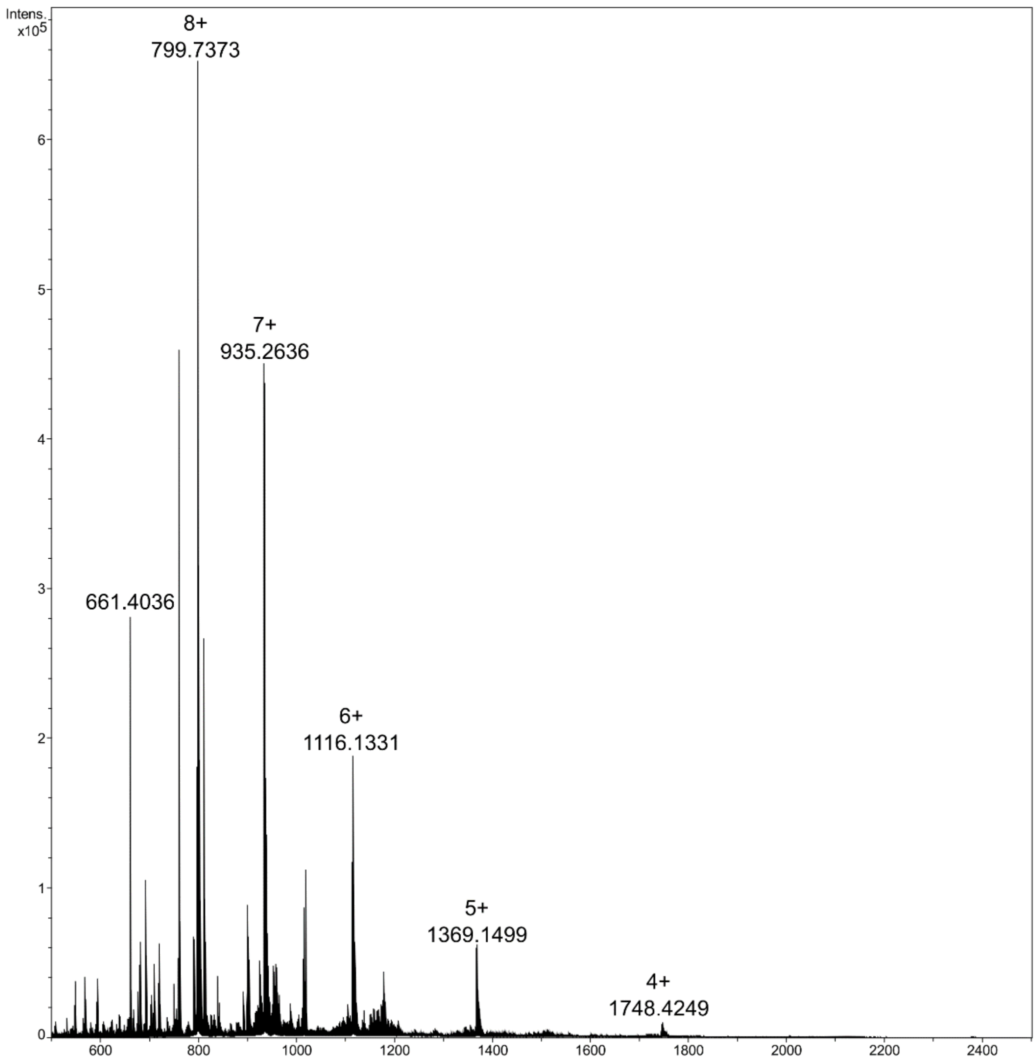


Figure S 1. CSI mass spectrum (full spectrum) of **1·Fe_4(Zn-L)$_6$** with a spray temperature of -40 °C and a dry gas temperature of -35 °C. The peak with m/z ratio of 661 belongs to demetallated cage building block.

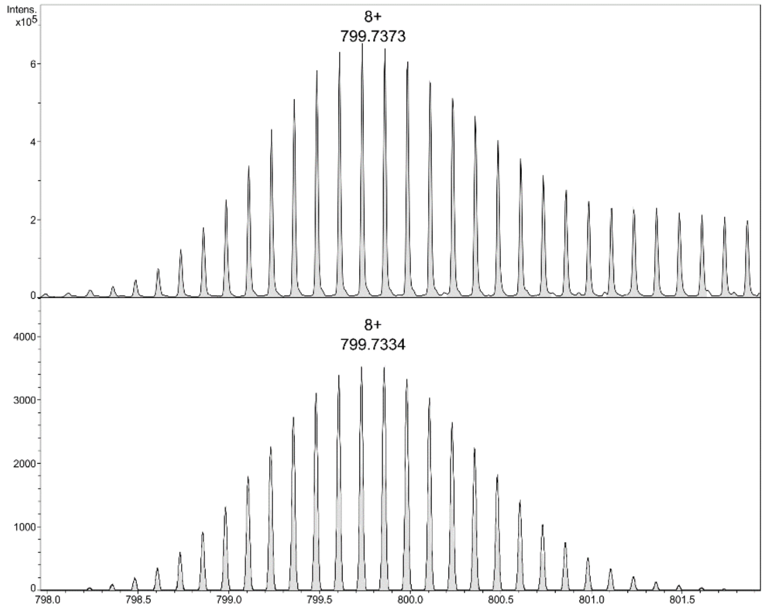


Figure S 2. Expanded spectrum for the charged species [**Fe_4(Zn-L)$_6$**(**1**)$_1$(OTf)$_0$]$^{8+}$ observed (above) in the CSI mass spectrum of the host-guest complex **1**·**Fe_4(Zn-L)$_6$** and simulated isotope distribution (below).

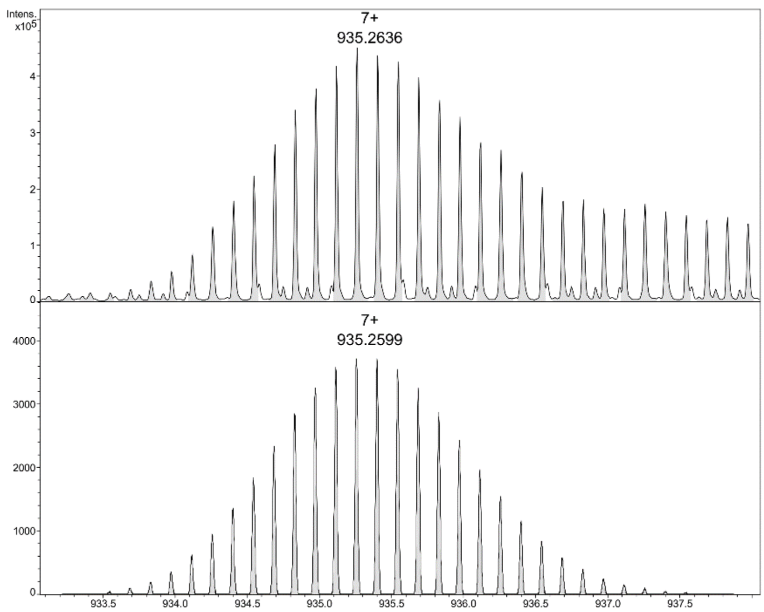


Figure S 3. Expanded spectrum for the charged species [**Fe_4(Zn-L)$_6$**(**1**)$_1$(OTf)$_1$]$^{7+}$ observed (above) in the CSI mass spectrum of the host-guest complex **1**·**Fe_4(Zn-L)$_6$** and simulated isotope distribution (below).

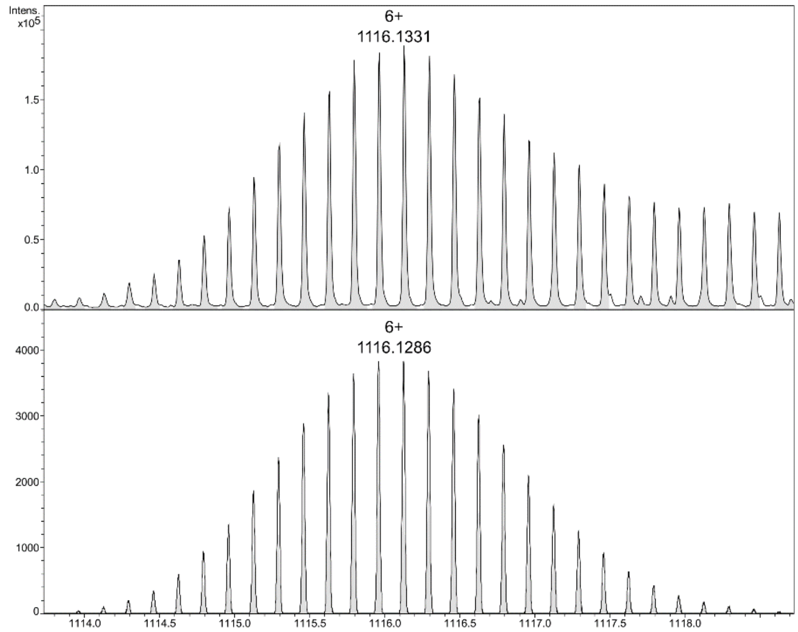


Figure S 4. Expanded spectrum for the charged species [$\mathbf{Fe_4(Zn\text{-}L)_6}$($\mathbf{1}$)$_1(OTf)_2$]$^{6+}$ observed (above) in the CSI mass spectrum of the host-guest complex $\mathbf{1}$·$\mathbf{Fe_4(Zn\text{-}L)_6}$ and simulated isotope distribution (below).

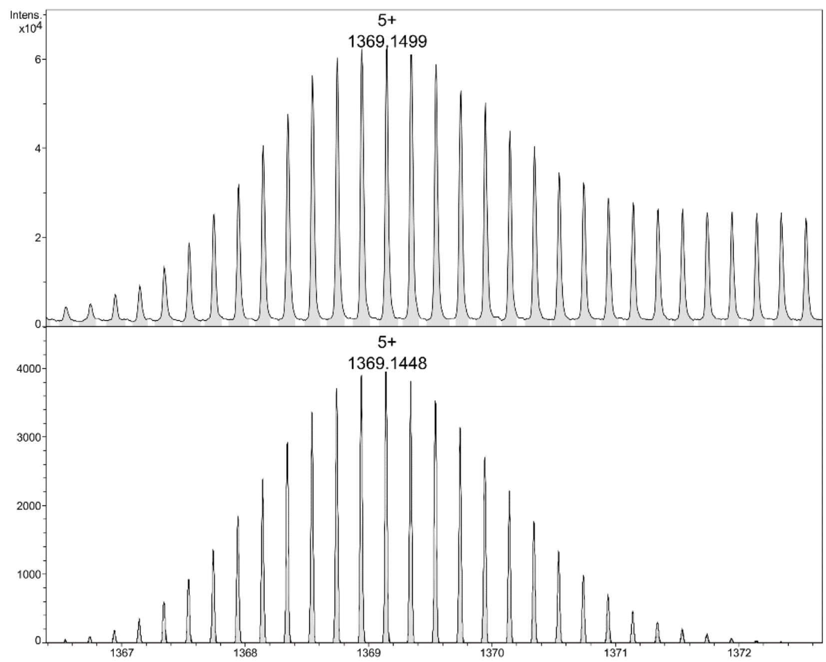


Figure S 5. Expanded spectrum for the charged species [$\mathbf{Fe_4(Zn\text{-}L)_6}$($\mathbf{1}$)$_1(OTf)_3$]$^{5+}$ observed (above) in the CSI mass spectrum of the host-guest complex $\mathbf{1}$·$\mathbf{Fe_4(Zn\text{-}L)_6}$ and simulated isotope distribution (below).

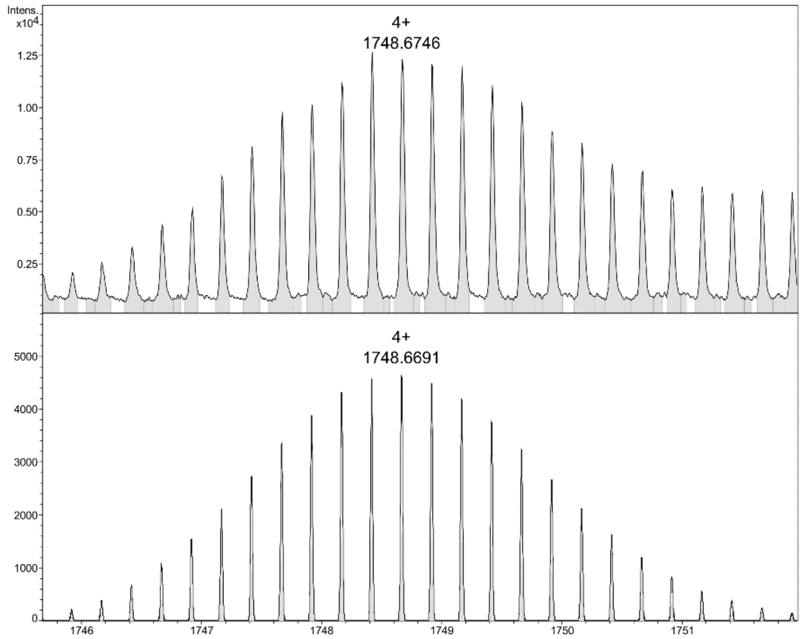


Figure S 6. Expanded spectrum for the charged species [$\mathbf{Fe_4(Zn\text{-}L)_6}$($\mathbf{1}$)$_1(OTf)_4$]$^{4+}$ observed (above) in the CSI mass spectrum of the host-guest complex **1**·$\mathbf{Fe_4(Zn\text{-}L)_6}$ and simulated isotope distribution (below).

3. ^{1}H NMR analysis of 1•$\mathbf{Fe_4(Zn\text{-}L)_6}$

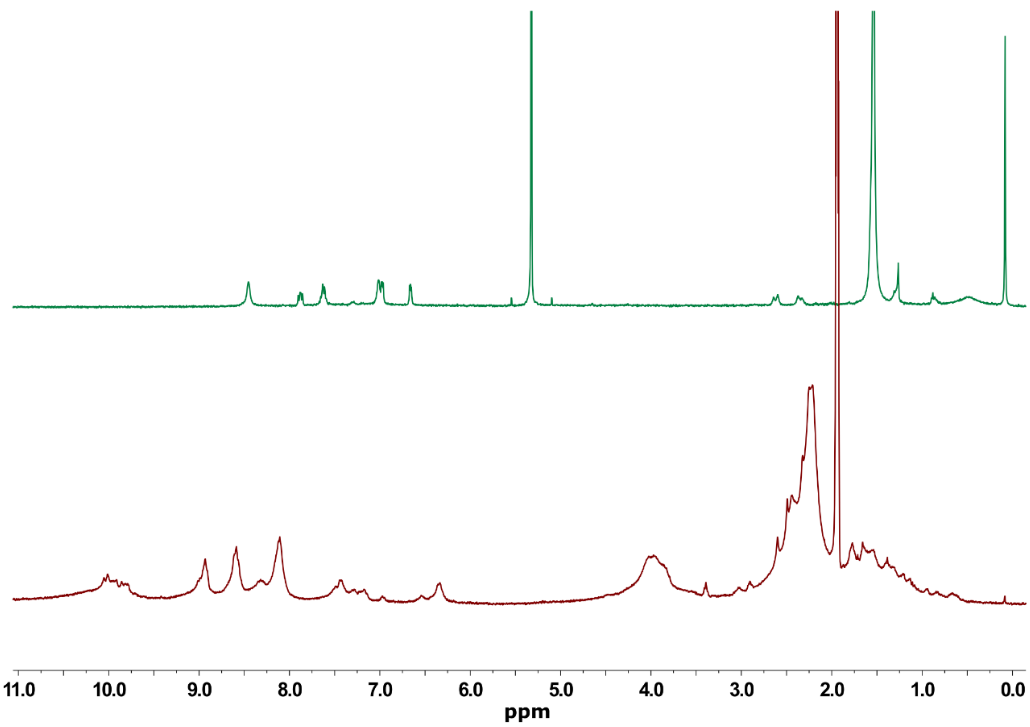


Figure S 7. ^{1}H NMR (300 MHz, 298 K) of **1** in CD_2Cl_2 (top) and **1**·$\mathbf{Fe_4(Zn\text{-}L)_6}$ in CD_3CN (bottom). The bottom spectrum is obtained from a 1:1 mixture of **1** and $\mathbf{Fe_4(Zn\text{-}L)_6}$.

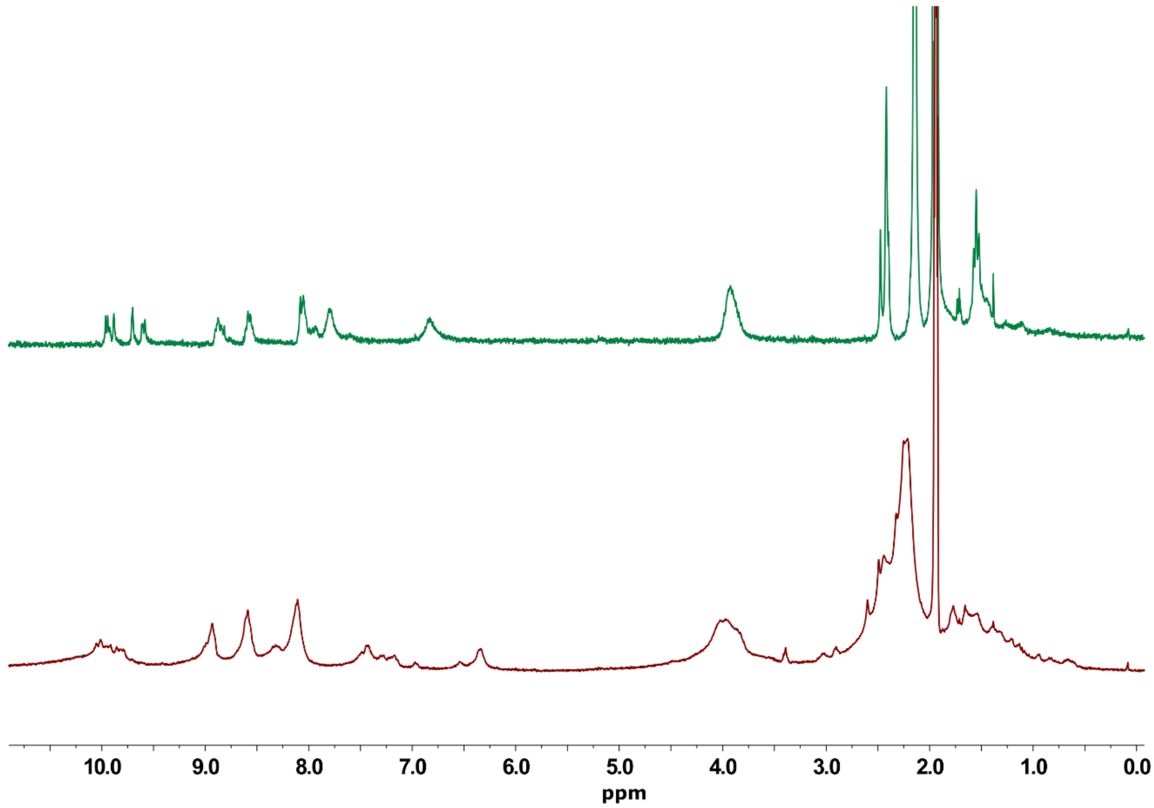


Figure S 8. [1]H NMR (300 MHz, 298 K) of **Fe_4(Zn-L)$_6$** (top) and **1·Fe_4(Zn-L)$_6$** in CD_3CN (bottom). The bottom spectrum is obtained from a 1:1 mixture of **1** and **Fe_4(Zn-L)$_6$**.

4. UV-vis binding study between 1 and Fe_4(Zn-L)$_6$

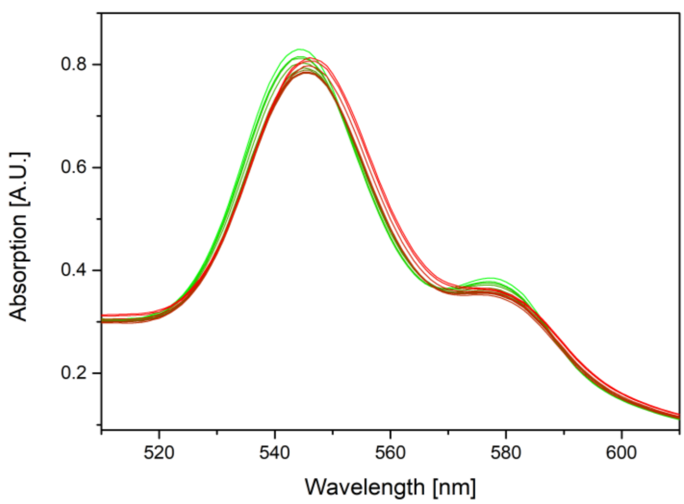


Figure S 9. Overlay of UV-vis spectra of the titration of **Fe_4(Zn-L)$_6$** (host) with **1** (guest), at a fixed host concentration of 7.7 µM in acetonitrile at 298 K.

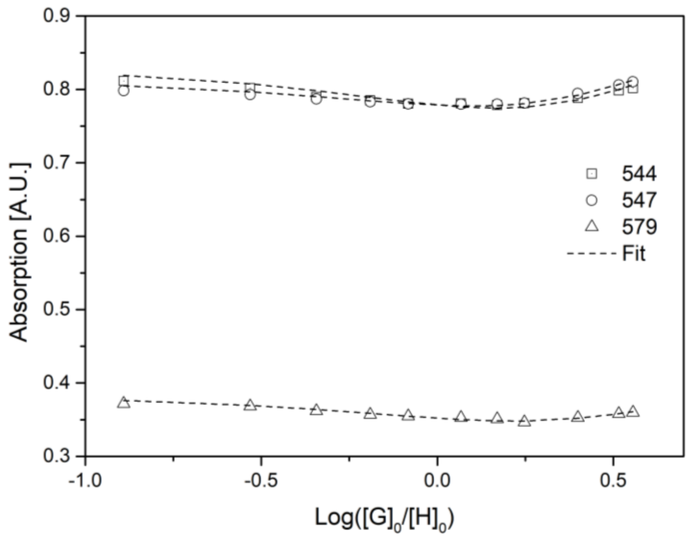


Figure S 10. Fitted UV-vis titration curves of **$Fe_4(Zn\text{-}L)_6$** (host) with **1** (guest) in acetonitrile at 298 K.

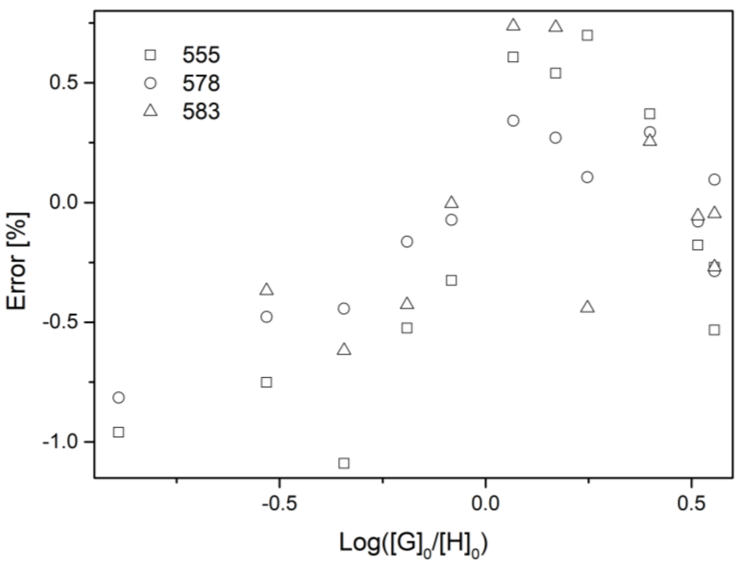


Figure S 11. The error distribution for the fitted titration curves of **$Fe_4(Zn\text{-}L)_6$** (host) with **1** (guest) in acetonitrile at 298 K.

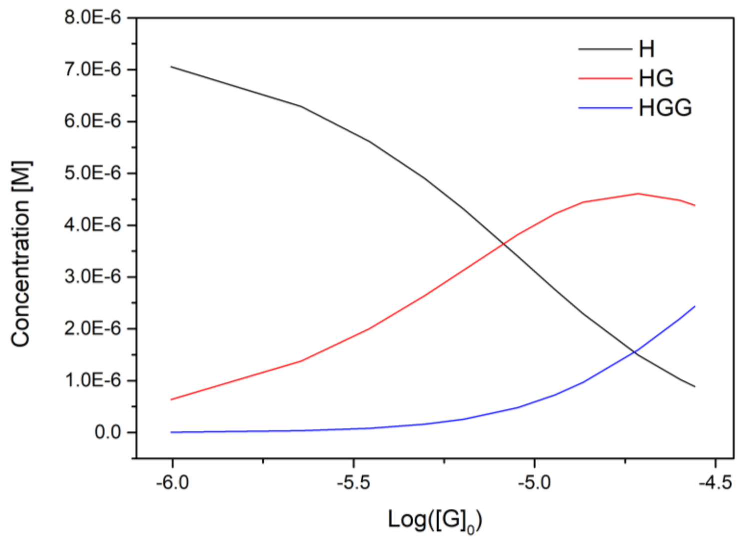


Figure S 12. Calculated species concentration of the titration of $\mathbf{Fe_4(Zn\text{-}L)_6}$ (host) with **1** (guest) in acetonitrile at 298 K.

5. Fluorescence lifetimes of $Fe_4(Zn\text{-}L)_6$ and $1{\bullet}Fe_4(Zn\text{-}L)_6$

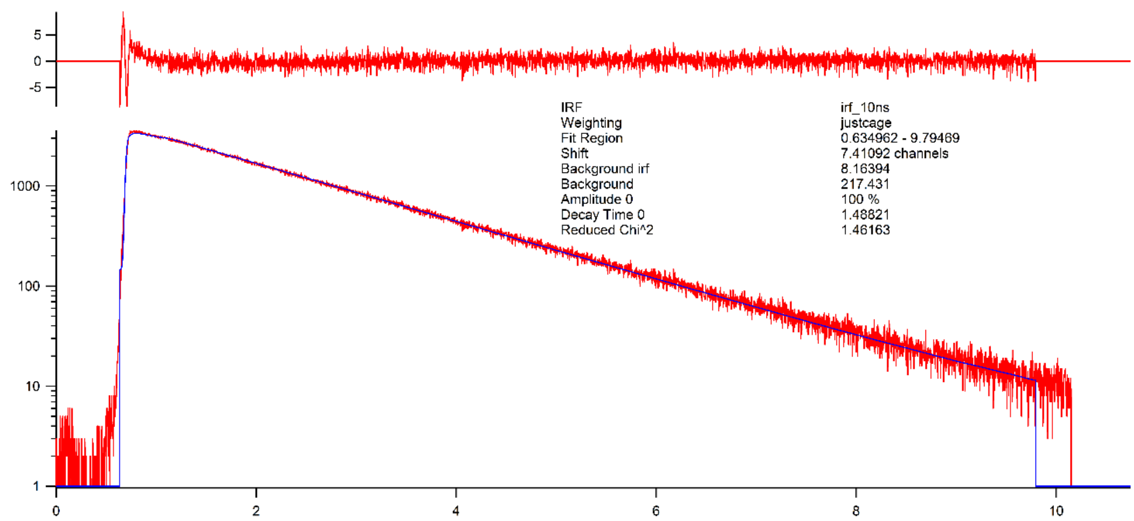


Figure S 13. Fluorescence decay of $\mathbf{Fe_4(Zn\text{-}L)_6}$ in acetonitrile. Monoexponential fit: τ = 1.49 ns. The Y-axis is the logarithm of the fluorescence intensity and the X-axis is the delay in ns.

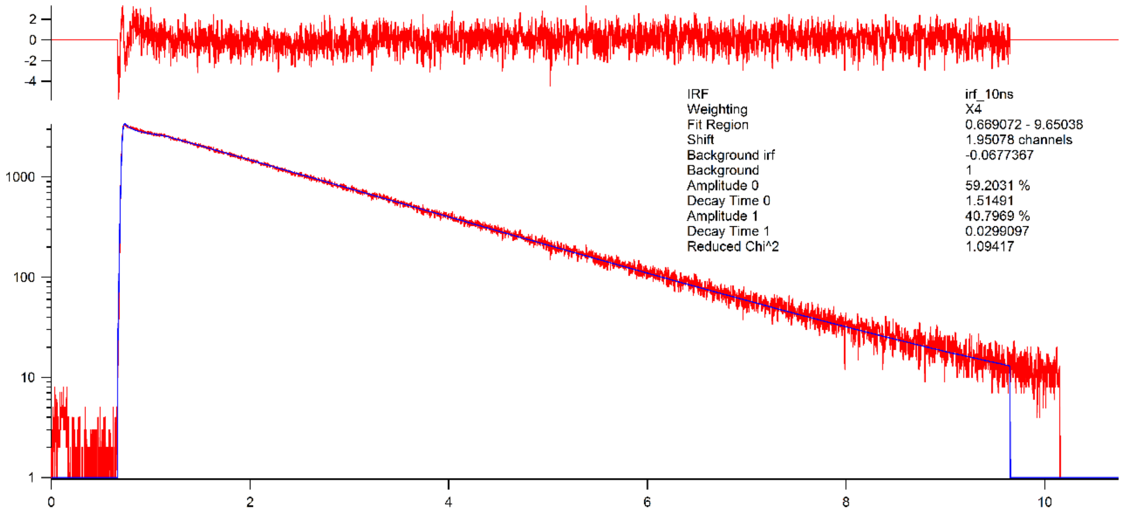


Figure S 14. Fluorescence decay of **1·Fe_4(Zn-L)$_6$** in acetonitrile. Biexponential fit: τ = 1.51 ns and τ = 0.03 ns. The amplitudes obtained from the fit are 59.2% and 40.8%, respectively. The Y-axis is the logarithm of the fluorescence intensity and the X-axis is the delay in ns.

6. Fitted species spectra from TR-IR measurements

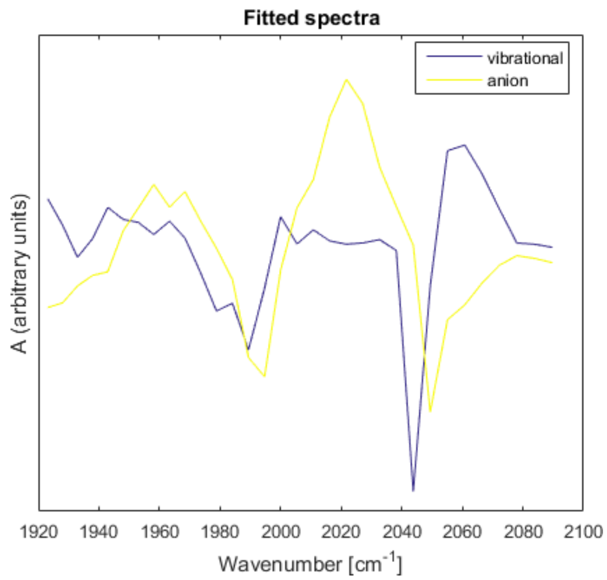


Figure S 15. Fitted differential spectra of the vibrational species and the anionic species observed in TR-IR.

7. Estimation of the electron transfer yield

We can estimate how much of the cage porphyrins are excited by one pulse of light during TR-IR measurements. The focal area of the pump pulse is around 200 µm wide and the sample cell is 500 µm long. With a cage concentration of 0.5 mM and 6 porphyrins per cage, the number of molecules in the excited area is around $5 \cdot 10^{13}$. The sample has an absorption of 0.4, so $1 - 10^{-0.4}$ = 60% of the photons is absorbed. A 2 µJ pulse of 2.1 eV (585 nm) light contains around $6 \cdot 10^{12}$ photons, of which $0.6 * 6 \cdot 10^{12}$ =

$4 \cdot 10^{12}$ photons are used to excite molecules. The percentage of excited molecules is then $4 \cdot 10^{12}$ / $5 \cdot 10^{13}$ is around 10%.

We can also estimate how much catalyst mono-anion is approximately formed. The catalyst concentration is also 0.5 mM, with an absorptivity of 10^4 $M^{-1}cm^{-1}$, leading to an absorption of 0.25 in the 500 µm cell. The ground-state depletion is around 0.25 mOD, and therefore 0.1% of the catalyst is reduced to the mono-anion. Dividing both ratios, we see that for each excited porphyrin, 1% of catalyst mono-anion is formed.

8. Gibbs free energy for photo-induced electron transfer

The Gibbs free energy for photo-induced electron transfer (ΔG_{ET}) is obtained by using the Rehm-Weller equation[5]:

$$\Delta G_{ET} = e\left[E^0_{\frac{D}{D^{+\cdot}}} - E^0_{\frac{A}{A^{-\cdot}}}\right] - \Delta E_{00} - \frac{e^2}{4\pi\varepsilon_0\varepsilon_{EC}R_c} - \frac{e^2}{8\pi\varepsilon_0}[\frac{1}{r^+} + \frac{1}{r^-}][\frac{1}{\varepsilon_{EC}} + \frac{1}{\varepsilon_s}]$$

The last term of the equation is a correction factor that is needed when the photoinduced electron transfer is studied in a different solvent than in which the potentials are determined. In our case all data are measured and calculated in acetonitrile and the last term equals zero. $E^0_{D/D^{+\cdot}}$ is the oxidation potential of the porphyrin cage, $E^0_{A/A^{-\cdot}}$ is the first reduction potential of the diiron catalyst, ΔE_{00} is the energy difference between the HOMO and the excited state from which electron transfer occurs of the porphyrin cage, *e* is the elementary charge, ε_0 is the vacuum permittivity, ε_{EC} is the dielectric constant of the used solvent (acetonitrile) and R_c is the center to center distance between the donor and the acceptor pair (determined from the molecular model of the host-guest complex to be 7.5 Å).

Table S 2. Potentials used for the calculation of the Gibbs free energy.

Photosensitizer	$E^0_{D/D^{+\cdot}}$	$E^0_{A/A^{-\cdot}}$	ΔE_{00}	ΔG_{ET}
$F_e(Zn\text{-}L)_6$	0.53 V *vs* $Fc^{0/+}$	-1.2 V *vs* $Fc^{0/+}$	1.94 eV	-0.26 eV
ZnTPP[6,7]	0.89 V *vs* $Fc^{0/+}$	-1.2 V *vs* $Fc^{0/+}$	2.05 eV	-0.18 eV

9. Time-resolved UV-vis spectra of $Fe_4(Zn\text{-}L)_6$ and $1 \bullet Fe_4(Zn\text{-}L)_6$

Comparing the two samples (with and without catalyst), it seems that they are almost the same, and the catalyst has no real influence on the bulk behavior of the porphyrins in the cage. For the time-resolved UV-vis data, it can be seen qualitatively that there is a fast (~10 ps) and a slow (few ns) decay present after excitation:

The absorption data contained a large apparent bleach signal around the excitation wavelength due to scattering of the pump pulse and long integration time of the detector. The wavelength region between 500 and 600 nm was therefore excluded from the data fitting procedure. The measured absorption data was fitted to $A(\lambda; t) = \sum c_s(t) \cdot \epsilon_s(\lambda)$ using the Matlab function `lsqcurvefit`, yielding the concentration profiles $c_s(t)$ and spectra $\varepsilon_s(\lambda)$ for all species. The concentration profiles were a function of the rate constants, but independent of the initial excited state concentration $[\widetilde{S_1}]_0$ (since they all contain it as a pre-factor).

To be able to interpret the data, kinetic equations for the concentration time-dependence of all species was determined. Since we could not discriminate between non-radiative (IC) and radiative (f) ground state reformation, we could only determine their sum $k_f + k_{IC} = k_G$.

For the vibrationally hot singlet excited state decay:

$$\frac{d[\widetilde{S_1}]}{dt} = [\widetilde{S_1}]_0 - k_{IVR}[\widetilde{S_1}] \quad and\ thus \quad [\widetilde{S_1}](t) = c_{\widetilde{S_1}}(t) = [\widetilde{S_1}]_0 \exp(-k_{IVR}t)$$

The (cooled) singlet excited state decay $\frac{d[S_1]}{dt} = k_{IVR}[\widetilde{S_1}] - (k_G + k_{ISC})[S_1]$ then leads to a double-exponential decay weighed by the rate constants as:

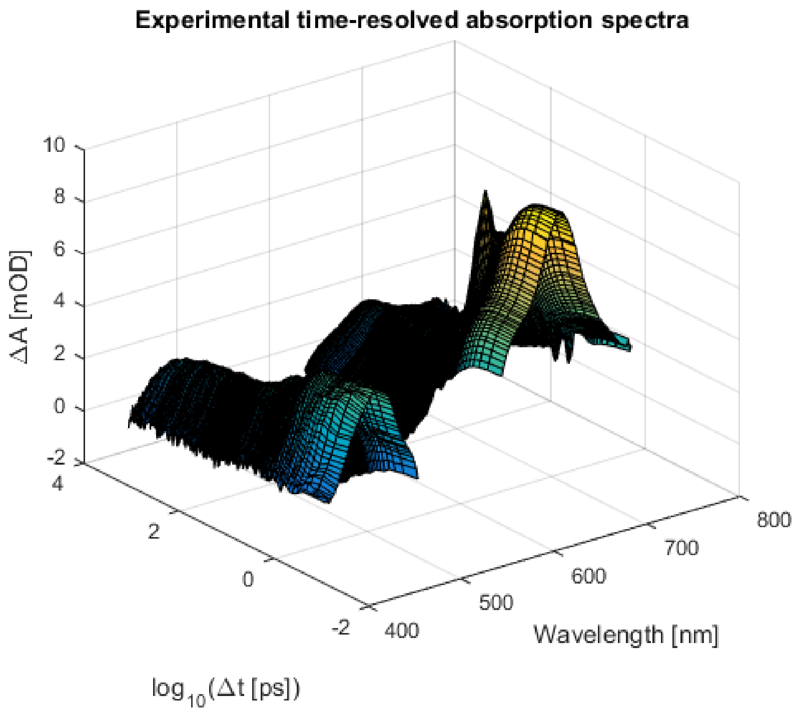
$$[S_1](t) = c_{S_1}(t) = \frac{k_{IVR}}{k_{IVR} - k_G - k_{ISC}}\left(\exp(-(k_G + k_{ISC})t) - \exp(-k_{IVR}t)\right)$$

The concentration profiles of the triplet and ground state are weighed integrated forms of $c_{S1}(t)$:

$$[T](t) = c_T(t) = k_{ISC} \cdot \frac{k_{IVR}}{k_{IVR} - k_G - k_{ISC}}\left(\frac{\exp(-k_{IVR}t) - 1}{k_{IVR}} - \frac{\exp(-(k_G + k_{ISC})t) - 1}{k_G + k_{ISC}}\right)$$

$$[G](t) = c_G(t) = k_G \cdot \frac{k_{IVR}}{k_{IVR} - k_G - k_{ISC}}\left(\frac{\exp(-k_{IVR}t) - 1}{k_{IVR}} - \frac{\exp(-(k_G + k_{ISC})t) - 1}{k_G + k_{ISC}}\right) - 1$$

where the "– 1" in $c_G(t)$ accounts for the depleted ground state concentration at t=0, since all equations are normalized to $[\widetilde{S_1}]_0 = [G] - [G]_0$. The fitting procedure thus yielded values for the rate constants k_{IVR}, k_G and k_{ISC}, and the spectra for all species.



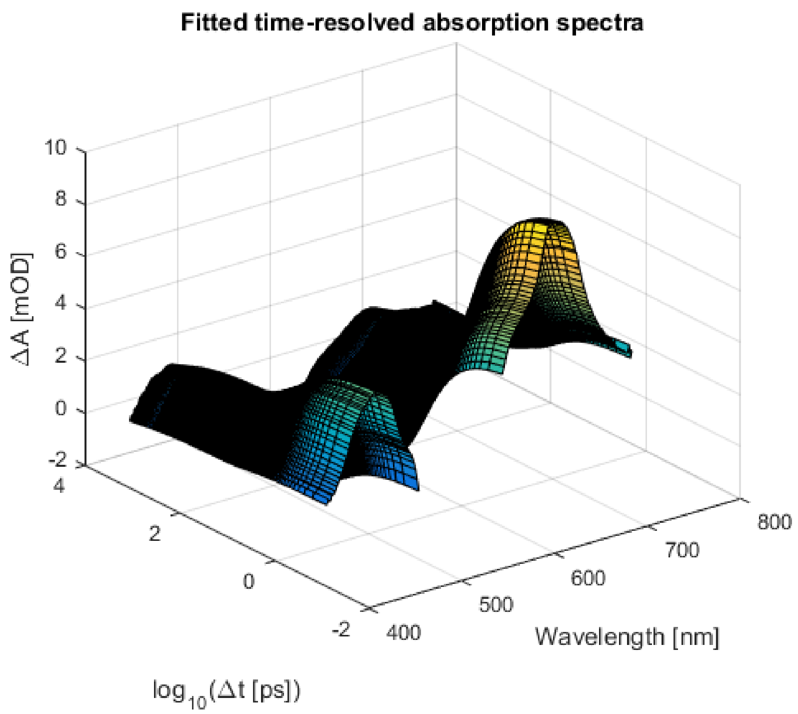


Figure S 16. Time-resolved absorption spectra of 13 µM $\mathbf{Fe_4(Zn\text{-}L)_6}$ with different delay times. (top) Experimental data. (bottom) Fitted data.

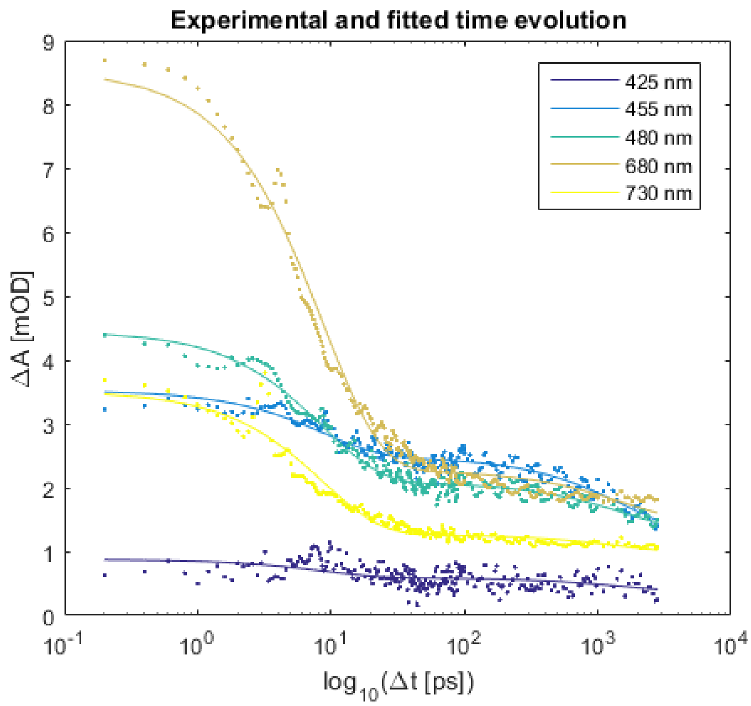


Figure S 17. Experimental and fitted kinetic trace of the time-resolved absorption spectra at five different wavelengths with different delay times of 13 µM **$Fe_4(Zn\text{-}L)_6$** in acetonitrile.

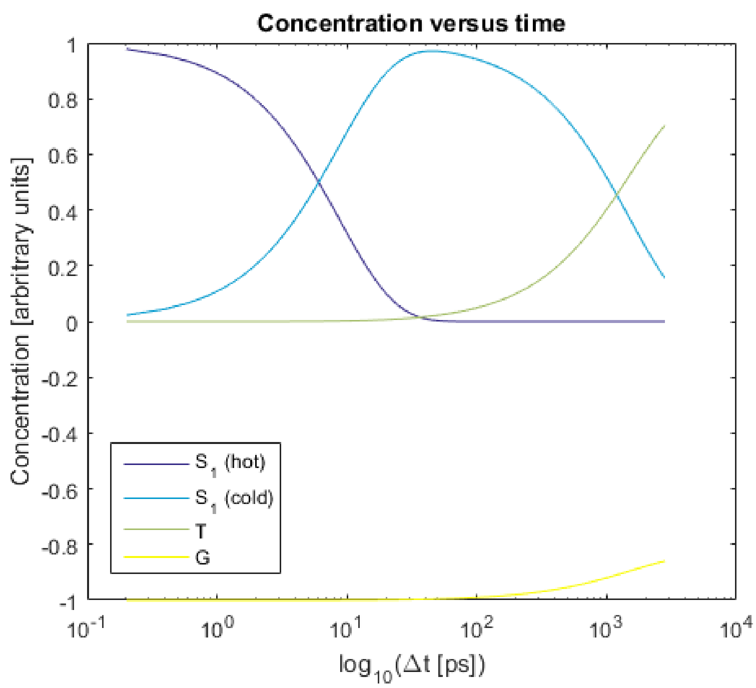


Figure S 18. Fitted species concentrations of the different species of the time-resolved absorption spectra as a function of time of 13 µM **$Fe_4(Zn\text{-}L)_6$** in acetonitrile.

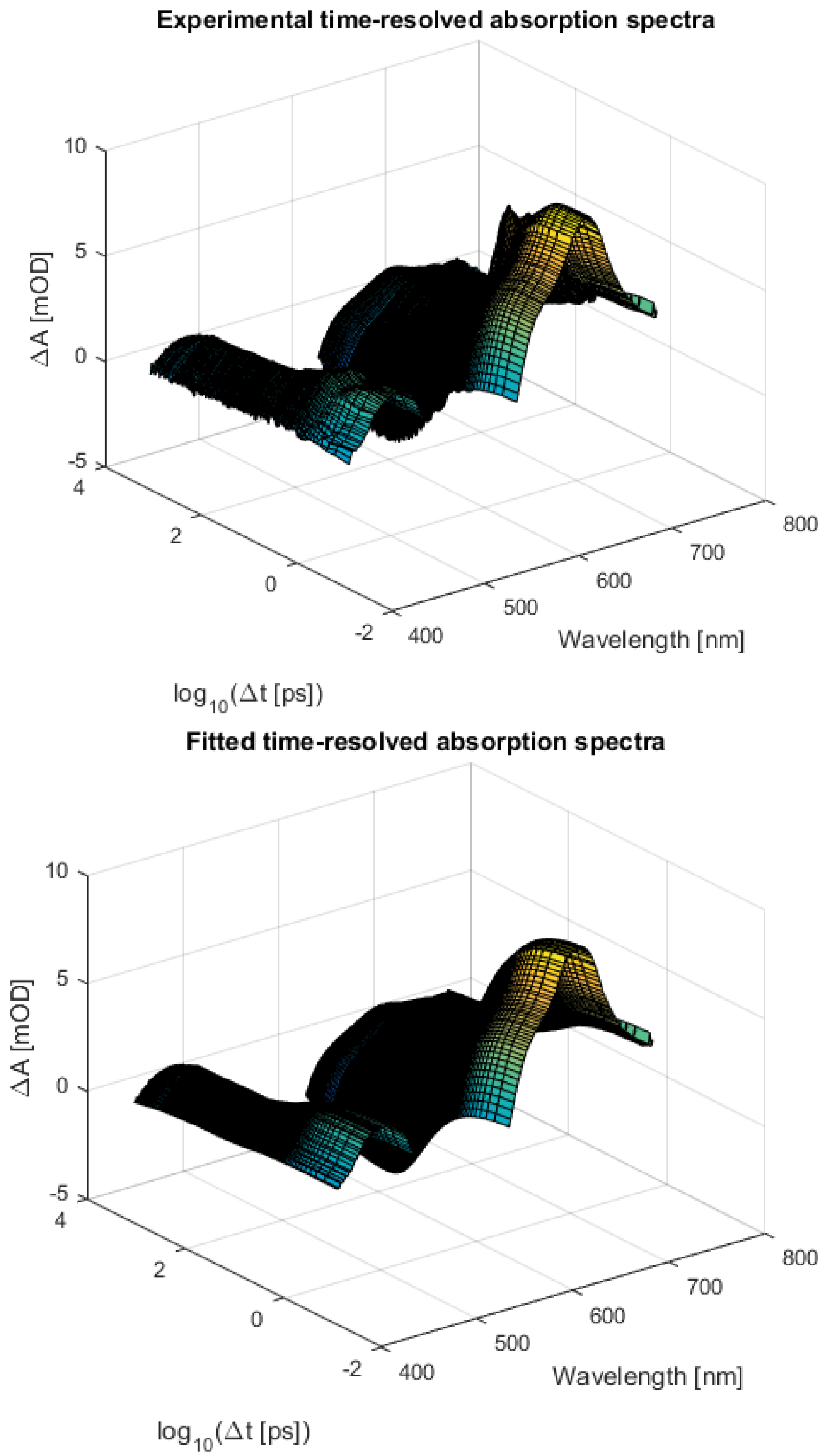


Figure S 19. Time-resolved absorption spectra of 13 µM **1·Fe_4(Zn-L)$_6$** with different delay times. (top) Experimental data. (bottom) Fitted data.

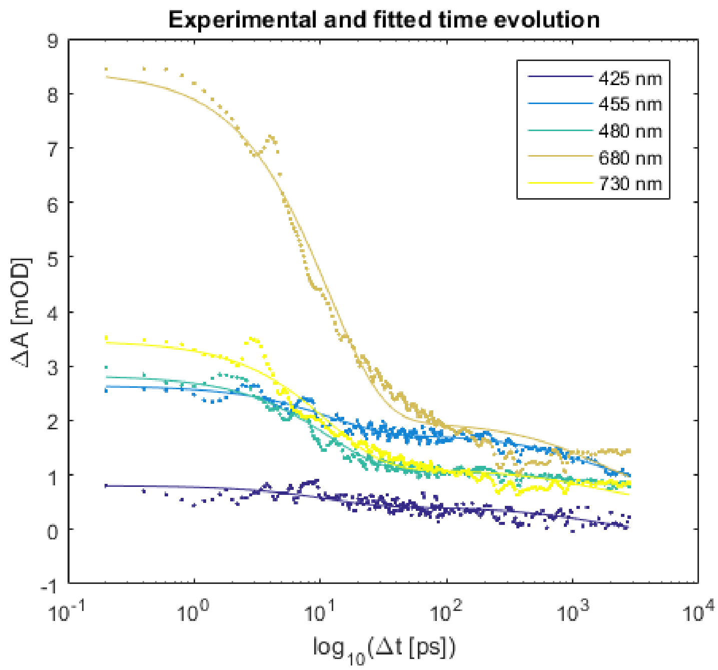


Figure S 20. Experimental and fitted kinetic trace of the time-resolved absorption spectra at five different wavelengths with different delay times of 13 µM **1·Fe_4(Zn-L)$_6$** in acetonitrile.

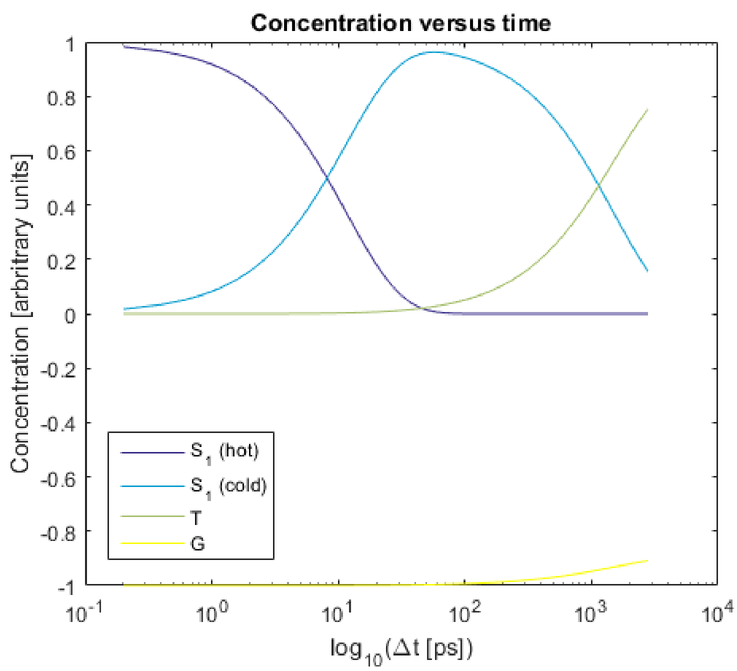


Figure S 21. Fitted species concentrations of the different species of the time-resolved absorption spectra as a function of time of 13 µM **1·Fe_4(Zn-L)$_6$** in acetonitrile.

10. Full system description

The general scheme for porphyrin excited state chemistry is as follows. Q-band excitation leads to population of the (vibrationally hot) singlet excited state $\widetilde{S_1}$ from the ground state G at time t = 0. This state then "cools" to the (vibrationally cold) singlet excited state S_1 with a rate constant k_{IVR}:

$$\widetilde{S_1} \xrightarrow{k_{IVR}} S_1$$

For ZnTPP the lifetime for this hot singlet state $\widetilde{S_1}$ is 10 to 20 ps, depending on the solvent. Next, the (cold) singlet excited state S_1 decays via two pathways: radiative (fluorescence, f) and non-radiative (inter-system crossing, ISC, and internal conversion, IC). The fluorescence pathway (with rate constant k_f) and the internal conversion pathway (with rate constant k_{IC}) reform the ground state G through:

$$S_1 \xrightarrow{k_f} G + h\nu \quad and \quad S_1 \xrightarrow{k_{IC}} G + heat$$

The inter-system crossing pathway forms the triplet state with a rate constant k_{ISC}:

$$S_1 \xrightarrow{k_{ISC}} T$$

Since these triplet states generally live for milliseconds (τ_T for ZnTPP in benzene is 1.2 ms), and our measurement window is only a few nanoseconds, we do not include the triplet decay in our models.

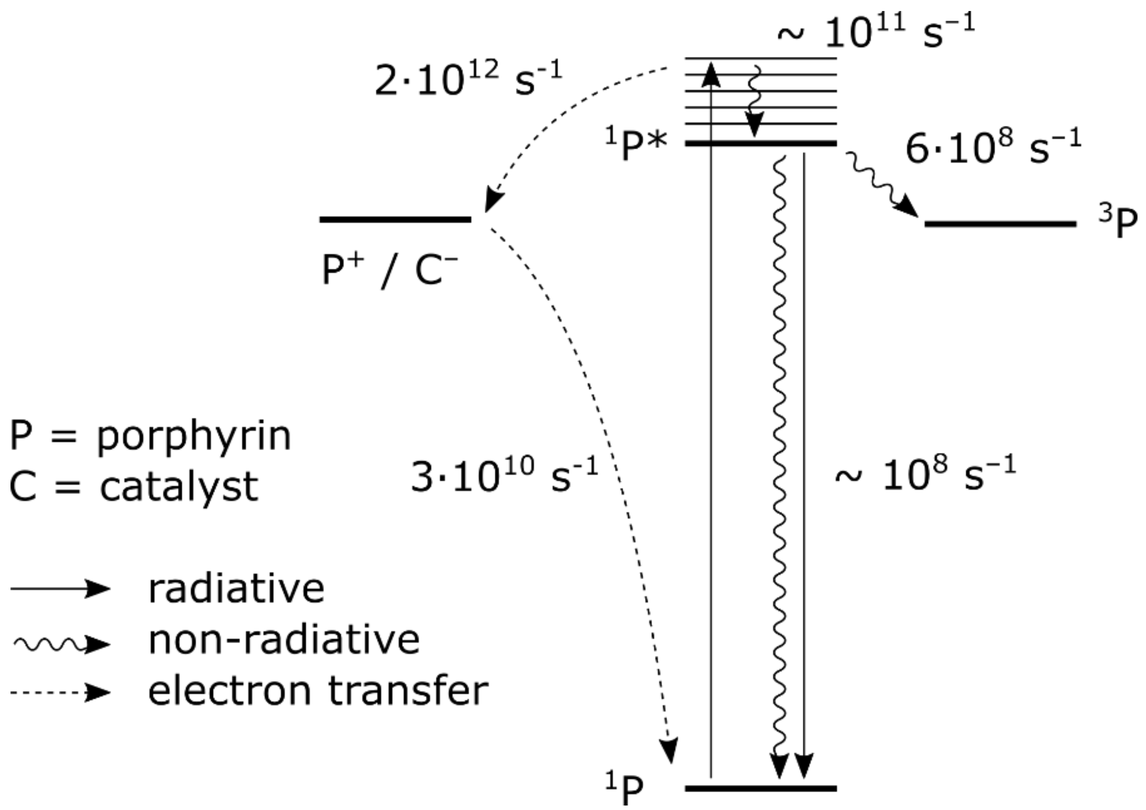


Figure S 22. Full system description in the form of a Jablonski diagram.

11. FOTW analysis and Tafel plot

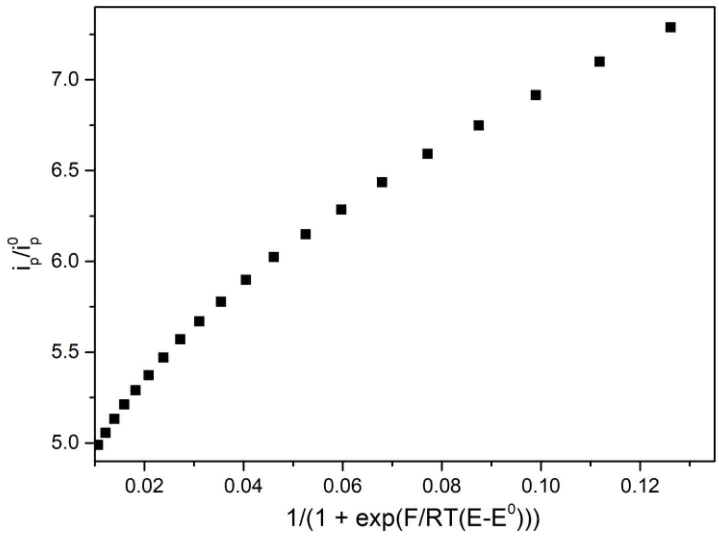


Figure S 23. FOTW analysis of the voltammograms of **1•Fe_4(Zn-L)$_6$** in the presence of weak acid ($HNEt_3PF_6$) in acetonitrile. One single plot is shown here for clarity, but the analysis was averaged over several acid concentrations.

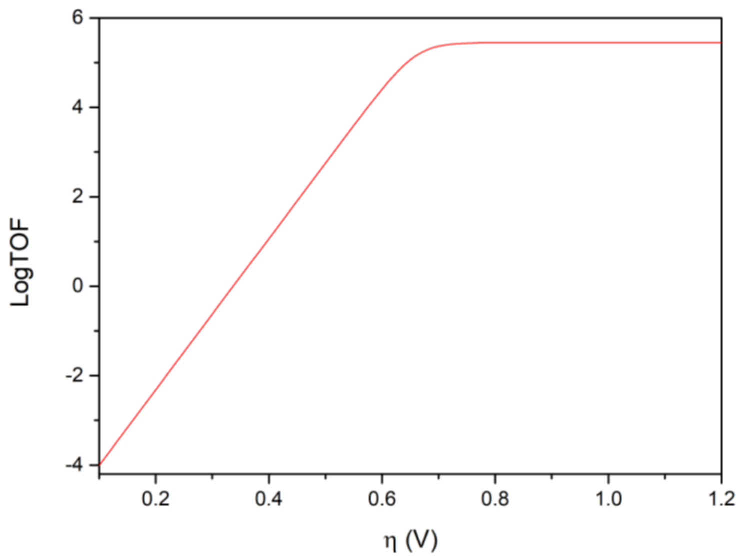


Figure S 24. Tafel plot of catalyst **1•Fe_4(Zn-L)$_6$** in the presence of weak acid ($HNEt_3PF_6$) in acetonitrile. The value of TOF_{max} is extrapolated for a 1 M concentration of acid.

12. Coordinates of xTB calculations

FE	7.10314077176956	7.29018478863480	6.96310728567300
ZN	-0.37113880806427	7.32265856867648	-0.29822326280423
N	9.03636742772793	7.59547953780841	6.66658072982952

N	7.07763944981381	7.41239835879369	5.01517633726583
N	0.12104362086916	8.17552761471695	1.49093608997466
N	1.59128920416542	6.74448610566648	-0.44345135070566
C	10.02876884519785	7.64990923574308	7.55443321827838
H	9.76198939916203	7.54088215286025	8.59823952563422
C	11.35453953215744	7.84412566067249	7.19876993419540
H	12.11456598186327	7.88083225439756	7.96385299221578
C	11.68579679866628	7.99235910130208	5.85640206977345
H	12.71059417730980	8.14579598985634	5.55405324292640
C	10.66773472630538	7.94281711087221	4.92103358694348
H	10.86987097586812	8.05744463777278	3.86666086624776
C	9.35599443760919	7.74321242462290	5.35525191485670
C	8.21906450238541	7.68895200030776	4.48285540091245
H	8.32314728275638	7.89036656921493	3.41964421630839
C	5.94525778425940	7.47506727968086	4.16644244068043
C	5.30832150912440	6.30547253903969	3.76704463279094
H	5.70859431328669	5.35198329635920	4.07267755272599
C	4.18573475609185	6.36755328246102	2.96525410122586
H	3.69021464050028	5.45717650401692	2.65899195763326
C	3.68195885203284	7.59306132598358	2.53486538524134
C	4.34200089791051	8.76165240325803	2.91367451226327
H	3.98003614487133	9.71689123154172	2.56110243485700
C	5.46983264912707	8.70598884918467	3.71387467201116
H	5.98273299593068	9.61695510741971	3.99519305374774
C	2.09239497577767	6.02893272626030	-1.48238104637990
C	3.51639978034863	5.85015342103549	-1.32383142180361
C	3.86461943471554	6.52467895940905	-0.18715344078261
C	2.62822553070743	7.01931079719328	0.39710953468505
C	2.48200897935918	7.59516086126275	1.66550334928805
C	1.27540524077657	8.06166257964176	2.20488745072141
C	1.02718556971305	8.45010482790138	3.58330934582161

C	-0.28050570373380	8.83928274778436	3.65071939169946
C	-0.83043461659333	8.66291616766259	2.32885183286296
C	1.39281590720942	5.65816356738709	-2.61648208799921
H	1.93494859144032	5.05952961916316	-3.33578457420399
C	4.42770891320549	5.11469060027588	-2.24842925600680
H	5.27816582021097	5.75282607616750	-2.50245138918821
H	3.91074931994200	4.87754128266721	-3.17880315085003
C	4.94903470121894	3.82071003482157	-1.63265189491238
H	5.53157506081329	4.02856782462811	-0.74002481798319
H	5.58439679344162	3.29740616596839	-2.34287211302905
H	4.12040955895799	3.16659200645668	-1.36264021979147
C	5.26741838124878	6.79137165902133	0.23140497876340
H	5.89261100386592	6.82885556756333	-0.65865135841037
H	5.64782044045771	6.00603220426814	0.88195327853838
H	5.35286123272568	7.74532945634733	0.74374015343741
C	1.94986370954810	8.37884223027864	4.75126074545687
H	2.67742346612228	9.18980289048633	4.72986750403422
H	2.49032159072126	7.43451122205379	4.76306436480262
H	1.36958294714255	8.45575371774869	5.66837846571405
C	-1.05623676929130	9.28364170981753	4.84332240222003
H	-1.74873408288830	10.07742028882955	4.55929545586313
H	-0.38176081417112	9.69460329416167	5.59643325695573
C	-1.83960753433309	8.12315081068028	5.44702917555915
H	-2.53184964299390	7.71252738191332	4.71586566015505
H	-2.40307109225797	8.46360940406946	6.31140629236197
H	-1.16036307385602	7.33186129749448	5.75694373155718
N	-9.40657634995014	7.75872604878390	-7.76460200308304
N	-7.38139085712146	7.65111552085621	-6.15842016991196
N	-0.70978191611523	6.84884426740841	-2.26746092346938
N	-2.20461362162358	8.23474875111451	-0.34386678569717
C	-10.44238630093819	7.75833063484095	-8.60341564203729

H	-10.26920543271633	7.37635202859695	-9.60154417787479
C	-11.70075619468258	8.22531157042666	-8.25686126692265
H	-12.49953335935133	8.20033168551884	-8.98186164006719
C	-11.91425660183076	8.72405824490931	-6.97643315617431
H	-12.88394996499373	9.09622388404785	-6.68265031121083
C	-10.85081313415210	8.73294888633580	-6.09230123645599
H	-10.96163073414938	9.11129086959237	-5.08719947426605
C	-9.61189907412632	8.24381250207259	-6.51348565518017
C	-8.44611160545104	8.20758098650438	-5.68216431023590
H	-8.46942536068639	8.63579671656133	-4.68268837985387
C	-6.23113820891408	7.72042041021338	-5.34054377140445
C	-5.62857032979530	6.55046709902831	-4.88762077714276
H	-6.02109294726522	5.59764541383476	-5.20622803887599
C	-4.55980131378501	6.61286219110854	-4.01531856905442
H	-4.11963216893472	5.69729833136471	-3.64526669605350
C	-4.04306259144681	7.84096333517261	-3.59751346627208
C	-4.61696937257841	9.01129967160343	-4.09851998875066
H	-4.20436266613331	9.96863015512916	-3.81587949239867
C	-5.71075148604031	8.95504431970399	-4.94300746570392
H	-6.15814166131246	9.86806780639622	-5.31436350040383
C	-2.77613930324044	8.73118325394344	0.78219368871003
C	-4.17269802511910	9.01374794152988	0.54774504127968
C	-4.42694313192995	8.67099340538943	-0.74896245773567
C	-3.16381909157419	8.21894084599161	-1.31405836177589
C	-2.91418086550462	7.83142981140550	-2.63540136737726
C	-1.70233003161784	7.28555779150996	-3.09095873141133
C	-1.37772844498127	6.92749835032930	-4.46263108135649
C	-0.27510238613446	6.11767053572340	-4.40197827911092
C	0.15869448913984	6.12979969531553	-3.02671068491491
C	-2.14460697976436	8.93400010740949	1.99566766874061
H	-2.75568770622578	9.35611759853430	2.78237424981668

C	-5.11433993960933	9.55242551187462	1.57033670864678
H	-5.96961140403739	10.01696210199420	1.07808709698824
H	-4.61266767732032	10.32897157435637	2.15103871515693
C	-5.61139444198561	8.46277596850575	2.51386548197068
H	-6.18850947623735	7.72246689266355	1.96584102162773
H	-6.24513530542149	8.89992277135536	3.28033802213696
H	-4.77401788888307	7.96047414526733	2.99364564337117
C	-5.77428564743109	8.71893185510274	-1.38071606262549
H	-6.53335755849119	8.75483233480087	-0.60274418212778
H	-5.94987538306133	7.84157722407303	-1.99944312453009
H	-5.88778089234227	9.60778368093778	-2.00026072243609
C	-1.89224505981011	7.55686321432342	-5.71248659004953
H	-1.29852947949310	8.45279818169095	-5.90579033577931
H	-2.93062237294966	7.86212693886482	-5.64322470567662
H	-1.76084950760441	6.88523488587407	-6.55800365102456
C	0.39369702939756	5.36901376246201	-5.50616339016663
H	1.45136819252371	5.63854304661387	-5.55103310012036
H	-0.05736935831952	5.64288885225610	-6.46104034221958
C	0.26808893564617	3.85878140138867	-5.32611418447432
H	0.79086606307517	3.52754407653980	-4.43230824778644
H	0.68446545087731	3.34490146601741	-6.18932872935153
H	-0.77755985685836	3.57346585888541	-5.22622233956129
FE	-7.54202330885647	7.16609566662047	-8.06477190495546
ZN	-0.13645372671773	-0.18546568087497	8.59669029937123
N	6.64343048624940	9.21149561035956	6.93016872636720
N	5.18819219962394	7.11533274156397	7.15280436150049
N	1.84834484577062	0.15501854142135	8.65850050785434
N	-0.38537818227260	1.79245088264591	8.19608131045927
C	7.44335719597865	10.27368783235845	6.84538963934386
H	8.50998499620172	10.08816128078650	6.87064012419581
C	6.96871974986862	11.57181262869913	6.73848607943670

H	7.66517889537954	12.39361667848190	6.67576318013584
C	5.59653726410327	11.79639668108153	6.71749169083941
H	5.20271114138865	12.79791146549310	6.63354021755720
C	4.75141186371705	10.70550061591967	6.81536625581991
H	3.67853017756898	10.82621595060446	6.81433354562494
C	5.30338267234997	9.42801077538315	6.92239473992384
C	4.53672098689192	8.22527912586491	7.07383637334293
H	3.45434038275018	8.26358543085375	7.16236204209767
C	4.40876960069922	5.95076774715506	7.39311882125586
C	3.75401230972747	5.31736882618986	6.34143890274765
H	3.84450196651382	5.71404973681121	5.34303761817361
C	3.00114733567573	4.18056345348118	6.57074768316062
C	2.82756506310263	3.69736641624487	7.86404265517103
C	3.45305018559301	4.36078052818611	8.91965840534034
H	3.29552236303484	4.01433911366998	9.93095835601817
C	4.25439452571489	5.46531660794976	8.68936055003315
H	4.73044179723013	5.97390075060308	9.51733494154074
C	-1.60451422176569	2.40067319747115	8.17483984044562
C	-1.44576600946902	3.80723549512342	7.91528822177702
C	-0.10259200455883	4.04370700650317	7.82321065276387
C	0.56141091723164	2.76356146717867	8.02076522946780
C	1.94113243057140	2.52989201628379	8.10120997377346
C	2.54137590367194	1.31087283009420	8.43116724824428
C	3.95970311205373	1.05955049167913	8.63249786089331
C	4.07155017453158	-0.22556755731933	9.07960519320121
C	2.74936419560393	-0.79522036584480	9.03361405563908
C	-2.81831296106386	1.78956838616375	8.42569001315575
H	-3.67948823735674	2.44031814288951	8.48565266581077
C	-2.57369246115741	4.75878867779080	7.70797259046053
H	-2.25180320929184	5.77970511149641	7.91652306344283
H	-3.38935738152142	4.52735840307558	8.39454168039107

C	-3.08462949199341	4.68110689653488	6.27314676721172
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H	-3.90838018391533	5.37565996154563	6.13330412888116
H	-3.42838606937303	3.67390894661980	6.04883193335735
C	0.48677163769003	5.39607563034469	7.61508224258418
H	-0.28818424832094	6.14625712789205	7.75239815432624
H	0.89060610699009	5.50394586257662	6.60800974065751
H	1.28082573889324	5.59687058176629	8.32969811007237
C	5.12257225604302	1.94803480492860	8.35144921088260
H	5.25686490382418	2.69703931982538	9.13123899622600
H	4.99400748404787	2.45685733093778	7.39925506043645
H	6.02540949929533	1.34447870825338	8.29541253308636
C	5.30040130520951	-0.94932282381555	9.51349781320351
H	5.05685406642867	-1.61764329177440	10.34123046216700
H	6.03318594601123	-0.22761743147670	9.87950901632218
C	5.91608059418989	-1.75312810310851	8.37658430035840
H	5.24951939000330	-2.55201427390026	8.06400475309380
H	6.85865904646443	-2.18961415767425	8.69605967929959
H	6.09178324900875	-1.10314728727299	7.52302749560810
N	-7.16008168751503	-9.38012640542228	6.84963700725949
N	-5.53395570955876	-7.39688437384849	7.07213940877450
N	-2.13014631729302	-0.54534704890731	8.44638925359875
N	0.11186379231190	-2.20640772794913	8.66440340679041
C	-8.03233488980968	-10.38039595810477	6.72726333934694
H	-9.07536675529997	-10.11411376579594	6.61248991733085
C	-7.66408329063656	-11.71649509630674	6.75157933831686
H	-8.41809632702075	-12.48156525523824	6.65004883534381
C	-6.32374905608028	-12.05207243440472	6.91106043976231
H	-6.01173455958211	-13.08515450612347	6.93268856389887
C	-5.40503524853021	-11.02789587664274	7.04869849549813
H	-4.35365884093132	-11.23272878336649	7.18407547557994

C	-5.85207441526726	-9.70498913469259	7.01575528356779
C	-4.99967041374211	-8.56702723076770	7.18523124110508
H	-3.94782149222661	-8.69403863936863	7.42919641594041
C	-4.69619641943051	-6.29911757976448	7.39037715459789
C	-4.21046981512305	-5.47009944395870	6.38656741549899
H	-4.45847727448056	-5.67924580312441	5.35858817451386
C	-3.39482169648201	-4.40200799483644	6.70843088697278
H	-3.01838945660226	-3.76065841425404	5.92262429937198
C	-3.04114652502045	-4.14823810360409	8.03057524460450
C	-3.50621180945817	-5.00049007450637	9.02911365033686
H	-3.21749118894734	-4.82737203394304	10.05589352956114
C	-4.32482392099186	-6.07050961912590	8.71489184439911
H	-4.68112191440262	-6.73180542093276	9.49421557029921
C	1.31513171549504	-2.80271493686139	8.86495450909144
C	1.20126598681947	-4.22560853273571	8.66206939966622
C	-0.10047900487359	-4.47202069538573	8.32920510465261
C	-0.79363691544557	-3.19597710764505	8.39460552593593
C	-2.16925058114240	-2.98001829515552	8.31735389275922
C	-2.79442073800047	-1.73746736748961	8.47790670476117
C	-4.20656246846969	-1.49175922483370	8.69634529863976
C	-4.35782569168835	-0.13850029285895	8.81723891060459
C	-3.05833740708146	0.44060634513661	8.59817844841000
C	2.49811477663623	-2.14714656703132	9.15451171160012
H	3.33977556769316	-2.77020000163019	9.42264820890538
C	2.35153671601646	-5.17093042197711	8.71283051458384
H	1.99378801670661	-6.19448687423292	8.83049449843321
H	2.97632453184905	-4.94073360867853	9.57772026414752
C	3.19180541676137	-5.07058331017846	7.44424732337269
H	2.60536426847349	-5.36151097521781	6.57542828546524
H	4.05574565425177	-5.72555976276263	7.51729934524169
H	3.53087617529878	-4.04717188972989	7.29947662651710

C	-0.65154160430681	-5.80449462114655	7.95728473386176
H	0.16585452636260	-6.51058979366724	7.83574869434967
H	-1.20973103749277	-5.75463443539064	7.02285225869612
H	-1.31518151837360	-6.18485662300311	8.73233085813457
C	-5.30318570024171	-2.48847766566899	8.84276660221917
H	-5.12938456970304	-3.13146440969920	9.70434540154787
H	-5.38671951663694	-3.11897419533215	7.95908760176254
H	-6.24526163099710	-1.96414446178704	8.98449096810292
C	-5.58894173496124	0.63256177214114	9.15244262616232
H	-5.32177159650288	1.47500149595942	9.79289074363791
H	-6.27255433110172	-0.00179719715670	9.71948473352719
C	-6.30247833851706	1.15223509429760	7.91245985473516
H	-5.68113810699664	1.87799168401851	7.39673754307355
H	-7.23392885909628	1.63336483382189	8.19766834838299
H	-6.52095832337113	0.33486635169653	7.22945586559198
FE	7.71689023518146	-7.55255429808501	-7.66781510884864
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C	-2.70557790078106	-0.96462012609804	-2.23324189018132
H	-3.55265300374232	-1.62482402819499	-2.34922405509024
C	-2.10042426511199	-0.84726859339530	-0.99370214342743
H	-2.46667607957949	-1.42032256279241	-0.15339082281804
N	-1.00776746420068	5.45063521992029	0.56144992815208
C	-1.57189011373973	4.54890736905326	-0.23131432337336
H	-1.92667753739790	4.91602507517566	-1.18286275017720
C	-1.69018216433227	3.21475050557406	0.10692509700006
H	-2.14570975640482	2.51230695359746	-0.57594812449648
C	-1.20436415713023	2.78200579604076	1.34087329847369
C	-0.65189006859211	3.74436121467477	2.18667097714892
H	-0.25730533358432	3.46418891438780	3.15299513463157
C	-0.57128049264533	5.05276138226594	1.75028110956465
H	-0.12672602910642	5.81551609582761	2.37261738373805
C	-1.20482999220122	1.35859906568609	1.68233349817109
C	-1.83789020560390	0.74403692266982	2.71107524571365
C	-2.72337486329049	1.44498425930376	3.69323249200424
H	-2.30210522259919	2.41945267211722	3.94632450084971
H	-3.69405360342894	1.62287143752835	3.21710982513405
C	-2.93126993722098	0.60958592343516	4.94713714146578
H	-3.65557763345939	1.09513207418168	5.60070868044020
H	-1.99633110816263	0.51515817659278	5.50259645844424
C	2.51842578599795	0.13979003219373	-0.83654860640207
O	2.85766711057345	-0.35142352492637	-1.81507777425125
S	2.90357656901750	-0.94313218365238	1.79379965495762
C	2.01037644644120	-0.99637596030644	3.31960797755246
C	1.76417680355422	-2.15349861727947	4.03131583662404
H	2.14404812525188	-3.10178208043236	3.68110318587637

C	1.01665289797874	-2.06207271678736	5.19964788036491
H	0.81581061966867	-2.95312935214400	5.77657013694104
C	5.11900940093780	0.51867455347665	0.65037632641639

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