Hydrogen Gas Generation by a Metal-Free Fluorinated Porphyrin

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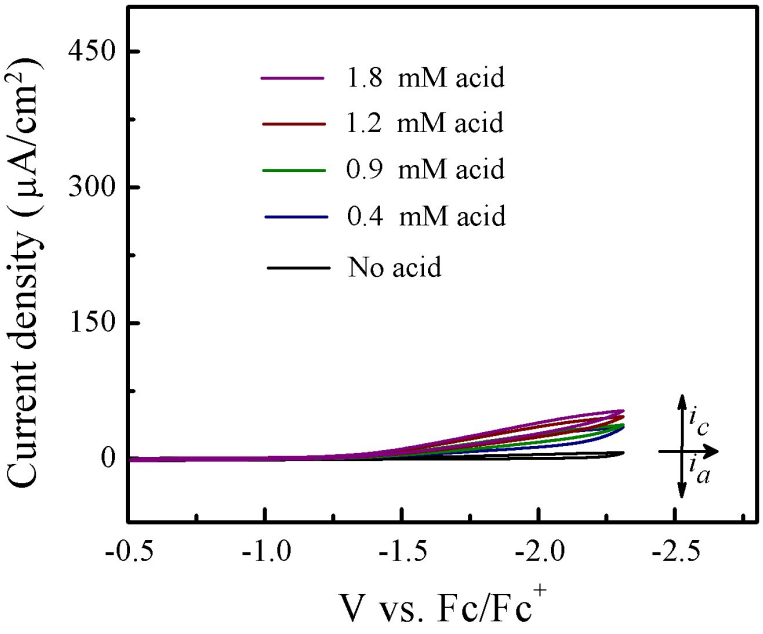

Figure S1. Cyclic voltammogram of *p*-toluenesulfonic acid in THF (no catalyst added); Scan rate: 100 mV/s; glassy carbon working electrode.

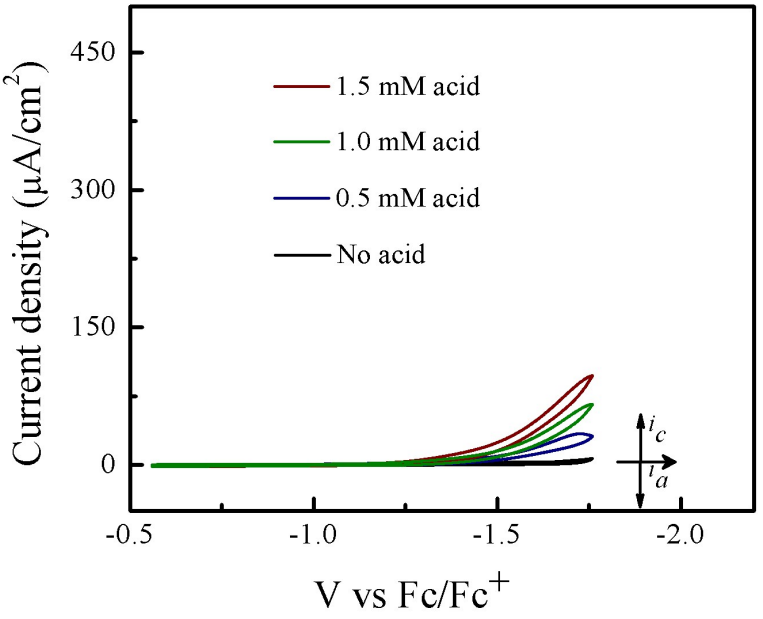

Figure S2. Cyclic voltammogram of *p*-toluenesulfonic acid in THF (no catalyst added); Scan rate: 100 mV/s; gold working electrode.

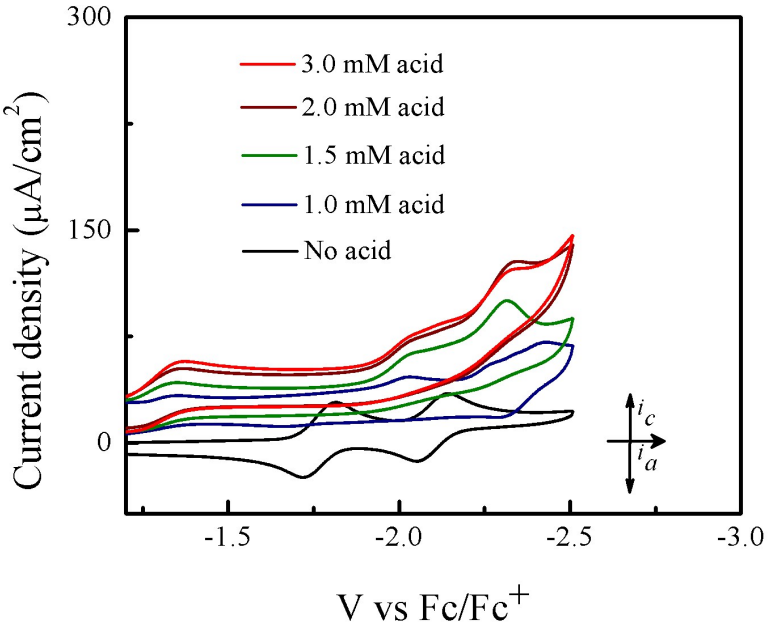

Figure S3. Cyclic voltammograms of *meso*-tetraphenylporphyrin with 0.1 M $TBAPF_6$ in THF and titrating with *tosic* acid: 100 mV/s; glassy carbon working electrode.

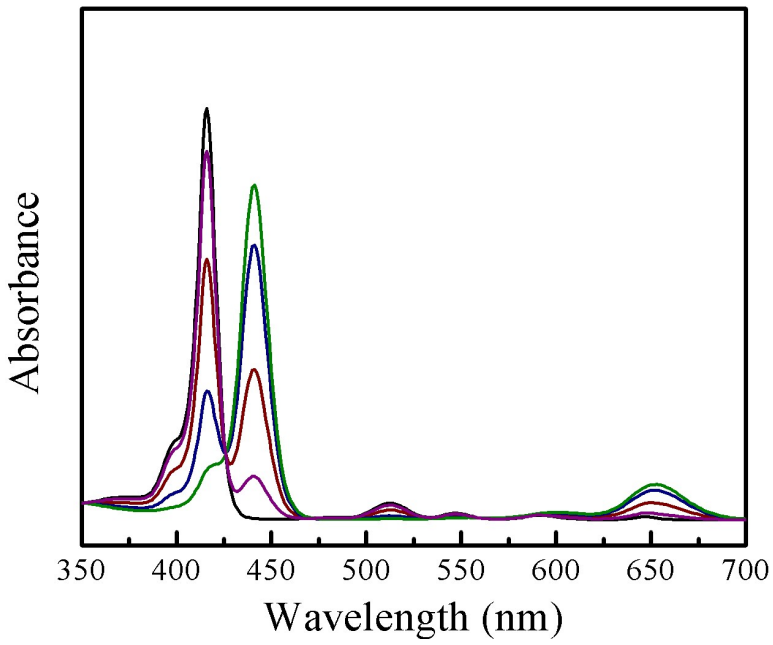

Figure S4. UV-vis spectra of *meso*-tetraphenylporphyrin (black line) and *meso*-tetraphenylporphyrin with addition of *tosic* acid (colored lines). This indicates that the free-base porphyrin is doubly protonated by *tosic* acid.

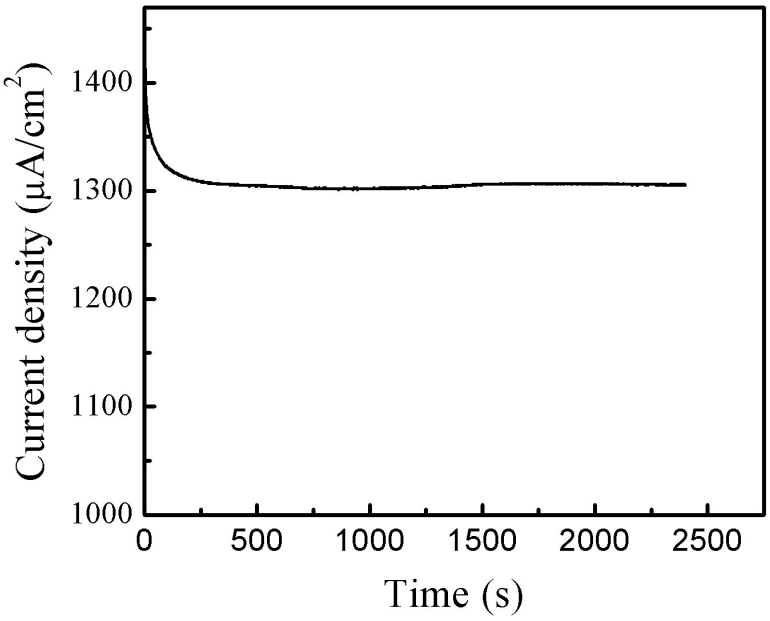

Figure S5. Plot of current density versus time of controlled -potential electrolysis experiment containing 50 mL THF solution of 1 mM of **1**, 0.1M $TBAPF_6$ and 10 mM *tosic* acid on a carbon rod electrode at –1.7 V vs Fc/Fc^+.

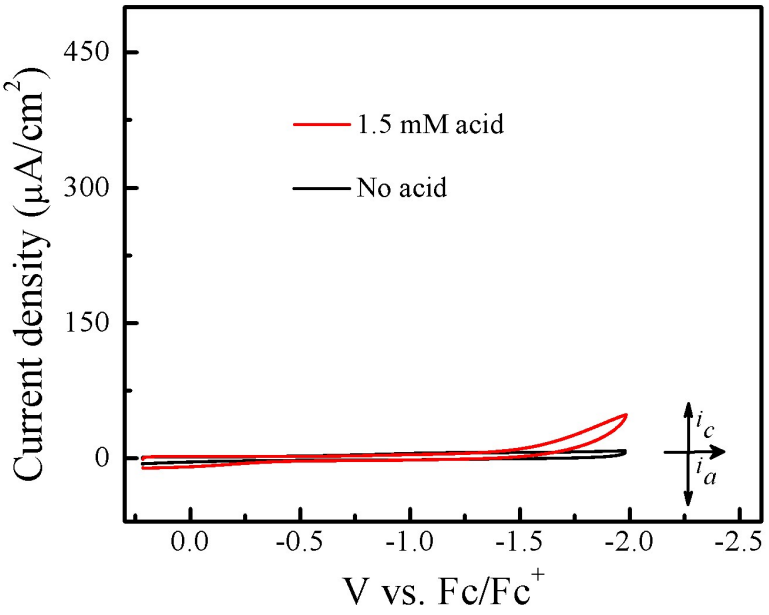

Figure S6. Cyclic voltammograms recorded using the rinsed glassy carbon electrode after performing bulk electrolysis in the presence of 0.1 mM **1** at –1.7 V vs. Fc/Fc^+ for an hour. Scan rate: 100 mV/s; glassy carbon working electrode.

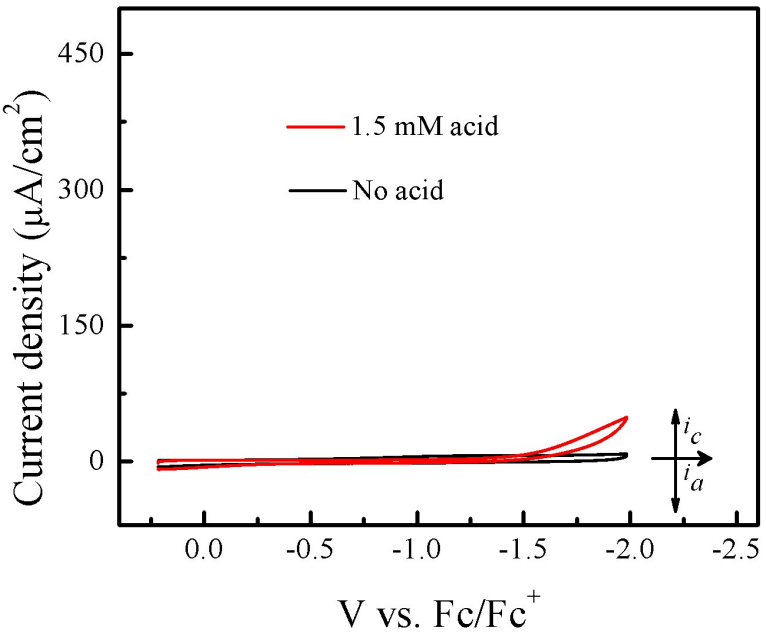

Figure S7. Cyclic voltammograms recorded using the rinsed glassy carbon electrode after performing bulk electrolysis in the presence of 0.1 mM **1** and 10 equiv *tosic* acid at –1.7 V vs. Fc/Fc^+ for an hour. Scan rate: 100 mV/s; glassy carbon working electrode.

Table S1. Charge passed, Volumes of H_2 measured and corresponding Faradaic efficiencies.

Catalyst	Solvent	Potential/V vs Fc/Fc^+	Time/min	q/C	V_{H_2}/mmol	f/%
1	THF	–1.7	40	3.18	0.0149	90
None	THF	–1.7	40	0.32	0	0

Calculation of overpotential.

Overpotential is calculated through $|E_{H+} - E_{cat/2}|$, where E_{H+} is the equilibrium potential of H^+/H_2 of *tosic* acid in THF and $E_{cat/2}$ is the potential at $i_{cat/2}$. E_{H+} is equal to the open circuit potential of *tosic* acid in THF solution using a platinum electrode at 1 atm hydrogen gas atmosphere.[1]

Table S2. Hammett constants for substituents.[2]

Substituent	σ_m	σ_p
C_6F_5	0.26	0.27
Cl	0.37	0.23
F	0.34	0.06

Calculation of k_{obs} from foot-of-the-wave analysis (FOWA).

Foot-of-the-wave analysis (FOWA) was used to determine the observed rate constant (k_{obs}) of hydrogen generation of **1**. For an ECEC mechanistic process: [3]

$$i = \frac{2FAC_p^0\sqrt{Dk_{obs}}}{1 + e^{\left[\frac{F}{RT}\left(E - E_{cat/2}\right)\right]}} \qquad \text{Eq. S1}$$

Where i is the catalytic current density (A/cm^2), F is the Faraday constant (96485 C/mol), A is the surface area of the working electrode (cm^2), C_p^0 is the concentration of the catalyst (mol/L), T is the temperature (298 K), D is the diffusion coefficient (cm^2/s) and k_{obs} is the observed rate constant, according to the Randles-Sevcik equation, the peak current i_p of a reversible catalytic wave can be described as: [4]

$$i_p = 0.4463\, FAC_p^0\sqrt{\frac{F\nu D}{RT}} \qquad \text{Eq. S2}$$

From Eq. S1 and Eq. S2, we can obtain:[3]

$$\frac{i}{i_p} = \frac{2\sqrt{\frac{RT}{F\nu}}\sqrt{k_{obs}}}{0.4463} * \frac{1}{1 + e^{\left[\frac{F}{RT}\left(E - E_{cat/2}\right)\right]}} \qquad \text{Eq. S3}$$

Then $\frac{i}{i_p}$ is plotted versus $\frac{1}{1 + e^{\left[\frac{F}{RT}\left(E - E_{cat/2}\right)\right]}}$ and the linear portion was selected to yield a line with a slope of m, which can be represented by:

$$m = \frac{2\sqrt{\frac{RT}{F\nu}}\sqrt{k_{obs}}}{0.4463} \qquad \text{Eq. S4}$$

Thus k_{obs} can be calculated through:

$$k_{obs} = \frac{(m)^2(0.4463)^2 F\nu}{4RT} \qquad \text{Eq. S5}$$

The catalytic rate constant (k_{cat}) is expressed as:

$$k_{cat} = \frac{k_{obs}}{[H^+]} \qquad \text{Eq. S6}$$

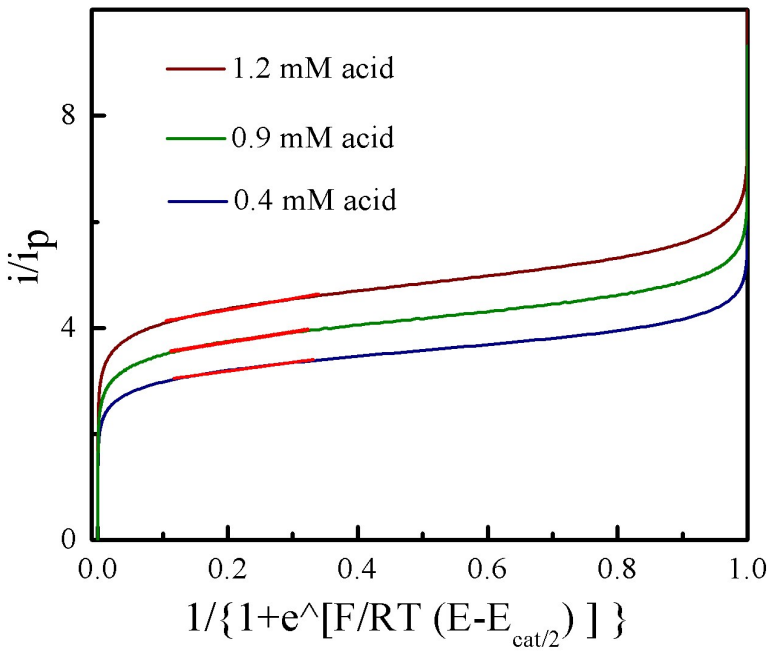

Figure S8. FOWA linear fit of **1** for hydrogen generation: 1.2 mM acid: slope= 2.144, R^2= 0.9874; 0.9 mM acid: slope= 1.956, R^2= 0.9876; 0.4 mM acid: 1.651, R^2= 0.9901.

Table S3. Summary of m, and k_{obs} at different acid concentration.

$[H^+]$ (mM)	m	k_{obs} (s^{-1})
0.4	1.651	0.528
0.9	1.956	0.742
1.2	2.144	0.891

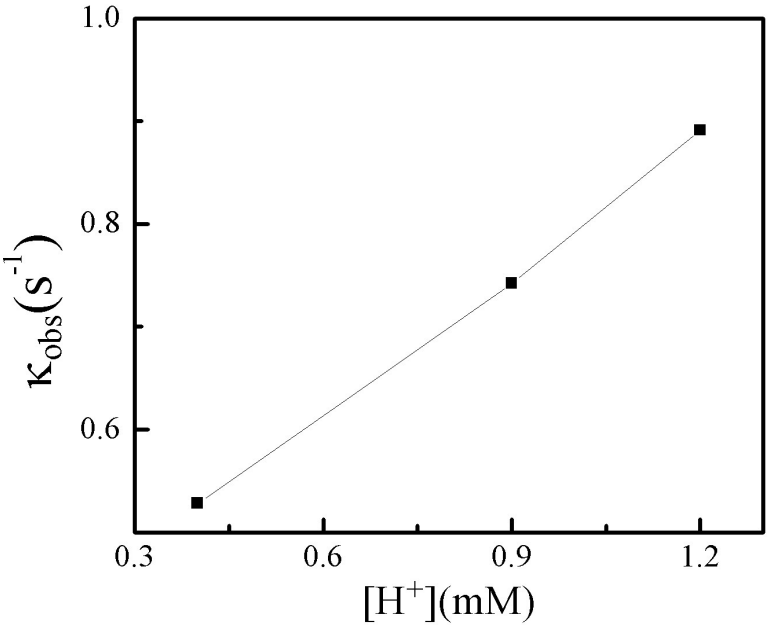

Figure S9. Plot of observed rate constant versus acid concentration. (R^2=0.9967)

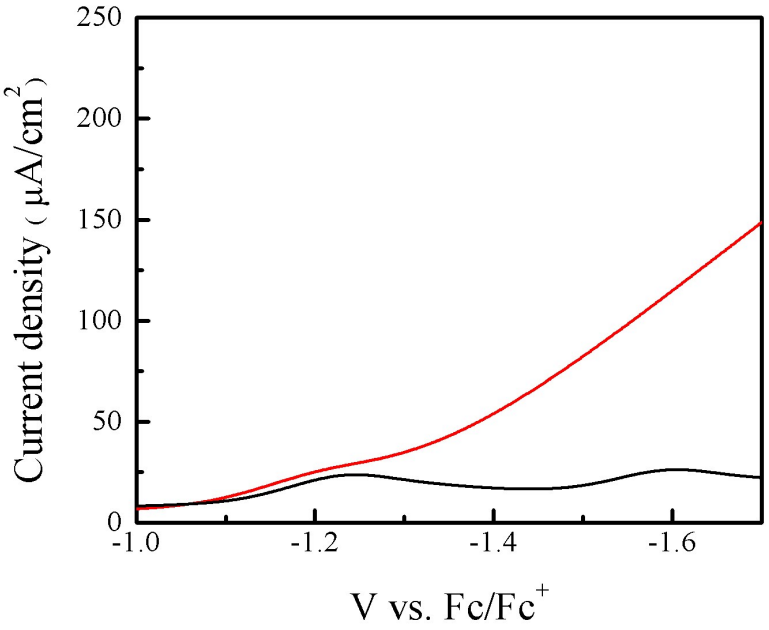

Figure S10. Linear sweep voltammograms of 0.1 mM **1** (black) and **1** with 12 equivalent deuterated *tosic* acid (red).

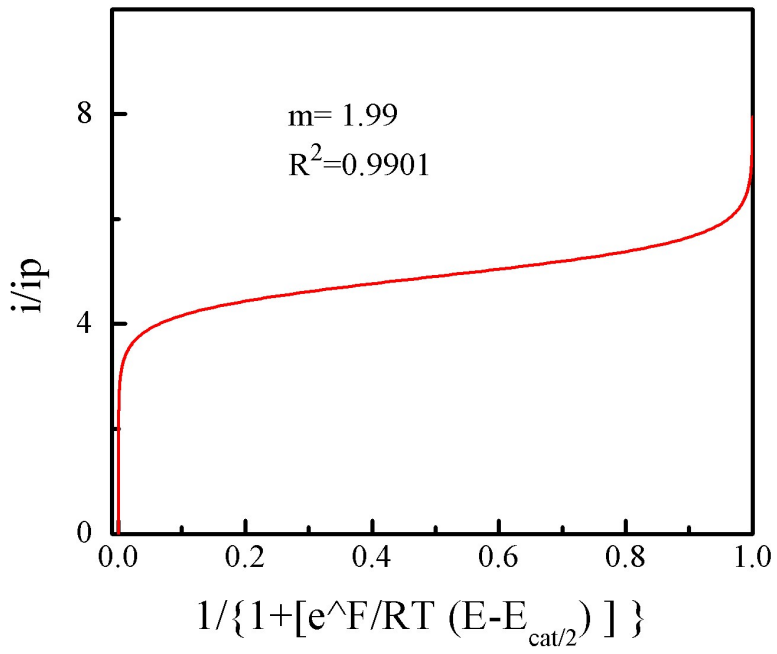

Figure S11. FOWA linear fit of 1 for hydrogen generation using 1.2 mM deuterated *tosic* acid.

Kinetic isotope effect (KIE) was analyzed using deuterated *tosic* acid ($C_7H_7SO_3D$). The calculated k_{cat} using $C_7H_7SO_3H$ is 742.5 $M^{-1}s^{-1}$ while k_{cat} using $C_7H_7SO_3D$ is 640.0 $M^{-1}s^{-1}$, resulting in KIE= $k_{cat,\ C7H7SO3H}/k_{cat,\ C7H7SO3D}$ = 1.16.[5]

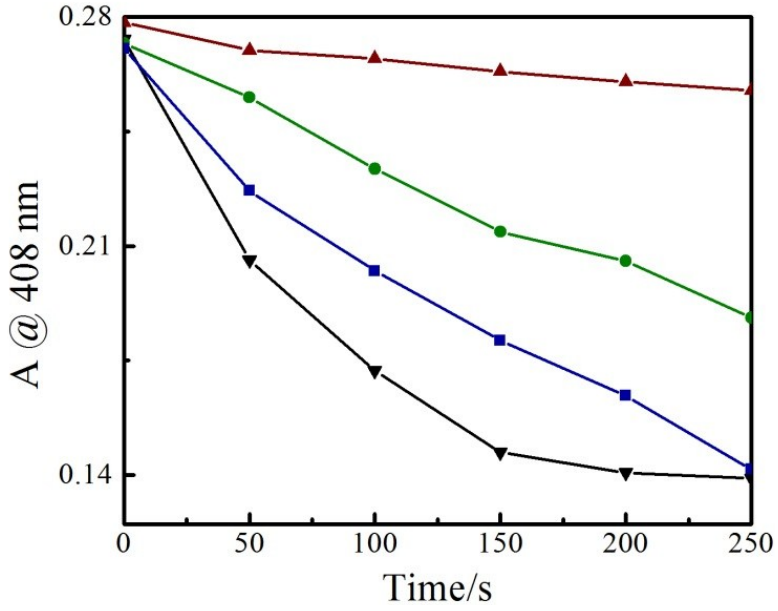

Figure S12. Change of absorption of **1** at 408 nm over time during electrolysis containing 1 M $TBAPF_6$ in THF. (From bottom to top) (▼) –1.7 V without acid; (■) –1.35V without acid; (●) – 1.35 V with *p*-toluenesulfonic acid); (▲) –1.7 V with *p*-toluenesulfonic acid (Potentials referred to Fc/Fc^+).

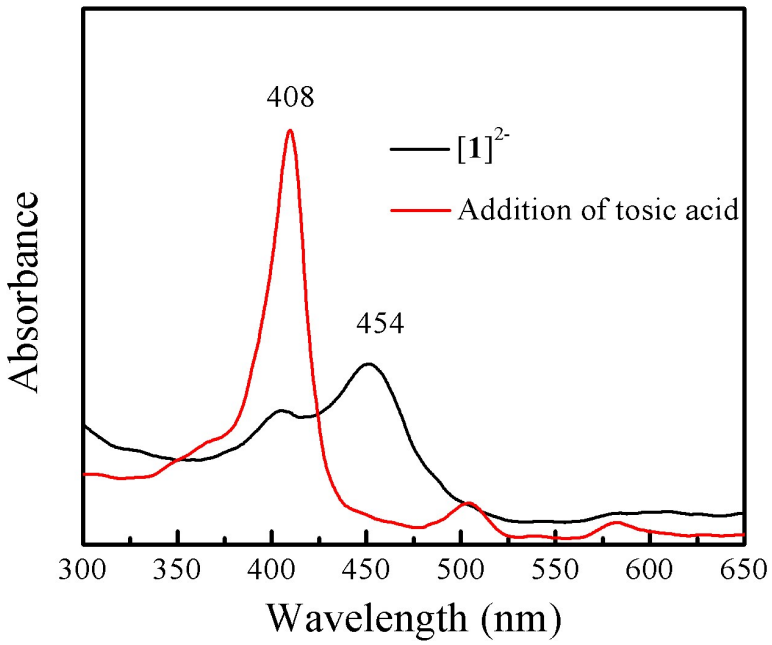

Figure S13. Uv-vis spectrum of $[\mathbf{1}]^{2-}$ (black) and the spectrum recorded upon addition of *tosic* acid to $[\mathbf{1}]^{2-}$ (red).

Uv-vis spectroelectrochemical study was performed using **1** at a potential of –1.7 V vs. Fc/Fc^{+} to obtain the dianion species, $[\mathbf{1}]^{2-}$ (black line in Figure S10). Subsequently, *tosic* acid was added to the solution and **1** was spontaneously obtained according to the spectrum (red line in Figure S10). This implies catalysis occurred upon addition of acid and **1** was regenerated. It should be noted that *E-E-P-P* pathway is also feasible for the generation of hydrogen gas.

Table S4. Experimental[6] and calculated pK_a's for acetic acid, benzoic acid, *tosic* acid and phenol in acetonitrile.

Compound	***pK_a Exp***	***pK_a Calc***
Acetic acid	23.51	20.76
Benzoic acid	21.51	19.93
Tosic acid	8.45	8.74
Phenol	29.14	27.47

Table S5. Calculated redox potentials and pK_a's in THF, values in parentheses correspond to the experimental values obtained in this work.

	B3LYP	***B3P86***	***B3LYP***	***B3P86***
Reaction	***E° (V vs Fc/Fc^+)***		***pK_a***	
TsOH + AcO^- → TsO^- + AcOH			11.8	10.8
[**1**] + e^- → [**1**]$^{\cdot -}$	–1.10 (–1.14)[a]	-0.95		
[**1**]$^{\cdot -}$ + e^- → [**1**]$^{2-}$	–2.12 (–1.54)[a]	-1.99		
[**1-H**]$^-$ + AcO^- → [**1**]$^{2-}$ + AcOH			37.7	35.3
[**1-HH**] + AcO^- → [**1-H**]$^-$ + AcOH			22.1	21.6
[**1-H**]$^+$ + AcO^- → [**1**] + AcOH			5.9	3.5
[**1-HH**]$^{2+}$ + AcO^- → [**1-H**]$^+$ + AcOH			–9.5	-11.1
[**1-H**]$^+$ + e^- → [**1-H**]	–0.25	-0.08		
[**1-HH**]$^{2+}$ + e^- → [**1-HH**]$^+$	0.69	0.85		
[**1-HH**]$^+$ + e^- → [**1-HH**]	–0.16	0.02		
[**1-H**] + e^- → [**1-H**]$^-$	–1.09	-0.99		
[**1-H**] + AcO^- → [**1**]$^{\cdot -}$ + AcOH			20.3	18.3
[**1-HH**]$^+$ + AcO^- → [**1-H**] + AcOH			6.3	4.6

[a]Experimental value

Table S6. Metal-free porphyrin core bond lengths and distances.[7]

	Distance (Å)
N(2)–H	0.80(7)
H···H	2.6(1)
N(2)···N(2)	4.144(3)
N(1)···N(1)	4.069(3)
N(1)···N(2)	2.911(3)
N(1)···H	2.37(6)

Cartesian coordinates of the DFT optimized structure [1] in the gas phase

C	-1.13619700	-2.90862300	-0.00003100
C	-0.68764800	-4.27446000	-0.00009500
C	0.68806400	-4.27439300	-0.00009400
C	1.13648100	-2.90851300	-0.00007700
N	0.00010300	-2.11362300	-0.00010300
C	-2.44483100	-2.42335300	0.00002600
C	2.44506800	-2.42311800	-0.00004800
C	2.89692700	-1.10017600	0.00009500
C	4.29711900	-0.68020700	0.00022600
C	4.29701700	0.68070800	0.00016700
C	2.89688100	1.10049500	0.00006900
N	2.05569100	0.00011900	0.00028500
C	2.44476800	2.42353600	0.00000900
C	1.13625400	2.90873400	-0.00010600
C	0.68762700	4.27453100	-0.00020200
C	-0.68804300	4.27446500	-0.00019100
C	-1.13653800	2.90862400	-0.00014100
N	-0.00010300	2.11362500	-0.00032000
C	-2.44500500	2.42330100	-0.00005600
C	-2.89698900	1.10021400	0.00002000
C	-4.29708500	0.68028900	0.00010500
C	-4.29705200	-0.68062500	0.00020600
C	-2.89681900	-1.10045500	0.00011700
N	-2.05569100	-0.00007800	0.00025900
H	-1.33819200	-5.13327300	-0.00009800
H	1.33869200	-5.13314300	-0.00010500
H	0.00005300	-1.09933300	-0.00015900
H	5.15069700	-1.33900700	0.00025300
H	5.15046600	1.33966300	0.00016700
H	1.33795400	5.13351000	-0.00022000
H	-1.33845200	5.13338200	-0.00021100
H	-0.00005400	1.09935300	-0.00047700
H	-5.15060000	1.33915800	0.00007100
H	-5.15056400	-1.33951100	0.00024000
Cl	3.74053100	3.72087200	0.00011900
Cl	-3.74089200	3.72051300	-0.00001200
Cl	-3.74043800	-3.72107700	0.00002900
Cl	3.74079900	-3.72071600	-0.00015300

Cartesian coordinates of the DFT optimized structure [1] $^-$ in the gas phase

C	-1.13915300	2.94027700	-0.00001300
C	-0.69876900	4.28974800	-0.00002600
C	0.69938800	4.28964900	-0.00001800
C	1.13957900	2.94011400	-0.00001100
N	0.00015600	2.14336500	-0.00005500
C	-2.45560200	2.42261600	-0.00000300
C	2.45595300	2.42226300	0.00000100
C	2.89928800	1.10799900	0.00000300
C	4.30274200	0.67934500	0.00000900
C	4.30265600	-0.67992900	0.00000800
C	2.89916600	-1.10842000	0.00000400
N	2.05640900	-0.00012800	0.00001800
C	2.45559000	-2.42256200	-0.00000400
C	1.13915600	-2.94026800	0.00000000
C	0.69877100	-4.28973200	0.00000300
C	-0.69939000	-4.28963200	0.00000000
C	-1.13958200	-2.94010500	0.00000300
N	-0.00015600	-2.14336900	0.00003100
C	-2.45594100	-2.42221000	0.00000200
C	-2.89932700	-1.10800400	0.00001100
C	-4.30275500	-0.67930900	0.00000900
C	-4.30264300	0.67996500	0.00001700
C	-2.89912700	1.10841600	0.00000400
N	-2.05640900	0.00016600	0.00002900
H	-1.34687300	5.15072700	-0.00002700
H	1.34761400	5.15053500	-0.00001300
H	0.00008300	1.12814000	-0.00008500
H	5.15713000	1.33847100	0.00000800
H	5.15696500	-1.33916100	0.00000600
H	1.34688000	-5.15070500	-0.00000200
H	-1.34762100	-5.15051400	-0.00000500
H	-0.00008400	-1.12814200	0.00004900
H	-5.15716000	-1.33841700	0.00000400
H	-5.15693600	1.33921500	0.00001600
Cl	-3.76745000	-3.73385800	-0.00001300
Cl	-3.76687300	3.73435000	0.00000600
Cl	3.76741400	3.73380800	0.00001700
Cl	3.76690900	-3.73440000	-0.00001600

Cartesian coordinates of the DFT optimized structure $[1]^{2-}$ in the gas phase

C	1.12980800	-2.98360400	-0.00000200
C	0.69071800	-4.31902900	0.00000700
C	-0.73053400	-4.31252500	0.00001300
C	-1.15737000	-2.97311400	0.00000700
N	-0.01012200	-2.18058000	-0.00001500
C	2.45450700	-2.43649000	-0.00001000
C	-2.47697400	-2.41383200	0.00000500
C	-2.90472900	-1.10274200	-0.00001300
C	-4.30909400	-0.65969900	-0.00002900
C	-4.30278900	0.69942100	-0.00004500
C	-2.89437600	1.12941400	-0.00001400
N	-2.05529100	0.00942300	-0.00003200
C	-2.45450700	2.43649000	-0.00000400
C	-1.12980800	2.98360400	0.00002000
C	-0.69071800	4.31902900	0.00003000
C	0.73053400	4.31252500	0.00002900
C	1.15737000	2.97311400	0.00003300
N	0.01012200	2.18058000	0.00011200
C	2.47697400	2.41383200	0.00001700
C	2.90472900	1.10274200	-0.00000100
C	4.30909400	0.65969900	-0.00004500
C	4.30278900	-0.69942100	-0.00003000
C	2.89437600	-1.12941400	-0.00001900
N	2.05529100	-0.00942300	-0.00002600
H	1.33385200	-5.18500800	0.00000900
H	-1.38155000	-5.17259900	0.00002000
H	-0.00543400	-1.16387000	-0.00002000
H	-5.16856900	-1.31443600	-0.00003200
H	-5.15614700	1.36211000	-0.00005800
H	-1.33385200	5.18500800	0.00001700
H	1.38155000	5.17260000	0.00001400
H	0.00543400	1.16387000	0.00017800
H	5.16856900	1.31443600	-0.00006000
H	5.15614700	-1.36211000	-0.00003700
Cl	-3.78215000	3.76762500	-0.00002900
Cl	3.81681600	3.73269200	-0.00000500
Cl	3.78215000	-3.76762500	0.00000300
Cl	-3.81681600	-3.73269200	0.00003000

Cartesian coordinates of the DFT optimized structure [1-H] in the gas phase

C	-1.14343900	-2.93229300	0.10314600
C	-0.69813400	-4.18076000	0.57538800
C	0.70640000	-4.17940200	0.57513500
C	1.14914300	-2.93010900	0.10267800
N	0.00206200	-2.16512500	-0.17434600
C	-2.46855900	-2.44420400	-0.05409700
C	2.47329700	-2.43952800	-0.05499100
C	2.92263100	-1.13489100	-0.13702400
C	4.28158900	-0.66788400	-0.32260500
C	4.28682600	0.70186000	-0.28124900
C	2.93454800	1.16058100	-0.08038200
N	2.13505200	0.01529900	-0.01372600
C	2.44125100	2.44610100	0.03609500
C	1.10142900	2.88945200	0.14720000
C	0.68180800	4.26932600	0.24928900
C	-0.69005800	4.26805200	0.24883400
C	-1.10704000	2.88736700	0.14668400
N	-0.00203400	2.04144700	0.10645800
C	-2.44599900	2.44148000	0.03519100
C	-2.93676300	1.15496900	-0.08098300
C	-4.28816100	0.69354900	-0.28154700
C	-4.28030700	-0.67620300	-0.32201000
C	-2.92039500	-1.14046300	-0.13647100
N	-2.13497000	0.01127200	-0.01408200
H	-1.34179700	-4.97852900	0.90866700
H	1.35173100	-4.97591800	0.90819700
H	0.00115800	-1.41200800	-0.84949000
H	5.12885400	-1.31796500	-0.46686300
H	5.14060700	1.35132900	-0.38649100
H	1.15579100	0.09045800	0.22503800
H	1.33568900	5.12482400	0.30283800
H	-1.34557100	5.12232500	0.30193500
H	-5.14320800	1.34130700	-0.38705800
H	-5.12632900	-1.32802200	-0.46573100
H	-1.15588200	0.08865200	0.22484400
Cl	-3.72557800	3.75556800	0.00743000
Cl	3.71834400	3.76271900	0.00937500
Cl	3.76090800	-3.74231200	-0.08158300
Cl	-3.75380500	-3.74942800	-0.07967500

Cartesian coordinates of the DFT optimized structure $[1\text{-H}]^-$ in the gas phase

C	-1.14869700	-2.93888700	0.18089800
C	-0.71182200	-4.09399200	0.82900500
C	0.71170000	-4.09401400	0.82900200
C	1.14860700	-2.93892200	0.18089400
N	-0.00003500	-2.23402100	-0.21232500
C	-2.47889100	-2.44234200	-0.06257000
C	2.47881500	-2.44241700	-0.06257700
C	2.92592900	-1.15102000	-0.14937200
C	4.28715100	-0.67158600	-0.37042300
C	4.29242700	0.69425900	-0.31982700
C	2.94350300	1.16463400	-0.08576800
N	2.14223600	0.00561500	-0.00740900
C	2.45294300	2.43550300	0.04150400
C	1.10752900	2.90699200	0.17938700
C	0.69578100	4.26558700	0.32538600
C	-0.69565200	4.26560800	0.32538100
C	-1.10744100	2.90702600	0.17938400
N	0.00003200	2.06111700	0.10823400
C	-2.45286800	2.43557800	0.04149800
C	-2.94346700	1.16472300	-0.08577200
C	-4.29240500	0.69438900	-0.31983100
C	-4.28717100	-0.67145700	-0.37042100
C	-2.92596500	-1.15093200	-0.14936800
N	-2.14223500	0.00567900	-0.00741000
H	-1.35775100	-4.83946100	1.26577300
H	1.35760800	-4.83950200	1.26576900
H	-0.00002500	-1.51173500	-0.91822300
H	5.13135800	-1.32239300	-0.53219800
H	5.14554800	1.34384800	-0.43692500
H	1.16209100	0.07950400	0.22383500
H	1.34697800	5.12271500	0.40239100
H	-1.34682300	5.12275700	0.40238300
H	-5.14550500	1.34400400	-0.43693400
H	-5.13139900	-1.32223800	-0.53219500
H	-1.16209000	0.07953800	0.22383900
Cl	3.76520900	-3.77421100	-0.18564800
Cl	3.74311600	3.76944600	-0.01769500
Cl	-3.74300000	3.76956000	-0.01770700
Cl	-3.76532600	-3.77409800	-0.18563300

Cartesian coordinates of the DFT optimized structure [1-HH] in the gas phase

C	1.14592600	-2.89175600	0.31828900
C	0.70926400	-4.05293300	0.96210100
C	-0.70758500	-4.05322200	0.96210200
C	-1.14472300	-2.89222900	0.31828200
N	0.00045400	-2.17490600	-0.05213800
C	2.47454300	-2.43808800	-0.00426700
C	-2.47352500	-2.43911000	-0.00428000
C	-2.90774100	-1.16326600	-0.21176500
C	-4.20156200	-0.68259800	-0.66773100
C	-4.20184400	0.68085000	-0.66771500
C	-2.90822900	1.16204400	-0.21172500
N	-2.11079700	-0.00044600	0.00543200
C	-2.47454400	2.43807300	-0.00423100
C	-1.14592900	2.89177400	0.31824500
C	-0.70926200	4.05310400	0.96178300
C	0.70758300	4.05339700	0.96177700
C	1.14472600	2.89224700	0.31824000
N	-0.00045400	2.17481300	-0.05198800
C	2.47352700	2.43909500	-0.00424200
C	2.90774300	1.16324600	-0.21173300
C	4.20156300	0.68259000	-0.66770600
C	4.20184200	-0.68085700	-0.66774100
C	2.90822800	-1.16206300	-0.21175700
N	2.11079600	0.00042500	0.00542900
H	1.35365400	-4.80940300	1.38099400
H	-1.35166700	-4.80995600	1.38099400
H	0.00030100	-1.42129900	-0.72412600
H	-5.01010500	-1.33144600	-0.96560500
H	-5.01065900	1.32936700	-0.96557000
H	-1.35364900	4.80966900	1.38050700
H	1.35166100	4.81023000	1.38049400
H	-0.00029900	1.42113700	-0.72390000
H	5.01010900	1.33144500	-0.96555700
H	5.01065300	-1.32936800	-0.96562100
H	1.40101700	0.00026700	0.72633900
H	-1.40101700	-0.00031200	0.72634100
Cl	3.71807000	3.77826200	-0.15477500
Cl	3.71961200	-3.77676100	-0.15487000
Cl	-3.71803700	-3.77830100	-0.15488700
Cl	-3.71964500	3.77672200	-0.15476100

Cartesian coordinates of the DFT optimized structure [1-HH]$^+$ in the gas phase

C	-1.15064300	2.89253900	0.26301600
C	-0.70836500	4.12396800	0.79370700
C	0.69083700	4.12691000	0.79379000
C	1.13833200	2.89737000	0.26309400
N	-0.00454900	2.13368300	-0.02481300
C	-2.47195300	2.44157700	-0.00380600
C	2.46152100	2.45207600	-0.00380900
C	2.90073700	1.15909100	-0.21432700
C	4.19113100	0.69458800	-0.66041100
C	4.19406600	-0.67675900	-0.66038300
C	2.90565600	-1.14676600	-0.21431000
N	2.11447200	0.00448200	0.00963600
C	2.47195300	-2.44161000	-0.00379200
C	1.15065900	-2.89253200	0.26306200
C	0.70836500	-4.12396900	0.79372000
C	-0.69083700	-4.12691600	0.79372800
C	-1.13832000	-2.89738200	0.26300700
N	0.00455300	-2.13371300	-0.02489800
C	-2.46153000	-2.45204000	-0.00382800
C	-2.90071900	-1.15907100	-0.21433500
C	-4.19117300	-0.69456800	-0.66038400
C	-4.19408500	0.67674900	-0.66041400
C	-2.90563000	1.14675000	-0.21432200
N	-2.11452000	-0.00448100	0.00961600
H	-1.35418800	4.91088900	1.14913100
H	1.33331200	4.91653900	1.14928100
H	-0.00285100	1.38354200	-0.70252700
H	4.99798700	1.34363900	-0.96188100
H	5.00370100	-1.32234900	-0.96182500
H	1.35417000	-4.91087500	1.14920900
H	-1.33332900	-4.91654600	1.14918100
H	0.00306500	-1.38360200	-0.70264800
H	-4.99802200	-1.34363500	-0.96184100
H	-5.00369600	1.32235800	-0.96188100
H	-1.37238100	-0.00291400	0.69698000
H	1.37263200	0.00291500	0.69735700
Cl	3.73265700	-3.74415300	-0.07057900
Cl	3.71663600	3.75999400	-0.07072400
Cl	-3.73265000	3.74411900	-0.07057500
Cl	-3.71664800	-3.75994800	-0.07067100

Cartesian coordinates of the DFT optimized structure $[1\text{-HH}]^{2+}$ in the gas phase

C	1.15715600	2.88728300	-0.23505800
C	0.70942800	4.15468000	-0.72322200
C	-0.67288500	4.16071900	-0.72329500
C	-1.13171100	2.89735700	-0.23495200
N	0.00932500	2.11744700	0.02125700
C	2.46851600	2.44682900	-0.00010600
C	-2.44688600	2.46854600	0.00012500
C	-2.88728900	1.15717300	0.23513800
C	-4.15470300	0.70945400	0.72324300
C	-4.16079800	-0.67287000	0.72319500
C	-2.89736800	-1.13171300	0.23508500
N	-2.11744700	0.00932300	-0.02111000
C	-2.46852900	-2.44690300	0.00003000
C	-1.15717200	-2.88727700	-0.23501100
C	-0.70946900	-4.15462200	-0.72335000
C	0.67284400	-4.16077500	-0.72317600
C	1.13169500	-2.89736200	-0.23500600
N	-0.00932200	-2.11744600	0.02125000
C	2.44687300	-2.46847100	-0.00001200
C	2.88729100	-1.15715200	0.23501000
C	4.15471200	-0.70943800	0.72317500
C	4.16081000	0.67285300	0.72312100
C	2.89737100	1.13169100	0.23495400
N	2.11743200	-0.00932300	-0.02115300
H	1.35793900	4.94972400	-1.05750800
H	-1.31437900	4.96139400	-1.05768500
H	0.00604100	1.37387600	0.70766900
H	-4.94976400	1.35793700	1.05754100
H	-4.96155000	-1.31433600	1.05744900
H	-1.35797800	-4.94960600	-1.05778500
H	1.31433800	-4.96151000	-1.05741500
H	-0.00607700	-1.37387100	0.70765900
H	4.94976200	-1.35795000	1.05745200
H	4.96155200	1.31434800	1.05735100
H	1.37362400	-0.00605800	-0.70729100
H	-1.37380600	0.00605800	-0.70744300
Cl	3.71191400	-3.74472000	0.00012000
Cl	-3.74471400	-3.71190300	-0.00014700
Cl	-3.71188300	3.74473400	0.00002400
Cl	3.74474600	3.71188800	-0.00005900

Cartesian coordinates of the DFT optimized structure of *p*-toluenesulfonic acid (TsOH) in the gas phase

C	-2.70639100	0.00323200	0.01153100
C	-1.98945400	1.21451900	-0.01436600
C	-0.59055900	1.22731600	-0.06625800
C	0.06356100	0.00104800	-0.08928500
C	-0.59327000	-1.22559600	-0.06585800
C	-1.99039300	-1.21080700	-0.01450300
H	-2.52700300	2.15740900	0.00561000
H	-0.03167000	2.15588800	-0.09389400
H	-0.03504600	-2.15457100	-0.09319800
H	-2.52953400	-2.15317200	0.00517100
C	-4.21766700	-0.00153700	0.04661300
H	-4.61491800	0.98190600	0.31519000
H	-4.63149400	-0.27061900	-0.93432300
H	-4.59733000	-0.73077500	0.77115400
S	1.92056700	-0.00065400	-0.14691400
O	2.49143300	1.40635000	-0.72948000
O	2.48835300	-1.40934400	-0.72839600
O	2.17480600	-0.00007200	1.66747600
H	3.14622500	-0.00013000	1.85086500

Cartesian coordinates of the DFT optimized structure of tosylate (TsO^-) in the gas phase

C	-2.68689900	-0.00053100	-0.00000200
C	-1.96233400	-1.21002400	-0.00000300
C	-0.56315200	-1.21004900	0.00000900
C	0.11218400	0.00904500	-0.00000800
C	-0.56754900	1.22035200	-0.00001500
C	-1.97172600	1.20918700	0.00001300
H	-2.49915400	-2.15672900	0.00001100
H	0.00065100	-2.13690300	0.00002500
H	0.00748700	2.14082400	-0.00000400
H	-2.51521200	2.15177400	0.00002000
C	-4.20256300	-0.01183700	-0.00000500
H	-4.60078100	-0.52821000	-0.88413600
H	-4.60079200	-0.52840700	0.88400500
H	-4.60518800	1.00743700	0.00011100
S	2.00583100	0.00433500	-0.00001100
O	2.41758300	-0.81555100	-1.39042200
O	2.41756900	-0.81561400	1.39039900
O	2.38633900	1.62416400	0.00004900

Cartesian coordinates of the DFT optimized structure of acetic acid (AcOH) in the gas phase

C	-0.07469800	0.13141800	-0.00007000
O	-0.61797500	1.23976300	0.00001000
C	1.39726400	-0.14320700	-0.00001000
H	1.66955000	-0.73161100	0.88256100
H	1.66944800	-0.73284900	-0.88174500
H	1.94500000	0.79925600	-0.00055300
O	-0.81248000	-1.04153700	-0.00000400
H	-1.77575100	-0.84987200	0.00016800

Cartesian coordinates of the DFT optimized structure of acetate (AcO^-) in the gas phase

C	0.19443700	0.00071300	-0.00002400
O	0.80637500	-1.13131900	-0.00000800
C	-1.35903900	-0.04379300	0.00003300
H	-1.74257600	0.48128500	0.88575800
H	-1.74272700	0.48243400	-0.88493600
H	-1.72137600	-1.07753900	-0.00057200
O	0.71791200	1.17785700	-0.00003000

Cartesian coordinates of the solvated DFT optimized structure [1] in THF

C	-1.13633000	2.91143200	-0.00019300
C	-0.68783000	4.27783000	-0.00038400
C	0.68781100	4.27783300	-0.00035100
C	1.13631700	2.91143700	-0.00019000
N	-0.00000500	2.11601900	-0.00031100
C	-2.44407200	2.42444700	-0.00008400
C	2.44406100	2.42445800	-0.00008300
C	2.89675000	1.10114800	0.00017400
C	4.29631900	0.68093900	0.00048600
C	4.29632100	-0.68092900	0.00043100
C	2.89673900	-1.10112800	0.00020700
N	2.05481800	0.00000500	0.00074800
C	2.44406900	-2.42443600	-0.00002200
C	1.13632300	-2.91142700	-0.00012300
C	0.68782900	-4.27783800	-0.00031500
C	-0.68781000	-4.27784100	-0.00026100
C	-1.13631000	-2.91143200	-0.00009700
N	0.00000500	-2.11602700	-0.00030300
C	-2.44405800	-2.42444700	0.00002600
C	-2.89673400	-1.10114100	0.00023200
C	-4.29631800	-0.68094800	0.00046700
C	-4.29632300	0.68092000	0.00046900
C	-2.89675500	1.10113600	0.00017600
N	-2.05481800	-0.00000400	0.00071100
H	-1.33498700	5.13925500	-0.00046100
H	1.33496400	5.13926100	-0.00040400
H	-0.00000200	1.10188000	-0.00040900
H	5.15215800	1.33697500	0.00050300
H	5.15216300	-1.33696200	0.00041300
H	1.33500800	-5.13924500	-0.00039400
H	-1.33498500	-5.13925100	-0.00029900
H	0.00000200	-1.10188700	-0.00045000
H	-5.15215700	-1.33698500	0.00047900
H	-5.15216500	1.33695200	0.00047300
Cl	3.74161100	-3.72156600	-0.00014000
Cl	-3.74159400	-3.72158300	-0.00002600
Cl	-3.74161000	3.72156500	-0.00018900
Cl	3.74159400	3.72158100	-0.00015900

Cartesian coordinates of the solvated DFT optimized structure [1] $^{-}$ in THF

C	-1.13944200	-2.94259700	0.00002800
C	-0.69833900	-4.29179500	0.00005900
C	0.70005400	-4.29151900	0.00004300
C	1.14062300	-2.94214500	0.00002800
N	0.00043200	-2.14443400	0.00013500
C	-2.45636100	-2.42474700	-0.00000100
C	2.45733500	-2.42377000	-0.00000100
C	2.89912200	-1.10898500	-0.00000900
C	4.30163500	-0.67888200	-0.00004700
C	4.30136500	0.68059200	-0.00003100
C	2.89868600	1.11014200	-0.00001200
N	2.05324700	0.00040500	-0.00004200
C	2.45636100	2.42474100	0.00000900
C	1.13944300	2.94260000	0.00000500
C	0.69834000	4.29179400	0.00000400
C	-0.70005500	4.29151800	0.00002000
C	-1.14062400	2.94214800	0.00000400
N	-0.00043200	2.14443700	-0.00005100
C	-2.45733400	2.42376500	0.00000700
C	-2.89913200	1.10898800	-0.00002200
C	-4.30163800	0.67887300	-0.00002700
C	-4.30136200	-0.68060100	-0.00007200
C	-2.89867600	-1.11013900	-0.00001700
N	-2.05324800	-0.00040900	-0.00006800
H	-1.34244300	-5.15592100	0.00005700
H	1.34450000	-5.15539000	0.00002900
H	0.00023100	-1.12974000	0.00021500
H	5.15885300	-1.33424300	-0.00006100
H	5.15832100	1.33629500	-0.00003300
H	1.34244300	5.15592000	0.00001200
H	-1.34450000	5.15538900	0.00003800
H	-0.00023100	1.12974300	-0.00009200
H	-5.15885800	1.33423100	-0.00001400
H	-5.15831500	-1.33630700	-0.00009200
Cl	-3.76665700	3.73222600	0.00005500
Cl	-3.76516200	-3.73371800	-0.00003200
Cl	3.76665500	-3.73222100	-0.00004200
Cl	3.76516400	3.73372100	0.00003700

Cartesian coordinates of the solvated DFT optimized structure $[1]^{2-}$ in THF

C	1.19229600	-2.95723900	0.00002200
C	0.78042500	-4.30035300	0.00001700
C	-0.64066900	-4.32326600	0.00002100
C	-1.09563600	-2.99421400	0.00002700
N	0.03540000	-2.17599000	0.00005800
C	2.50755400	-2.38651600	0.00000500
C	-2.42863900	-2.46624400	0.00001300
C	-2.87992900	-1.16455700	0.00000200
C	-4.29160000	-0.74891400	-0.00002400
C	-4.31378300	0.60940200	-0.00005600
C	-2.91639100	1.07087000	0.00000800
N	-2.04856000	-0.03302300	0.00000200
C	-2.50755400	2.38651600	0.00001100
C	-1.19229600	2.95723900	0.00005400
C	-0.78042500	4.30035300	0.00006200
C	0.64066900	4.32326600	0.00004500
C	1.09563600	2.99421400	0.00005700
N	-0.03540000	2.17599000	0.00020900
C	2.42863900	2.46624400	0.00001900
C	2.87992900	1.16455700	0.00002100
C	4.29160000	0.74891400	-0.00005500
C	4.31378300	-0.60940200	-0.00001000
C	2.91639100	-1.07087000	0.00000600
N	2.04856000	0.03302300	0.00002100
H	1.43690200	-5.15607800	0.00000100
H	-1.26921700	-5.19966300	0.00000800
H	0.01909500	-1.16024900	0.00008600
H	-5.13977000	-1.41748200	-0.00003600
H	-5.18340000	1.24979900	-0.00009100
H	-1.43690200	5.15607800	0.00003200
H	1.26921700	5.19966300	0.00000300
H	-0.01909500	1.16024900	0.00033100
H	5.13977000	1.41748200	-0.00009800
H	5.18340000	-1.24979900	-0.00002400
Cl	-3.85181300	3.68494100	-0.00008400
Cl	3.73079900	3.80686600	-0.00009300
Cl	3.85181300	-3.68494100	-0.00003500
Cl	-3.73079900	-3.80686600	-0.00000800

Cartesian coordinates of the solvated DFT optimized structure [1-H] in THF

C	-1.14242700	-2.93112800	0.10564600
C	-0.69930200	-4.16214900	0.62716400
C	0.70501200	-4.16124000	0.62693800
C	1.14636700	-2.92959200	0.10543500
N	0.00142200	-2.17810300	-0.20441300
C	-2.46676900	-2.44313600	-0.06194800
C	2.47003800	-2.43981900	-0.06248800
C	2.92176800	-1.13676000	-0.14909600
C	4.28189300	-0.67028500	-0.33630800
C	4.28810700	0.69876700	-0.28977700
C	2.93419400	1.15737200	-0.08438300
N	2.13591600	0.01280500	-0.01952100
C	2.44202000	2.44281300	0.03631800
C	1.10329300	2.89283900	0.14960900
C	0.68437600	4.27128700	0.26439300
C	-0.69014700	4.27039900	0.26409100
C	-1.10722700	2.89140600	0.14921800
N	-0.00141300	2.04691600	0.10015300
C	-2.44528100	2.43960800	0.03560000
C	-2.93570700	1.15346700	-0.08489900
C	-4.28903600	0.69299800	-0.28988200
C	-4.28101500	-0.67607400	-0.33571400
C	-2.92021900	-1.14066300	-0.14888800
N	-2.13585200	0.01000700	-0.01999000
H	-1.34117400	-4.94532600	0.99719800
H	1.34802000	-4.94360100	0.99674000
H	0.00088800	-1.46136100	-0.91893800
H	5.13064500	-1.31748600	-0.48537400
H	5.14410000	1.34539100	-0.39490100
H	1.15359900	0.08014400	0.20759100
H	1.33604900	5.12828500	0.32718000
H	-1.34296700	5.12654100	0.32661000
H	-5.14594700	1.33842700	-0.39489300
H	-5.12897000	-1.32445200	-0.48414900
H	-1.15344600	0.07890200	0.20633800
Cl	-3.72816400	3.75608600	0.01204800
Cl	3.72314700	3.76100100	0.01336600
Cl	3.75835300	-3.74627900	-0.08698400
Cl	-3.75339300	-3.75124900	-0.08567500

Cartesian coordinates of the solvated DFT optimized structure [1-H]$^-$ in THF

C	-1.14897800	-2.92242200	0.20970200
C	-0.71454900	-4.01568900	0.96128300
C	0.70852200	-4.01681000	0.96116500
C	1.14455000	-2.92412300	0.20966300
N	-0.00173200	-2.25953300	-0.24750400
C	-2.47943700	-2.44125800	-0.07005300
C	2.47572200	-2.44494600	-0.07012800
C	2.92727700	-1.15752500	-0.17094500
C	4.28612000	-0.67802300	-0.41184900
C	4.29348500	0.68662800	-0.35445600
C	2.94515200	1.15731700	-0.09740400
N	2.14621700	-0.00113000	-0.01115900
C	2.45805200	2.42774700	0.04178900
C	1.11176500	2.90106500	0.19580300
C	0.70098700	4.25387700	0.37925300
C	-0.69460300	4.25488400	0.37934400
C	-1.10736000	2.90270700	0.19566400
N	0.00158500	2.05863500	0.10074700
C	-2.45434300	2.43139500	0.04154900
C	-2.94334600	1.16170600	-0.09773700
C	-4.29240300	0.69305700	-0.35472100
C	-4.28713500	-0.67161000	-0.41194000
C	-2.92901200	-1.15316000	-0.17107400
N	-2.14611700	0.00206300	-0.01178800
H	-1.35840000	-4.71697800	1.46959400
H	1.35134800	-4.71909800	1.46939200
H	-0.00128000	-1.60737500	-1.01927700
H	5.13054000	-1.32471300	-0.58938800
H	5.14819800	1.33243600	-0.48094500
H	1.16229200	0.06281800	0.20432300
H	1.34959200	5.11091400	0.48101500
H	-1.34195700	5.11286000	0.48116500
H	-5.14615100	1.34015400	-0.48114500
H	-5.13256400	-1.31703300	-0.58928700
H	-1.16200100	0.06454600	0.20325300
Cl	3.74855200	-3.78761500	-0.21510500
Cl	3.74430300	3.76415200	-0.02484900
Cl	-3.73862000	3.76970900	-0.02486900
Cl	-3.75435600	-3.78199100	-0.21460200

Cartesian coordinates of the solvated DFT optimized structure [1-HH] in THF

C	1.05567700	-2.91327900	0.31949700
C	0.59419200	-3.99217500	1.08148300
C	-0.82282300	-3.94759500	1.09761900
C	-1.23199700	-2.84109600	0.34555400
N	-0.07227500	-2.21044600	-0.11634700
C	2.39473800	-2.51024200	-0.03330000
C	-2.54803400	-2.35668600	0.01111100
C	-2.94976600	-1.07055600	-0.20203700
C	-4.22599400	-0.55615200	-0.68092500
C	-4.18254600	0.80627100	-0.69745200
C	-2.87650600	1.24911400	-0.22754900
N	-2.13588300	0.06758400	0.02224200
C	-2.39474900	2.51011500	-0.03242400
C	-1.05568800	2.91327100	0.32007200
C	-0.59413200	3.99331500	1.08041600
C	0.82285700	3.94871600	1.09659600
C	1.23201300	2.84106600	0.34619100
N	0.07224400	2.20964300	-0.11459500
C	2.54804900	2.35654300	0.01206400
C	2.94981200	1.07045400	-0.20139600
C	4.22600500	0.55625400	-0.68058100
C	4.18252300	-0.80615900	-0.69780300
C	2.87651000	-1.24920200	-0.22798600
N	2.13594700	-0.06776300	0.02247100
H	1.22059000	-4.71814200	1.57627700
H	-1.48204900	-4.63396700	1.60599800
H	-0.06298000	-1.53025500	-0.86307700
H	-5.05180600	-1.18079300	-0.98329100
H	-4.96748500	1.47454800	-1.01493800
H	-1.22048200	4.72011600	1.57403400
H	1.48210300	4.63590900	1.60382700
H	0.06291000	1.52826100	-0.86022000
H	5.05180300	1.18102200	-0.98272300
H	4.96741100	-1.47430200	-1.01569500
H	1.36544300	-0.05435800	0.67470200
H	-1.36530100	0.05384700	0.67437300
Cl	3.82947200	3.67114000	-0.14825300
Cl	3.58676800	-3.90166000	-0.23008500
Cl	-3.82936700	-3.67134000	-0.14972500
Cl	-3.58694600	3.90145600	-0.22844100

Cartesian coordinates of the solvated DFT optimized structure [1-HH]$^+$ in THF

C	-1.38202500	2.78763000	0.26507300
C	-1.03866000	4.04566900	0.81125900
C	0.35406600	4.16484000	0.79444300
C	0.89339600	2.98209700	0.23822700
N	-0.18405000	2.13915400	-0.05834700
C	-2.66257200	2.22517800	0.01892100
C	2.24691400	2.64202300	-0.02707900
C	2.79797500	1.39010000	-0.21437200
C	4.12237700	1.03212700	-0.66558600
C	4.24017700	-0.33284100	-0.64802800
C	2.99496100	-0.90097000	-0.18740900
N	2.12132900	0.18073200	0.03915000
C	2.66257200	-2.22517800	0.01892800
C	1.38202400	-2.78763100	0.26507300
C	1.03865600	-4.04567100	0.81125400
C	-0.35407100	-4.16484100	0.79442800
C	-0.89339700	-2.98209800	0.23821000
N	0.18405000	-2.13915400	-0.05835400
C	-2.24691400	-2.64202300	-0.02710300
C	-2.79797400	-1.39009900	-0.21439400
C	-4.12237300	-1.03212400	-0.66561400
C	-4.24017400	0.33284300	-0.64805000
C	-2.99495900	0.90097100	-0.18742200
N	-2.12133100	-0.18073300	0.03913800
H	-1.74237600	4.76770700	1.19282400
H	0.93387900	4.99634400	1.16128200
H	-0.13021200	1.38725200	-0.73308100
H	4.86788700	1.74164600	-0.98678100
H	5.09660700	-0.91234800	-0.95314100
H	1.74236800	-4.76770900	1.19282300
H	-0.93388600	-4.99634600	1.16126300
H	0.13022000	-1.38725500	-0.73309300
H	-4.86788100	-1.74164300	-0.98681700
H	-5.09660200	0.91235200	-0.95316500
H	-1.36614400	-0.12571100	0.70995900
H	1.36615200	0.12570900	0.70998400
Cl	4.03377300	-3.42410700	-0.03178400
Cl	3.39220900	4.05629000	-0.11930400
Cl	-4.03377300	3.42410600	-0.03179200
Cl	-3.39220800	-4.05629000	-0.11933900

Cartesian coordinates of the solvated DFT optimized structure $[1\text{-HH}]^{2+}$ in THF

C	-0.81453200	-2.99612000	-0.23096500
C	-0.22667200	-4.19820700	-0.74162100
C	1.14418200	-4.04753000	-0.73525600
C	1.45173400	-2.74649800	-0.22122400
N	0.23416000	-2.11592000	0.05447900
C	-2.16570200	-2.70460400	-0.00915600
C	2.70465700	-2.16576300	0.00959500
C	2.99603600	-0.81458900	0.23164600
C	4.19859800	-0.22661400	0.74110500
C	4.04787300	1.14421200	0.73467300
C	2.74634300	1.45165600	0.22176400
N	2.11550200	0.23403300	-0.05294100
C	2.16572000	2.70460000	-0.00929900
C	0.81455300	2.99613900	-0.23106800
C	0.22663300	4.19829400	-0.74149300
C	-1.14422200	4.04761000	-0.73499300
C	-1.45172000	2.74650700	-0.22109400
N	-0.23410800	2.11589100	0.05437200
C	-2.70463400	2.16574400	0.00975800
C	-2.99601400	0.81457400	0.23177900
C	-4.19871100	0.22658300	0.74094900
C	-4.04800200	-1.14423900	0.73452500
C	-2.74634200	-1.45167500	0.22193000
N	-2.11543400	-0.23404900	-0.05256100
H	-0.78257500	-5.04980400	-1.09885600
H	1.87481300	-4.75797600	-1.08664900
H	0.14920900	-1.37241900	0.73618900
H	5.05060500	-0.78244600	1.09746600
H	4.75867800	1.87493500	1.08513800
H	0.78249000	5.04995500	-1.09864300
H	-1.87489500	4.75811000	-1.08618800
H	-0.14901600	1.37236400	0.73604500
H	-5.05082100	0.78241000	1.09706600
H	-4.75891700	-1.87497200	1.08474600
H	-1.37010100	-0.14897200	-0.73221200
H	1.37057500	0.14890500	-0.73306500
Cl	-4.11379600	3.29528900	0.02052200
Cl	3.29554100	4.11352600	-0.02140200
Cl	4.11381300	-3.29530900	0.02033600
Cl	-3.29553200	-4.11352000	-0.02144600

Cartesian coordinates of the solvated DFT optimized structure of *p*-toluenesulfonic acid (TsOH) in THF

C	-2.71175200	0.00000200	-0.01491500
C	-1.99502100	-1.21358300	0.00809400
C	-0.59717200	-1.22893300	0.05809300
C	0.05631800	0.00001200	0.08211600
C	-0.59717600	1.22894900	0.05808200
C	-1.99502900	1.21358700	0.00808400
H	-2.53181500	-2.15637900	-0.01249900
H	-0.04590200	-2.16153600	0.08129600
H	-0.04590800	2.16155300	0.08127600
H	-2.53182600	2.15638100	-0.01251700
C	-4.22166100	-0.00001200	-0.03747800
H	-4.61351900	-0.88776400	-0.54331300
H	-4.62281300	-0.00021900	0.98502900
H	-4.61354500	0.88792300	-0.54297100
S	1.91247200	-0.00001000	0.14078600
O	2.49950100	-1.39848900	0.74115100
O	2.49949500	1.39837400	0.74138100
O	2.20107400	0.00009200	-1.65993000
H	3.17418600	0.00023600	-1.84215400

Cartesian coordinates of the solvated DFT optimized structure of tosylate (TsO^-) in THF

C	-2.69346900	0.00223700	0.01069000
C	-1.97195900	-1.20857800	0.00066600
C	-0.57244500	-1.21562400	-0.02082300
C	0.09836800	0.00554500	-0.03773600
C	-0.57342200	1.22375300	-0.02103000
C	-1.97538500	1.21257200	0.00113700
H	-2.50797100	-2.15345100	0.01046600
H	-0.01795500	-2.14698600	-0.03550900
H	-0.02088100	2.15625800	-0.03475800
H	-2.51359100	2.15590000	0.01158600
C	-4.20623400	-0.00522100	0.01432900
H	-4.60076700	-0.28292500	-0.97224900
H	-4.59955900	-0.73014900	0.73624400
H	-4.60905500	0.98044500	0.26712800
S	1.97633500	0.00020700	-0.00058300
O	2.44518600	-1.34834000	-0.86105700
O	2.43240300	-0.09602100	1.60551300
O	2.44937100	1.43554700	-0.70157700

Cartesian coordinates of the DFT optimized structure of acetic acid (AcOH) in THF

C	-0.07469800	0.13141800	-0.00007000
O	-0.61797500	1.23976300	0.00001000
C	1.39726400	-0.14320700	-0.00001000
H	1.66955000	-0.73161100	0.88256100
H	1.66944800	-0.73284900	-0.88174500
H	1.94500000	0.79925600	-0.00055300
O	-0.81248000	-1.04153700	-0.00000400
H	-1.77575100	-0.84987200	0.00016800

Cartesian coordinates of the DFT optimized structure of acetate (AcO^-) in THF

C	0.19443700	0.00071300	-0.00002400
O	0.80637500	-1.13131900	-0.00000800
C	-1.35903900	-0.04379300	0.00003300
H	-1.74257600	0.48128500	0.88575800
H	-1.74272700	0.48243400	-0.88493600
H	-1.72137600	-1.07753900	-0.00057200
O	0.71791200	1.17785700	-0.00003000

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