Supporting Information

Developing Post-Modified Ce-MOF as Photocatalyst: A Detail Mechanistic insight of CO$_2$ Reduction towards Selective C2 Product Formation

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Experimental section:

Materials: All the reagents were commercially available and used as such without further purification. Ammonium cerium (IV) nitrate [$(NH_4)_2Ce(NO_3)_6$], purity $\geq$ 98.%, 2,2′ Bipyridine-5,5′-dicarboxylic acid were purchased from TCI chemicals. Ruthenium chloride ($RuCl_3 \cdot 3H_2O$) and 2,2′-bipyridine were purchased from Sigma-Aldrich Chemical Co. Ltd. N,N′ Dimethylformamide (DMF) and anhydrous acetone were purchased from Spectrochem Pvt. Ltd. All the photophysical studies were carried out using HPLC grade solvents. $^{13}CO_2$ cylinder was purchased from Sigma-Aldrich Chemical Co. Ltd.

Methods

Physical measurement:

Elemental analyses were performed in Thermo Scientific Flash 2000 CHN analyzer. Bruker FT-IR spectrometer was used to record infrared spectra. Samples were prepared as pellets using KBr for IR measurement. ^1H NMR spectra were recorded on Bruker AVANCE-400 spectrometer (at 400 MHz) with chemical shifts recorded as ppm, and all spectra were calibrated against TMS. Mettler Toledo-TGA 850 instrument was used to measure the thermal stability in N_2 atmosphere within the temperature range 30-800 °C at a heating rate of 5 °C/min. Powder X-ray diffraction patterns for all the MOFs were recorded in Bruker D8 discover instrument using Cu-K_α radiation. Morphological studies have been carried out using Bruker Leica-S440I Field Emission Scanning Electron Microscope (FE-SEM) by placing samples on a silicon wafer under a high vacuum with an accelerating voltage of 100 kV. Transmission Electron Microscopy (TEM) analysis has been performed using JEOL JEM-3010 with an accelerating voltage at 300 kV. N_2 adsorption measurements were carried out at 77 K in a QUANTACHROME QUADRASORD-SI analyzer. Samples were degassed at 100 °C and 1×10^{-1} Pa vacuum for 12 h before performing adsorption isotherm measurement. UV-vis studies were performed in solid state using Perkin Elmer Model Lambda 900 spectrophotometer instrument. The photoluminescence properties were performed in Fluorolog 3.21 spectrofluorimeter (Horiba Jobin-Yvon) instrument. The photoluminescence (PL) quantum yield was determined by an absolute method using the same fluorescence spectrometer equipped with a 120 mm integrating sphere with BENFLEC

coated inner face (Horiba Instruments). Fluorescence decay profiles were recorded using a Horiba Delta Flex time correlated single-photon-counting (TCSPC) instrument. A 405 nm laser diode with a pulse repetition rate of 1 MHz was used as the light source. The instrument response function (IRF) was collected using a scatterer (Ludox AS40 colloidal silica, Sigma-Aldrich).

XAS experiment:

XAS experiments at 300 K were performed at PETRA III, beamline P64, of DESY, Germany. Measurements of Ce-L3 edge and Ru K-edge were performed at ambient pressure in fluorescence as well as transmission mode using gas ionization chambers to monitor the incident and transmitted X-ray intensities. Monochromatic X-rays were obtained using a Si (111) double crystal monochromator which was calibrated by defining the inflexion point (first derivative maxima) of Ce foil as 5723 eV and Ru foil as 22117 eV. The beam was focused by employing a Kirkpatrick-Baez (K-B) mirror optic. Rhodium-coated X-ray mirror was used to suppress higher-order harmonics. A CCD detector was used to record the transmitted signals. Pellets for the ex-situ measurements were made by homogeneously mixing the sample with an inert boronitride matrix to obtain an X-ray absorption edge jump close to one. X-ray absorption near edge spectra (XANES) of the XAS spectrum were obtained by subtracting the pre-edge background from the overall absorption and normalizing to the spline fit using ATHENA software package. The k^2 -weighted extended X-ray absorption fine structure (EXAFS) was Fourier transformed over the limited range of k from 3 to 14 Å^{-1}.

The normalized, energy-calibrated Ce L$_3$-edge and Ru K-edge XANES spectra were obtained using standard data reduction techniques with Athena and Artemis software. The concentration of Ce^{3+} in both samples (**Ce-MOF** and **Ce-MOF-Ru^{II}-bpy**) was calculated using the following equations:

$$[Ce^{3+}] = A(Ce^{3+})/A(Ce^{3+}) + A(Ce^{3+})$$

Where, A(Ce^{3+}) and A(Ce^{4+}) correspond to the total integrated peak areas of the Ce^{3+} and Ce^{4+} associated peaks, respectively.

The EXAFS oscillations χ(k) as a function of photoelectron wave number k was extracted by following standard procedures. The theoretical paths were generated using FEFF and the

models were completed in a conventional way using a fitting program named Artemis. The theoretical phase and amplitude functions of Ru-N were calculated with FEFF.[1] CIF file was obtained for CCDC (No: 2005064). The values for the amplitude reduction factor (S_0^2) and the mean square disorder (σ^2) were determined by fitting the corresponding cif with FEFF. The EXAFS parameters were obtained by a least-squares fit in the R-space of the k^2-weighted Fourier transform (FT) data. Artemis evaluates a variety of statistical parameters relevant to the evaluation of the fit. For example, E_0 is rarely more than 10 eV or less than -10 eV, that S_0^2 and σ^2 should never be negative. σ^2 value in the range between 0.001 and 0.01 will not be got a penalty. ARTEMIS software thinks any fit which R-factor has 2% or less misfit between data and theory is not assessed a penalty.

TGA-MS:

TGA-MS measurement was carried out by TG-GCMS interface analyzer (PerkinElmer *TL 8500*). 8.2 mg Ce-MOF was heated on a *TL 8500* thermogravimetric analyzer from 30 °C to 650 °C at a rate of 5 °C min^{-1} under N_2 flow of 100 ml /min. The TGA instrument is equipped with a quadrupole mass spectrometer (MS) (Clarus® SQ 8T) to investigate the chemical nature of the species leaving the sample in the TGA run.

Transient absorption.

Transient absorption experiments were performed using an amplified Ti:sapphire laser (800 nm, 60 fs, 1 kHz, 3 mJ) from Amplitude Technologies, France and a pump-probe setup (Excipro) from CDP corporation Russia. For sample excitation, 400 nm laser pulse were generated from 800 nm fundamental light using a BBO crystal. For probing the transient species, a broad band (350–750 nm) pulse was generated by putting small amount of 800 nm laser pulse onto a rotating calcium fluoride plate. The pump and probe pulse was spatially overlapped in the rotating sample cell with 1mm optical path. The time-delay between the pump and probe pulse was maintained with the help of a stepper motor controlled optical delay stage. To get a pump induced changes in the optical absorbance in the sample the repetition rate of pump pulse was modulated to 500 Hz using a mechanical chopper. The probe pulse was dispersed in spectrograph and detected with photodiode array. The instrument response function of the TA set-up was 120 fs. For all TA experiments samples were dispersed in ethylene glycol.

Photocatalytic reaction:

The photocatalytic CO_2 reduction experiments were carried out in a 30 ml stopper vessel with magnetic stirring. 5 mg of the photocatalyst was dispersed in 10 ml water, and then pure CO_2 (99.99%) gas was passed into the reactor containing a well-dispersed solution for 1 h. The reaction mixture was irradiated with a 300 W Xenon lamp (Newport) through a visible bandpass filter (400–800nm) with constant stirring. We have measured the intensity of the light source using a power meter (Newport-843-R). The measured intensity during the catalytic reaction (λ= 400-800) is 99.5 mW/cm^2. (Note: The distance between light source and reactor is 8 cm.).

The gaseous products were analyzed using gas chromatography Mass Spectrometry SHIMADZU GC-2010 PLUS). The amount of products was quantified by using RT® Molecular sieve 5A column (45 m, 0.32 mm ID, 30 μm df) with a mass detector. The calibration was done by a standard gas mixture of H_2, CO, CH_4 of different concentrations in ppm-level. Importantly, GC-MS has a detection limit of 1.0 ppm for H_2, CO and CH_4. After the photocatalysis, the reaction mixture was filtered to remove the residual solid, and the solution was further analyzed to determine the amount of liquid product. 0.6 mL liquid product dispersed in 0.05 mL D_2O was analyzed by NMR spectroscopy (AVANCE-400 spectrometer at 400 MHz) using 50 μL solution of 4 mM DMSO and 20 mM phenol as the external standard. For $^{13}CO_2$ experiment, the reaction mixture was purged with $^{13}CO_2$. The content of H_2O_2 produced during the photocatalytic water splitting was measured by a UV-vis spectrophotometer. In an acidic environment (pH=1–2), Fe^{2+} can be oxidized into Fe^{3+} by H_2O_2, and Fe^{3+} can be combined with KSCN to form $[Fe(SCN)]^{2+}$. $[Fe(SCN)]^{2+}$ has a maximum absorption peak at 447 nm.

Selectivity was calculated by using this equation:

$$Selectivity_{CH3COOH} = \frac{8 * n_{CH3COOH}}{(8 * n_{CH3COOH}) + \left(2 * n_{H_2}\right)} \, x \, 100 \, \%$$

Computational details:

All the calculations are performed using density functional theory (DFT) in Gaussian 16 package of programs.[2] The calculations are performed utilizing B3LYP exchange-correlation functional along with 6-31G(d) basis set for all atoms except for Ru and Ce atoms.[3-8] For Ru

LANL2DZ, which utilizes a widely used effective core potential (ECP)- type basis set is used.[9,10] Whereas for Ce ECP-MWB28 basis set is used.[11] The implicit solvent effect of water is incorporated into all computations by polarisable continuum model (PCM). [12] Grimme's d3 dispersion is also used to tackle weak interactions.[4] The harmonic vibrational frequency analysis of the optimized geometries is performed to confirm the nature of stationary points. All the optimized intermediates revealed the absence of any imaginary vibrational mode, indicating the optimized geometries as minima on the potential energy surface (PES). The electronic absorption spectra are calculated using time-dependent DFT (TDDFT) method using the same level of theory as earlier. All thermochemical data are obtained with the ideal gas-rigid rotor-simple harmonic oscillator approximations at 298.15 K and 1 atm. Zero point-energy corrections are included in the Gibbs free energy values along with a concentration correction for c = 1 mol/ dm^3 condition in the solvent. The pictures of the optimized structures, molecular orbitals and spin density plots are taken from Gauss View 6.0.16. [13]

Electrochemical setup:

The Mott-Schottky and impedance measurement were carried out with a CHI760E workstation (CHI Instruments, USA) *via* a conventional three-electrode system in a 0.2 M Na_2SO_4 aqueous solution.

Preparation of working electrode for Mott-Schottky and impedance measurement: 2.5 mg of **Ce-MOF-Ru^{II}-bpy** was dispersed in a solution of 250 μL water, 250 μL isopropyl alcohol (IPA) and 10 μL of Nafion to prepare a homogenous slurry. Subsequently, 12 μL of the slurry was coated on a glassy carbon electrode and then dried at room temperature. The Ag/AgCl electrode was employed as the reference electrode, and the platinum plate was used as the counter electrode, respectively. During impedance measurement, a white LED lamp (LEICA KL1600 LED) was used for illumination.

Preparation of working electrode for transient photocurrent:

2.5 mg of compound (**Ce-MOF** and **Ce-MOF-Ru^{II}-bpy**) was dispersed in a solution of 250 μL water, 250 μL isopropyl alcohol (IPA) and 10 μL of nafion to prepare a homogenous slurry. Subsequently, 300 μL of the slurry was coated on ITO glass plate (1 cm x 1 cm) and then dried in room temperature. The Ag/AgCl electrode was employed as the reference electrode, and platinum plate was used as the counter electrode, respectively. The transient

photocurrent responses were carried out under visible-light irradiation conditions (300 W Xenon arc lamp).

Spectroelectrochemical set-up for *in-situ* UV-vis spectral changes under visible light irradiation:

In-situ UV-vis spectroscopy was carried out using an ocean optics set-up (Ser No: 057781227). The change of absorption spectra was monitored by dispersing **Ce-MOF-Ru^{II}-bpy** in aqueous medium. During the measurement, sample was irradiated with a visible light source (Leica KL1600 LED), and monitored the intensity change with pre and post-light irradiation. The light illumination time was 10 s before collecting any absorption spectra.
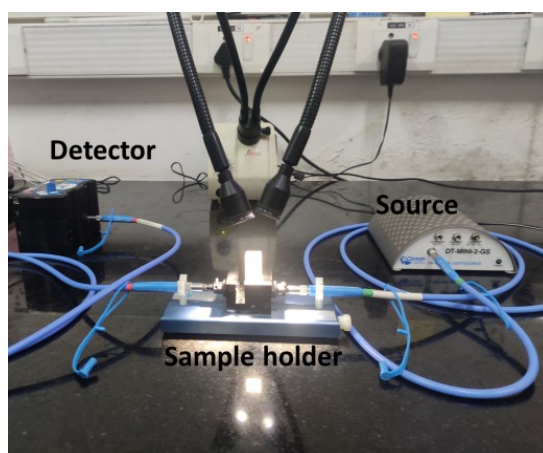
Scheme S1: Photograph of the *in-situ* UV-vis spectroscopy set-up.

Synthesis of Ce-UiO-66-bpydc (Ce-MOF) : Ce-UiO-66-bpydc was prepared by following a slight modification of the reported procedure. 2,2′-Bipyridine-5,5′-dicarboxylic acid (H$_2$bpydc, 52.1 mg, 213 µmol) was introduced into the glass reactor under inert conditions. After the addition of N,N-dimethylformamide (DMF; 1.2 mL), an aqueous solution of cerium(IV) ammonium nitrate [NH$_4$]$_2$[Ce(NO$_3$)$_6$] (400 µL, 0.533 M) was added to the mixture. The glass reactor was sealed and heated under stirring for 15 min at 100 °C. The yellow precipitate was centrifuged in the mother liquor, which was then decanted off before being re-dispersed twice in DMF (2 mL). To remove DMF from the product, the solid was washed afterwards and centrifuged with acetone (2 mL) four times. The resulting white solid was dried in air at 70 °C. Yield: 45 mg (38%).

a

b

14 Å

11 Å

Octahedral cage
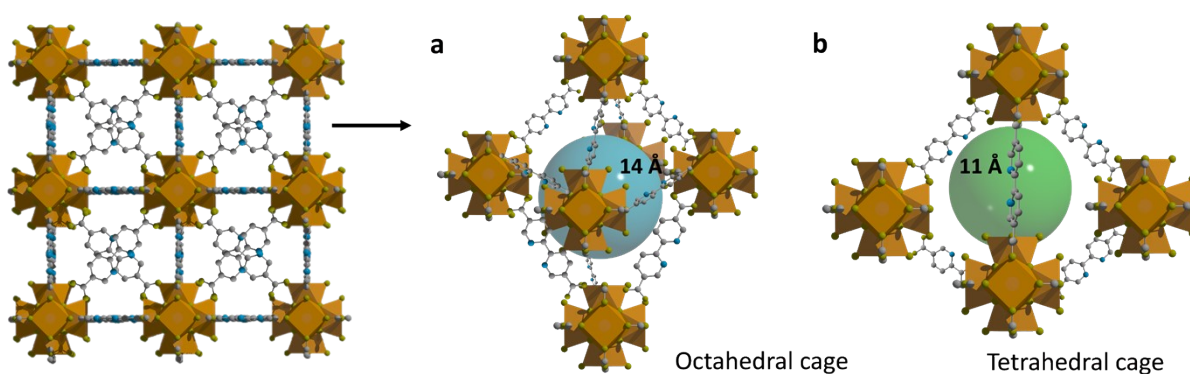
Tetrahedral cage

Fig. S1 Octahedral and tetrahedral cages of **Ce-MOF**.

○ **Yobs**
— **Ycalc**
— **Yobs -Ycalc**
| **Bragg position**

Intensity (a.u.)

10 20 30 40 50 60 70 80

2θ (degree)
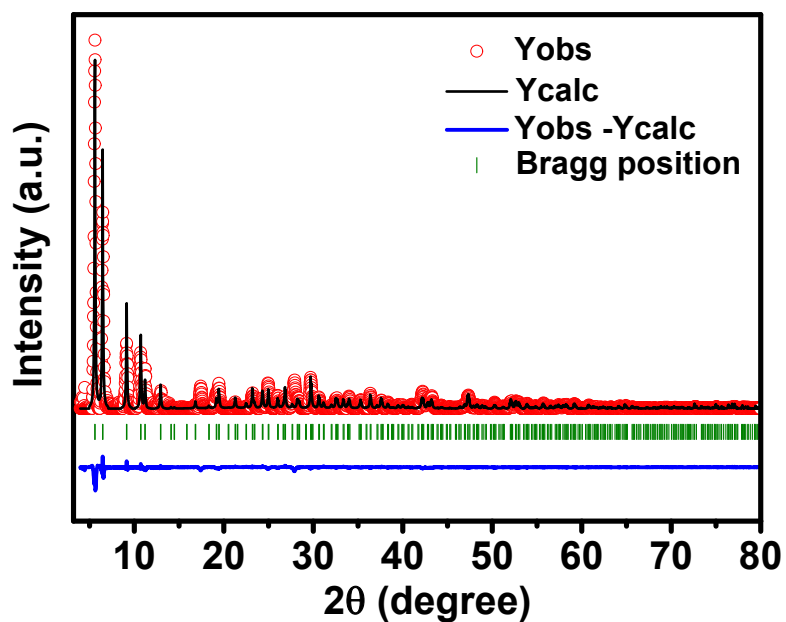
Fig. S2 Le Bail plot of **Ce-MOF**. The observed PXRD pattern (λ= 1.5401 Å) is shown in red, the calculated in black and the difference (observed - calculated) of both patterns is given in blue. The allowed positions of the peaks are given as green tics.

10 nm

1.4 nm
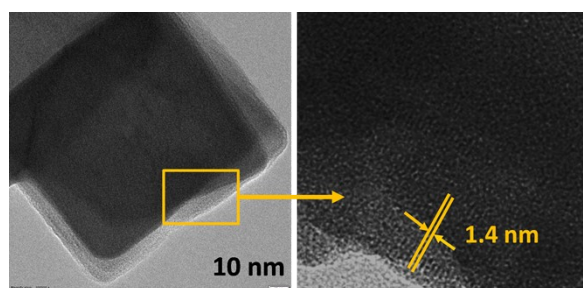
Fig. S3 High-resolution TEM images of **Ce-MOF.**
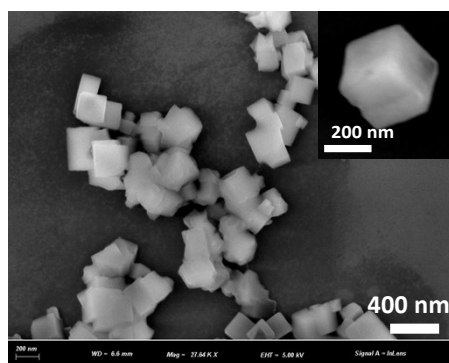
Fig. S4. FESEM images of **Ce-MOF.**
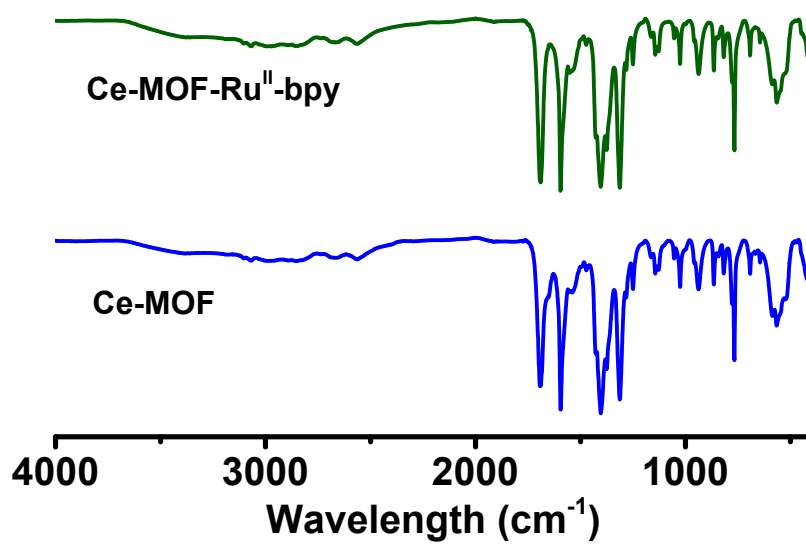
Fig. S5. FT-IR spectra of **Ce-MOF** and **Ce-MOF-Ru^{II}-bpy**.
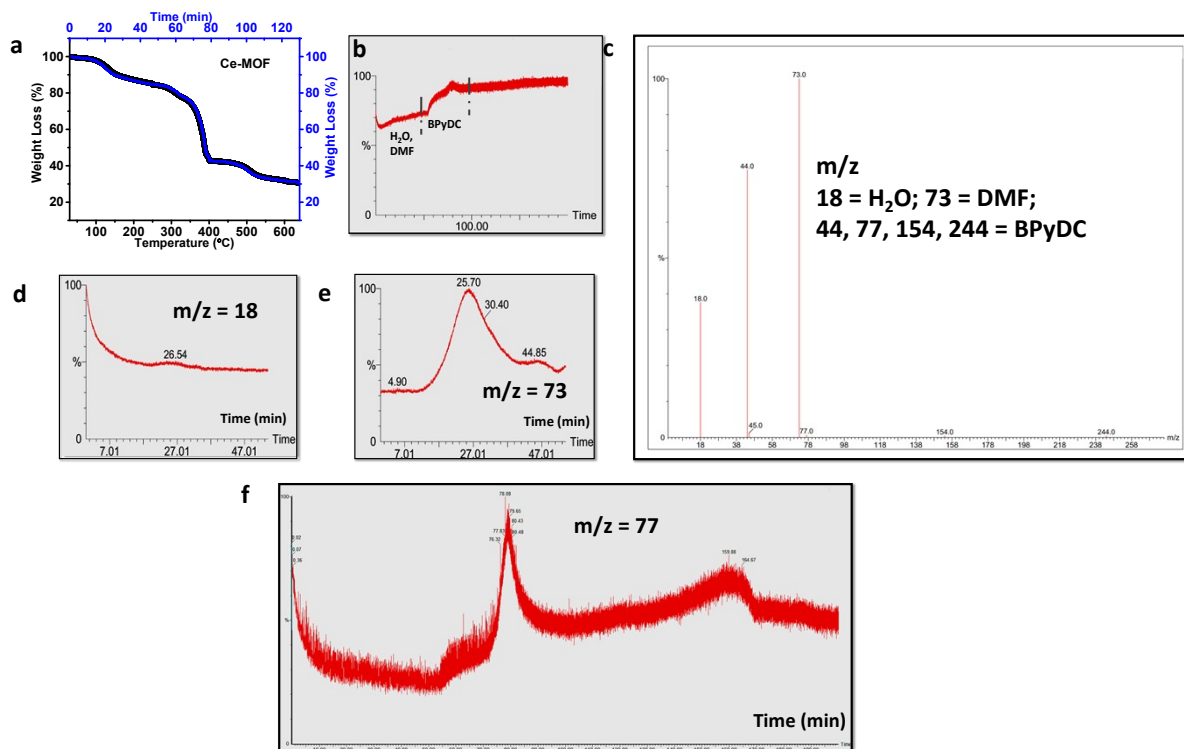
Fig. S6 Missing Linker defect of **Ce-MOF** investigated by TGA-MS. (a) TGA curve of **Ce-MOF** under N_2 atmosphere. (b) Corresponding mass signal of the **Ce-MOF** comes from the fragmentation of the thermogravimetric analysis. (c) m/z values of the **Ce-MOF** comes from the fragmentation of the thermogravimetric analysis. (d) Mass signal of water from TGA of **Ce-MOF**. (e) Mass signal of DMF from TGA of **Ce-MOF**. (f) Mass signal of the pyridine comes from the BPyDC linker of **Ce-MOF**.

Investigating the BpyDC linker weight % from TGA-MS analysis: The % of bpydc linker defect was calculated from the TGA-MS analysis. The weight loss data of **Ce-MOF** was represented with respect to temperature as well as time, and the corresponding mass signal was plotted with respect to time. Increasing temperature from 30 to 300 °C, **Ce-MOF** showed a progressive structural weight loss along with a clear shoulder band at 100 °C. Corresponding mass spectroscopy data suggested the loss of water and DMF molecule inside the MOF pore or coordinated with the Ce_6 cluster.

For defect-free MOF % of bpydc linker $= \dfrac{6 * \text{Molecular weight of bpydc}}{\text{Molecular weight of MOF}} * 100\%$

$= \dfrac{1092.2\ g/mol}{2063.6\ g/mol} * 100\%$

$= 52.92\%$

From the experiment, weight loss observed was about 44.08 % for the bpydc linker from 300-550 °C. Hence the as-synthesized pristine **Ce-MOF** exhibiting a difference of 8.84 wt % corresponds to the bpydc linker. This defect arose from missing linker which is well reported in the literature for UiO-66 architecture. Hence the molecular formula for **Ce-MOF** is $[Ce_6O_5(OH)_3(bpydc)_5(H_2O)_2]$
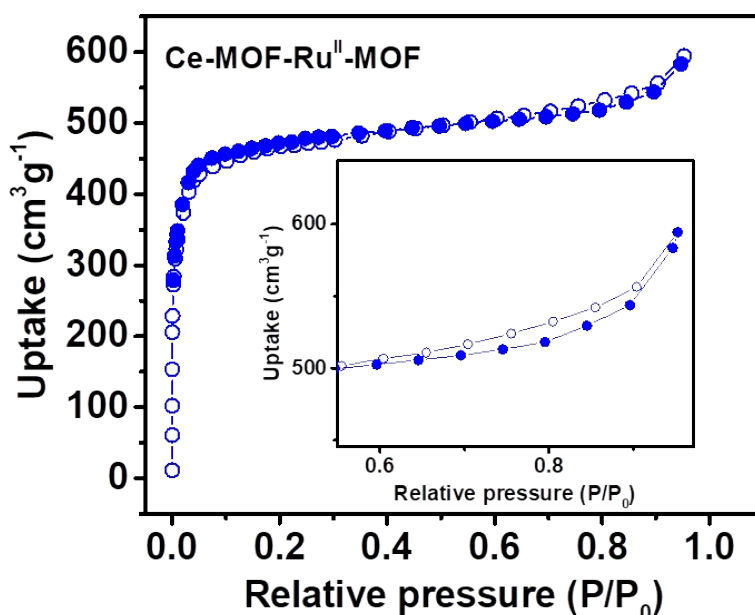
Fig. S7 N_2 adsorption-desorption isotherms of **Ce-MOF-Ru^{II}-MOF**. Inset shows the uptake in the pressure region of P/P_0 0.5 to 1.

Synthesis of [Ru(bpy)$_2$Cl$_2$]: [Ru(bpy)$_2$Cl$_2$] was prepared by following a previously reported literature. RuCl$_3$·3H$_2$O (1.000 g; 8.824 mmol), 2,2′-bipyridine (1.195 g; 7.649 mmol), and LiCl (1.074 g) were refluxed in a reagent grade dry DMF (10 ml) for 8 h with magnetic stirring. The reaction mixture was cooled to room temperature, and reagent grade acetone (30 ml) was added. The reaction mixture was then cooled to 0°C overnight. The mixture was then filtered, yielding a red-violet filtrate and a black crystalline substance. The solid was washed three times with 10 ml portions of water followed by three 10 ml portions of diethyl ether and was subsequently dried by suction (yield: 0.724 g; 39.1%). A high-resolution mass spectrometry was done. The ESI mass spectrum (Fig. S 8) shows the largest peak at 449 m/z, which is exactly 35 a.u. less than the molecular weight of the product, thus it corresponds to [Ru(bpy)$_2$Cl]$^+$ (loss of a Cl atom from the product). This may well have occurred during ionization, at attached Cl ligands are very labile and can be easily ionized. There is a small

peak at 484 m/z, indicating that a small amount of the product was ionized without disturbing the Cl ligands.
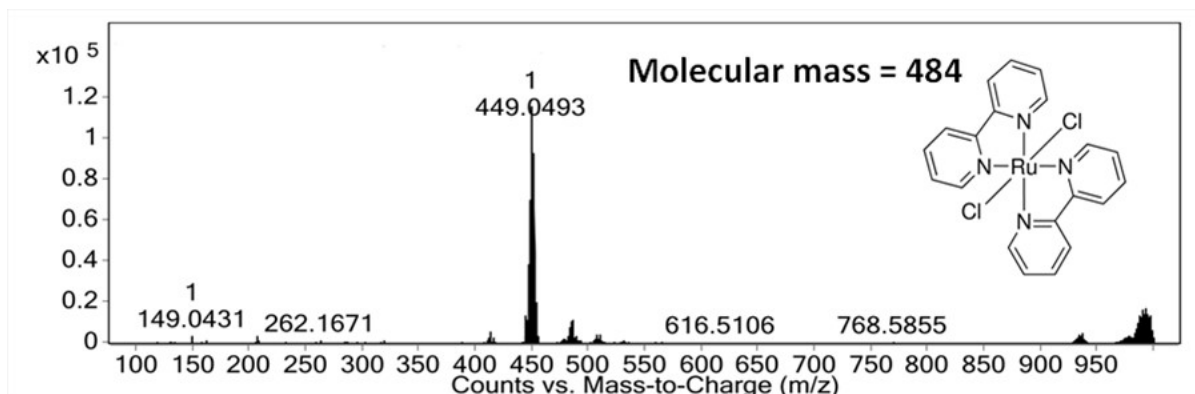
Fig. S8 HRMS of [Ru(bpy)$_2$Cl$_2$].
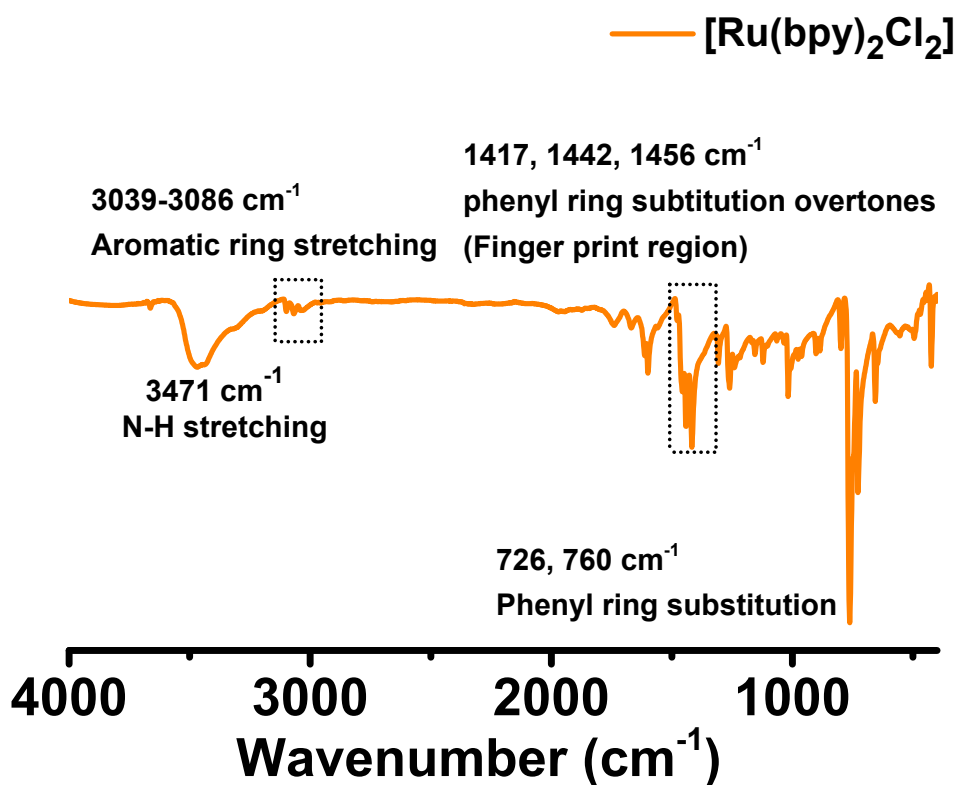
Fig. S9 FT-IR spectra of [Ru(bpy)$_2$Cl$_2$].

Synthesis of Ce-MOF-Ru^{II}-bpy: Ce-MOF (0.050 g) and [Ru(bpy)$_2$Cl$_2$] (2 mg, 3.84 µmol) were mixed in a 10 mL dry ethanol/toluene (1:1) in a schlenk tube. The suspension was heated at 90°C for 24 h. After the reaction, the product was filtered and washed with toluene

and ethanol to remove excess [Ru(bpy)$_2$Cl$_2$], affording orange colour **Ce-MOF-Ru^{II}-bpy**. Yield: 0.099 g.
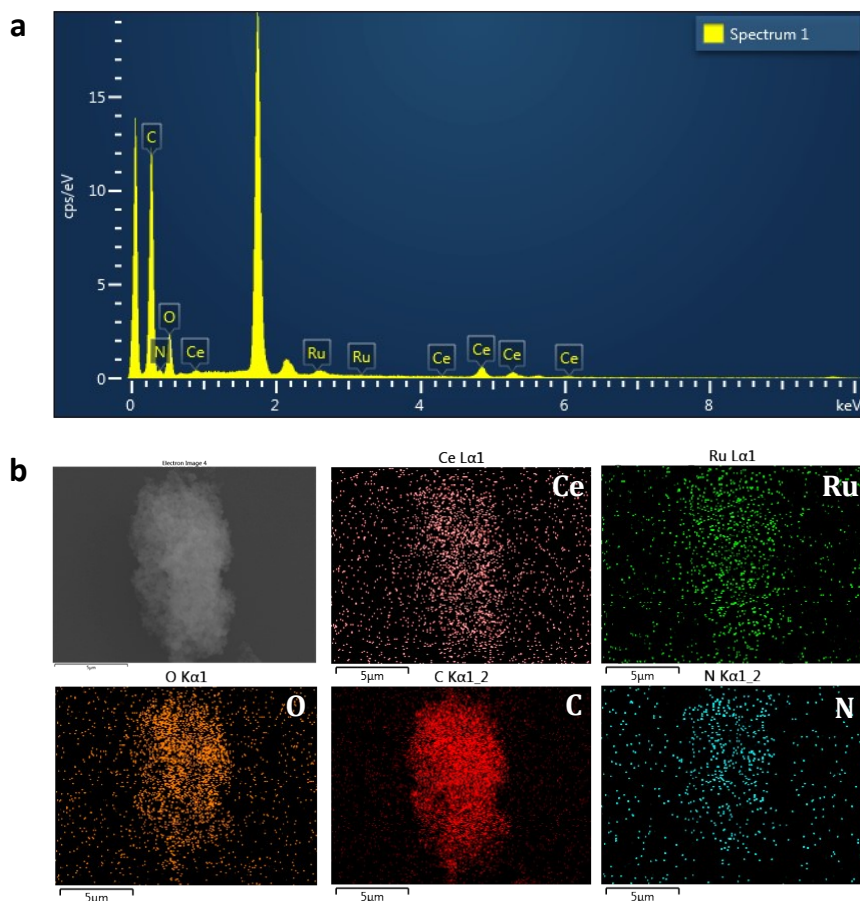
Fig. S9 EDX and elemental mapping of **Ce-MOF-Ru^{II}-bpy**.

Table S1 Table of Element Wt% from EDX analysis of **Ce-MOF-Ru^{II}-bpy**.

Element	Line Type	Apparent Concentration	k Ratio	Wt%	Wt% Sigma	Standard Label	Factory Standard	Standard Calibration Date
C	K series	2.48	0.02480	64.30	2.97	C Vit	Yes	
N	K series	0.05	0.00009	1.64	4.21	BN	Yes	
O	K series	0.98	0.00329	28.81	1.64	SiO2	Yes	

Ru	L series		0.01	0.00014	0.17	0.32	Ru (v)	Yes	
Ce	L series		0.41	0.00381	5.07	0.58	CeO$_2$	Yes	
Total:					100.00				
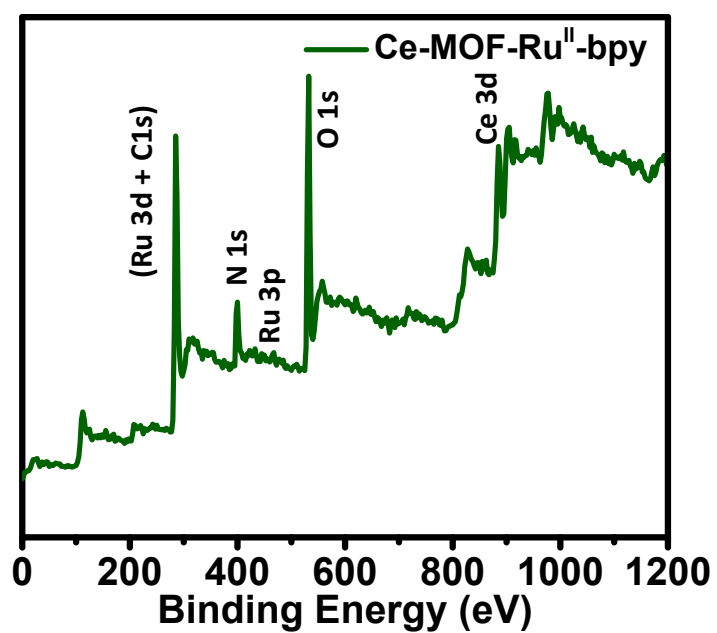
Fig. S10 XPS spectra of **Ce-MOF-Ru^{II}-bpy**.
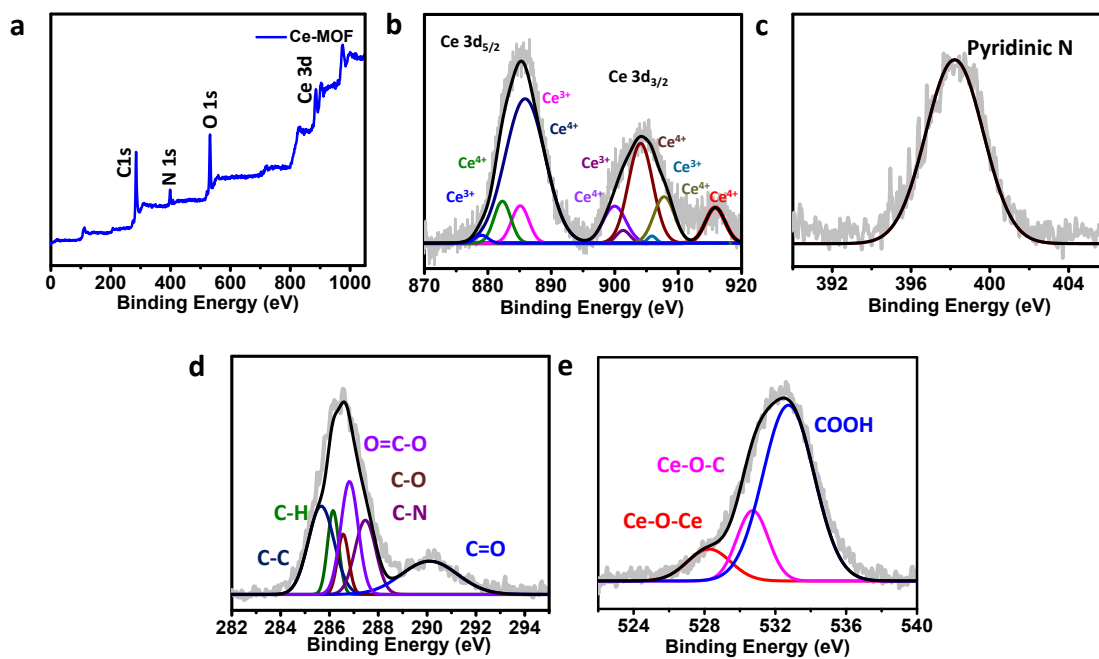
Fig. S11 (a) XPS spectra of **Ce-MOF**. (b) Ce 3d Xps spectra. (c) N 1s XPS spectra. (d) C 1s XPS spectra. (**e**) O 1s XPS spectra.
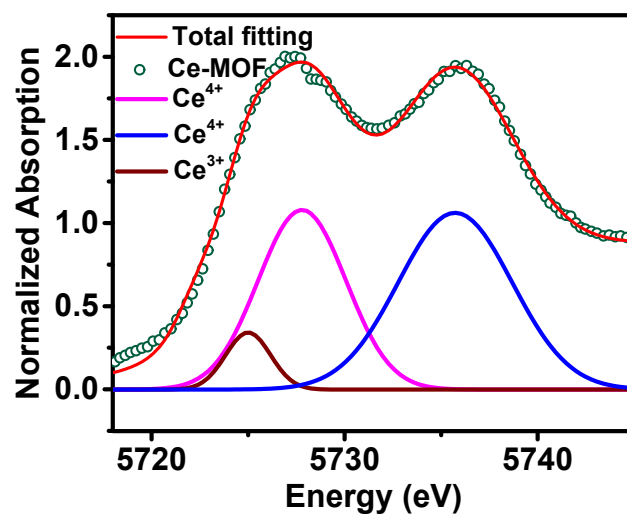
Fig. S12 Ce L3-edge XANES spectrum and fitting peaks of **Ce-MOF**.
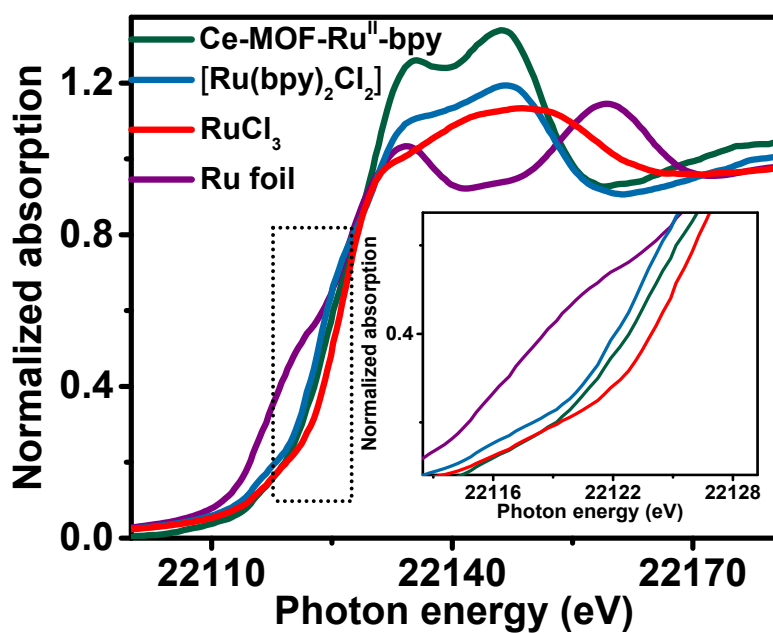
Fig. S13 Experimental Ru K-edge XANES spectra of **Ce-MOF-Ru^{II}-bpy** (green), [Ru(bpy)$_2$Cl$_2$], RuCl$_3$, Ru foil.
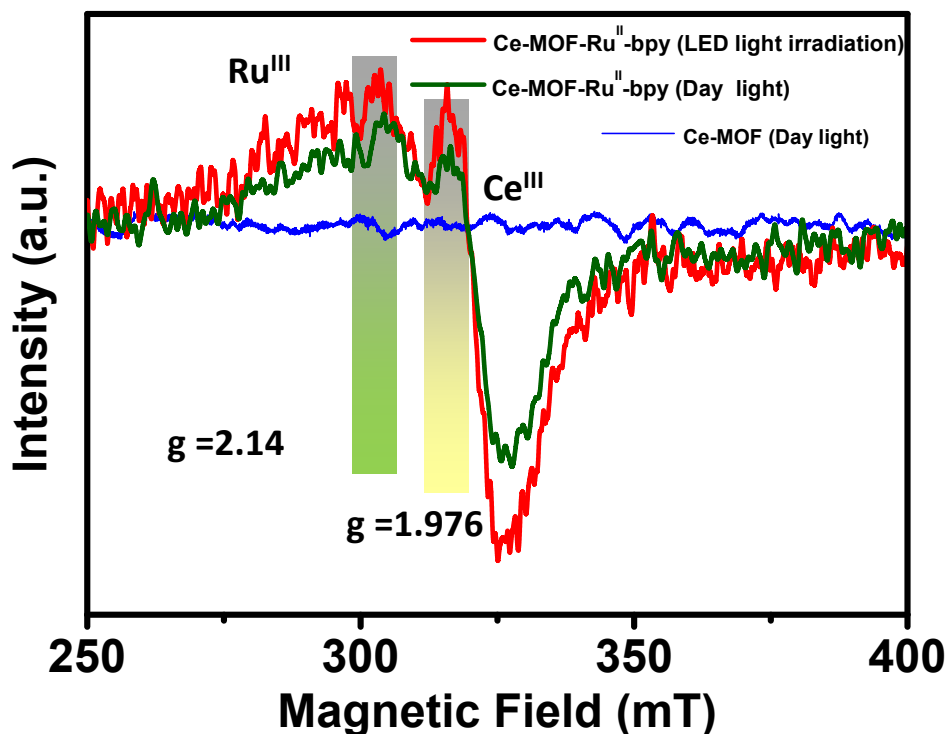
Fig. S14 EPR signals of **Ce-MOF** under visible light (blue) and **Ce-MOF-Ru^{II}-bpy** under daylight (green) and LED light (λ=380-780 nm) irradiation (red) condition.
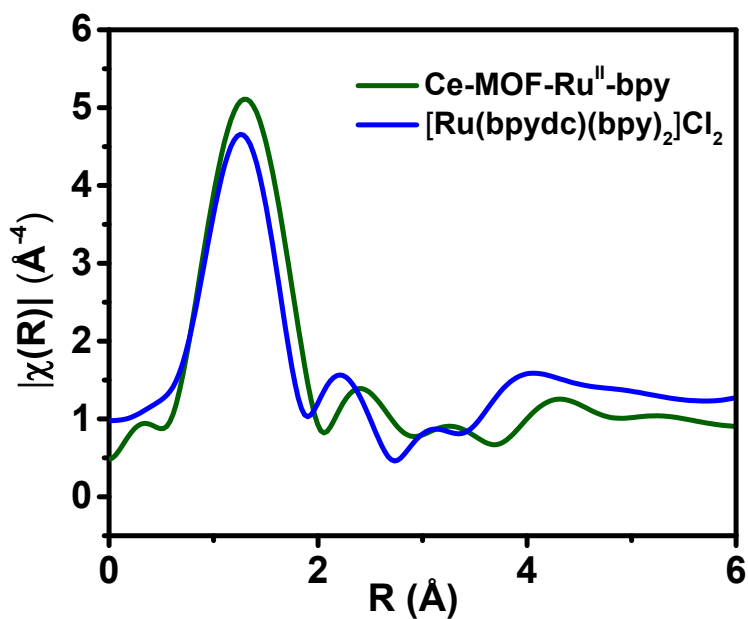
Fig. S15 A comparison of EXAFS data for **Ce-MOF-Ru^{II}-bpy** in comparison to their homogeneous components [Ru(bpydc)(bpy)$_2$]Cl$_2$.
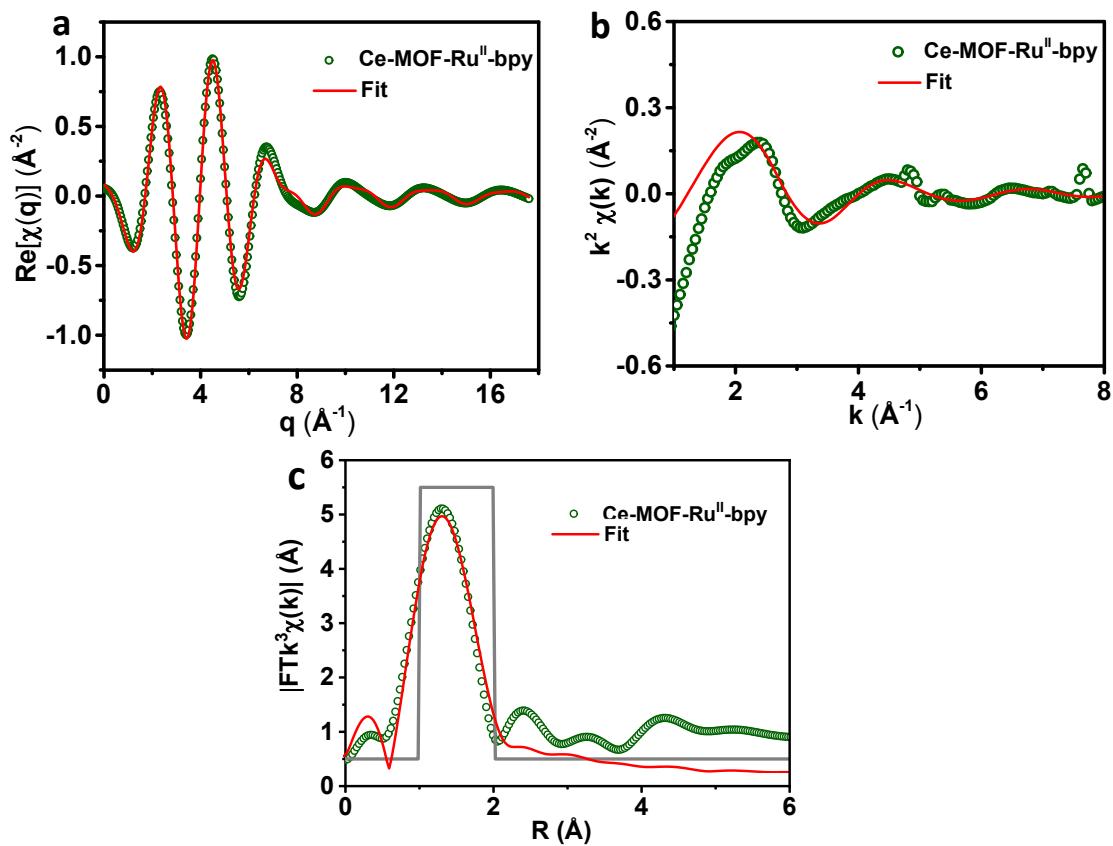
Fig. S16 Experimental and fitted EXAFS data in q space **a**, and K space **b**, and R space (k^3 weightage) **c**, of [Ru(bpydc)(bpy)$_2$]Cl$_2$ in **Ce-MOF-Ru^{II}-bpy**.

Table S2. Fitting parameter: CN, Coordination number, R, distance between backscatter atoms, σ^2, Debey-Waller factor (a measure of thermal and static disorder in absorber-scatterer distance); R factor is used to value the goodness of the fitting.

Sample	Path	CN	R(Å)	σ^2 (10^{-3} A^2)	R factor
Ce-MOF-Ru^{II}-bpy	Ru-N	6	2.07	3.28	0.014
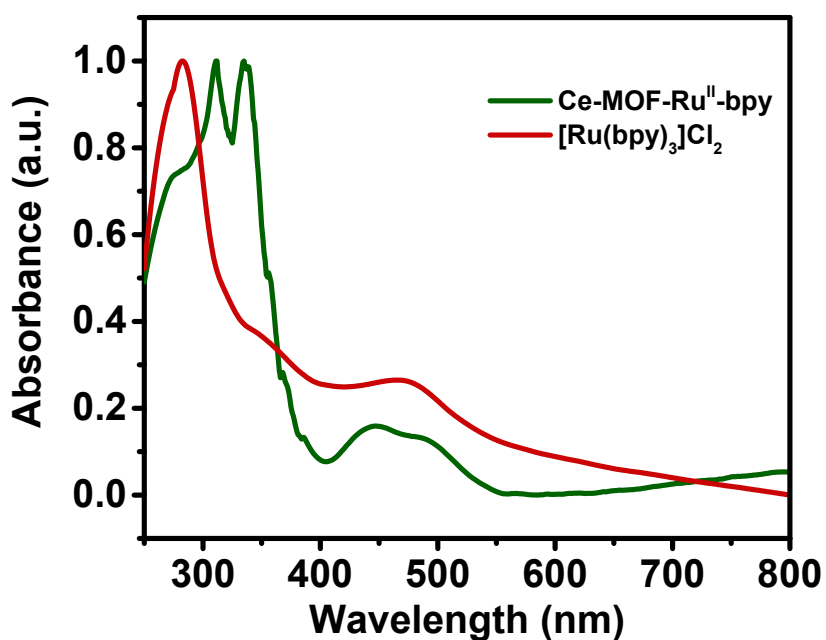
Fig. S17 UV-vis spectra of [Ru(bpy)$_3$]Cl$_2$ and **Ce-MOF-Ru^{II}-bpy**.
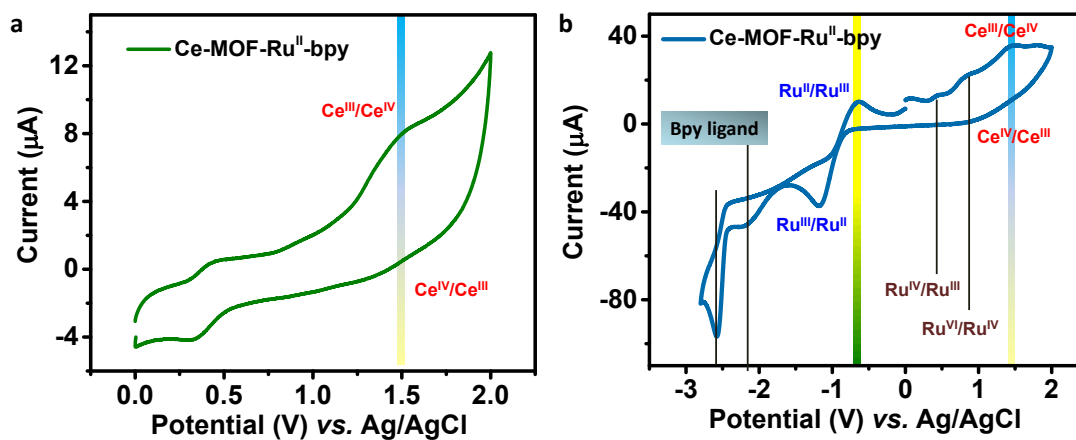
Fig. S18 (a) Cyclic voltammetry of **Ce-MOF-Ru^{II}-bpy** from 0 to 2 V vs Ag/AgCl. (b) Cyclic voltammetry of **Ce-MOF-Ru^{II}-bpy** from -3 to 2 V vs Ag/AgCl.
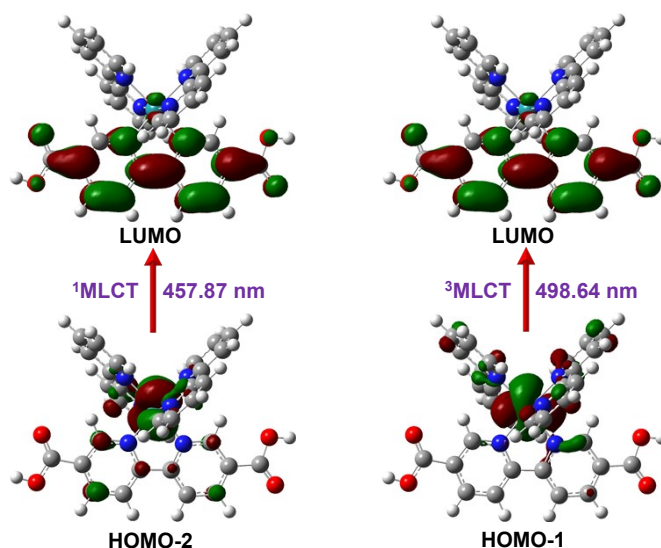
Fig. S19 HOMO and LUMO position of **¹MLCT** and **³MLCT** transition of [Ru(bpydc)(bpy)$_2$]Cl$_2$.

Table S3 Assignment of the ¹MLCT and ³MLCT band in the experimental solid-state absorption spectrum of Ce-MOF-Ru^{II}-bpy with different transitions.

Experimental absorption maximum	Theoretical band	Transition	Assignment	% Contribution
445 nm	457.87 nm	HOMO-2 → LUMO	^{1}MLCT	**91 %**
492 nm	498.64 nm	HOMO-1 → LUMO	^{3}MLCT	**81 %**
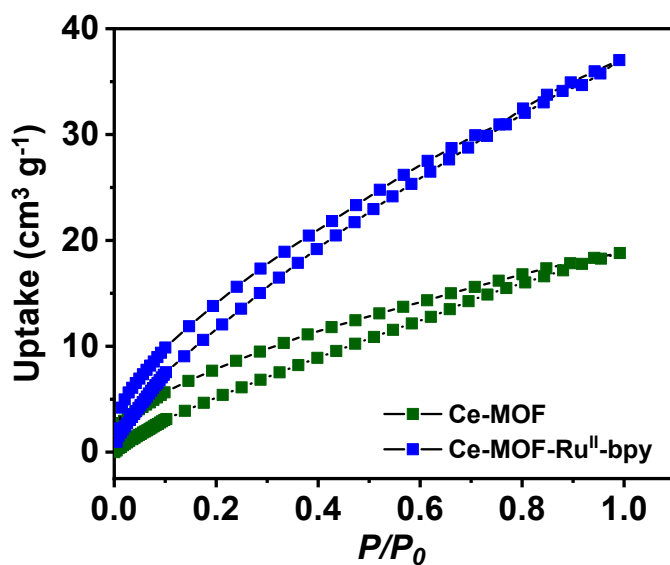
Fig. S20 CO$_2$ adsorption-desorption isotherms of **Ce-MOF** and **Ce-MOF-Ru^{II}-bpy** at room temperature (298 K).
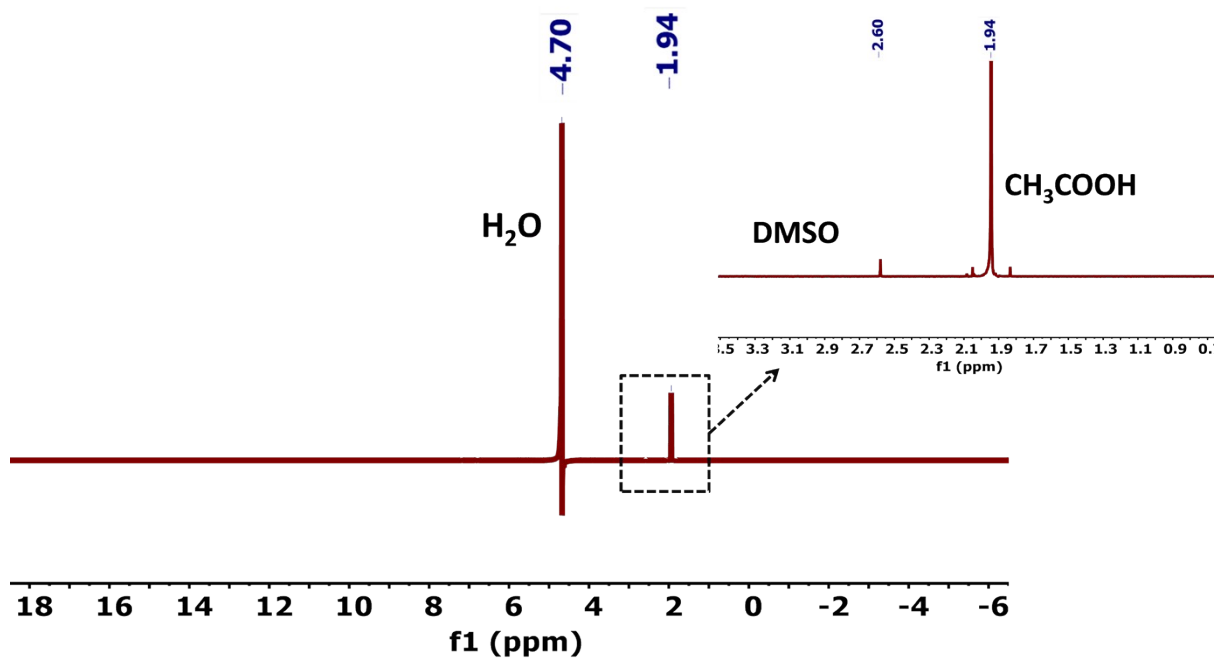
Fig. S21 ^{1}H NMR spectrum of standard acetic acid product in CO_2-saturated water. (DMSO is used as an external standard).
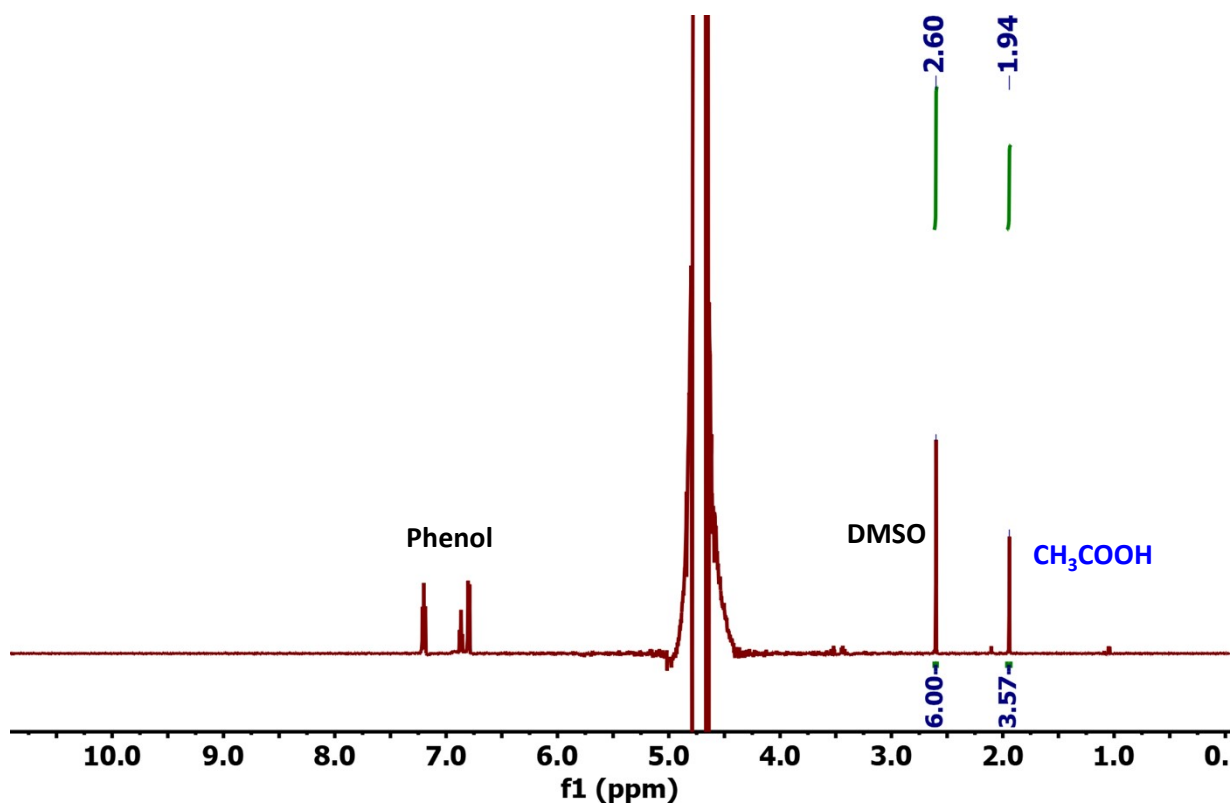
Fig. S22 ^{1}H NMR spectrum of the obtained acetic acid product in CO_2-saturated water solution after 10 h of photoirradiation. (DMSO and phenol are used as external standard).

NMR spectra of the obtained acetic acid product in water solution after 10 h of photoirradiation. (DMSO and phenol used as an external standard)

From Fig. S24, the ratio of [DMSO] and [CH$_3$COOH] was obtained using integration value.

[DMSO]/[CH$_3$COOH] = [6/6]/[3.57/3] = 0.84

[CH$_3$COOH] = [DMSO]/0.84 --(1)

Now, during NMR sample preparation 600 µL aliquot was taken along with 50 µL D$_2$O and 50 µL external standard (DMSO +Phenol).

Effective strength of DMSO in the NMR tube is 0.2857 mM;

From equation 1, we found [CH$_3$COOH] = 0.3401 mM

The amount of CH$_3$COOH = 0.2380 µmol

In total of 10 mL solution the amount of CH$_3$COOH = 3.4011 µmol

The yield of CH$_3$COOH $= \dfrac{3.4011\ \mu mol}{0.003\ g}$ = 1133 µmol g^{-1}
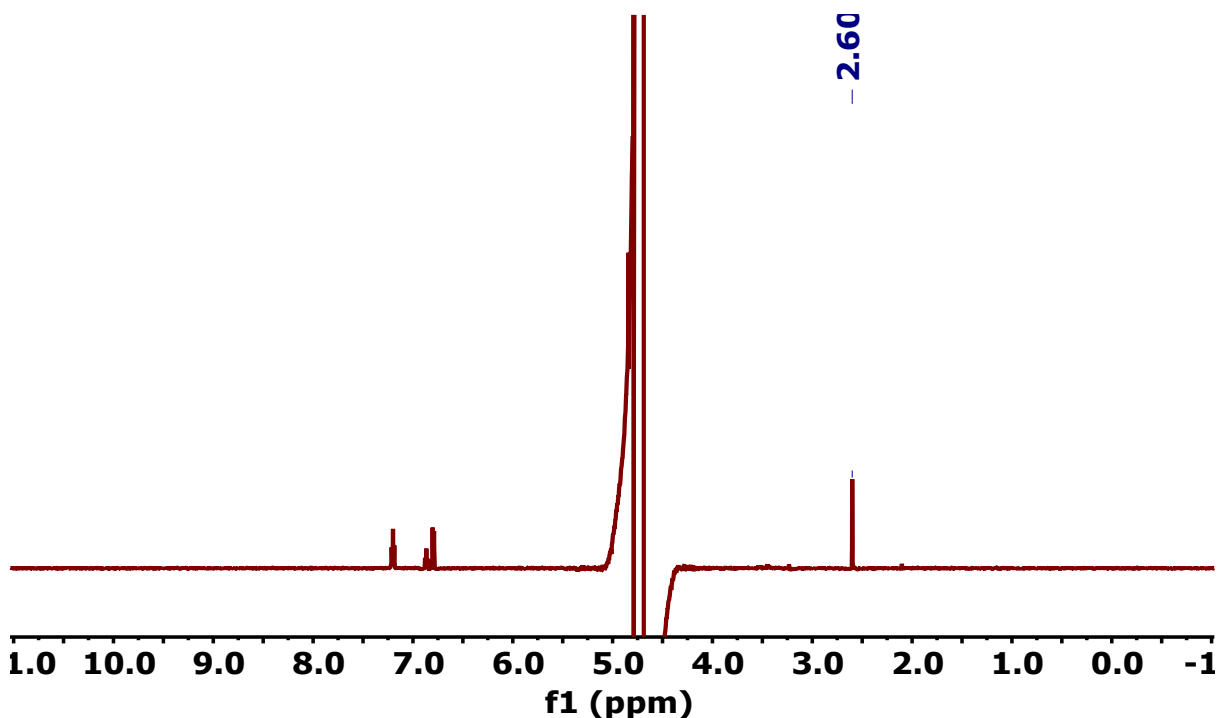
Fig. S23 ^{1}H NMR spectrum of liquid product in CO$_2$-saturated water solution without photoirradiation. (DMSO and phenol are used as external standard).
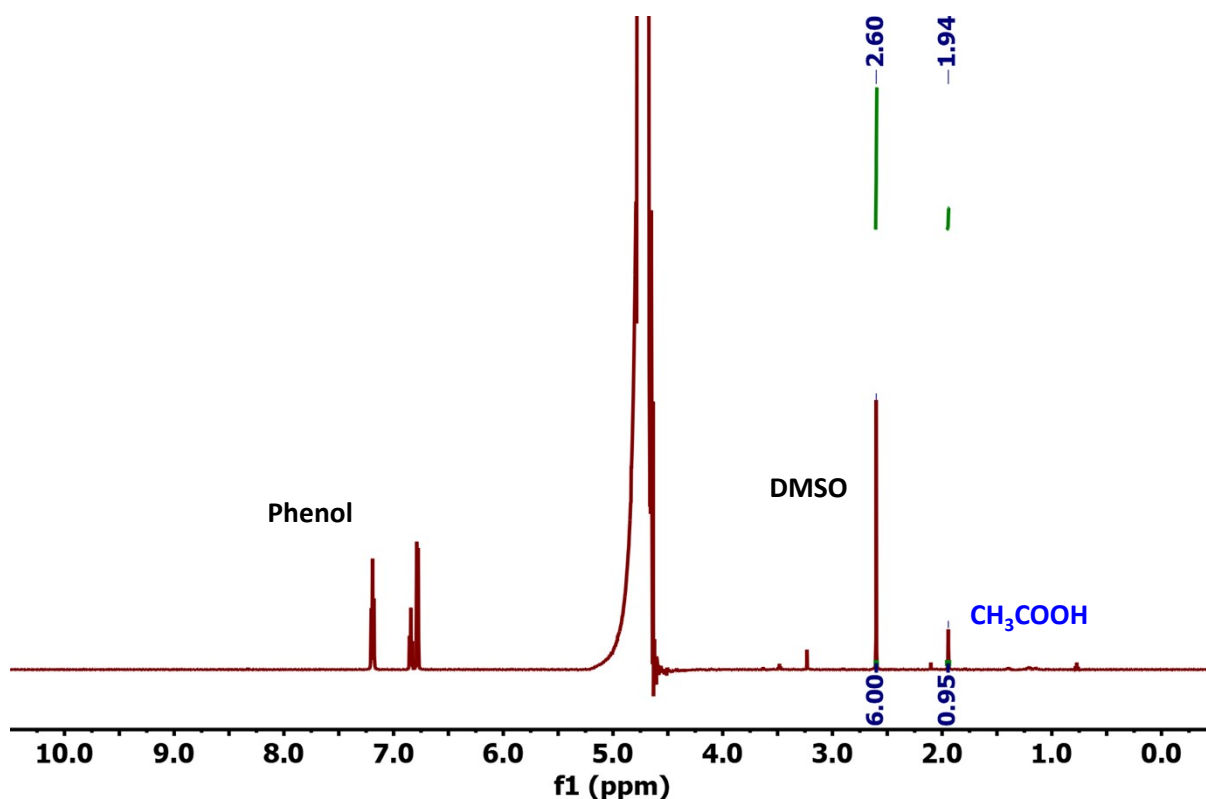
Fig. S24 ^{1}H NMR spectra of the obtained acetic acid product in CO_2-saturated water solution after 6 h of photoirradiation by applying a 450 nm bandpass filter. (DMSO and phenol used as external standard).

Apparent Quantum Efficiency Calculation:

Apparent quantum efficiency (AQE) is defined as the following equation: [1]

$$AQE = \frac{Number\ of\ reacted\ electrons}{Number\ of\ incident\ photons} \times 100\% \qquad Eq.\ 1$$

Eight electrons are required to convert CO_2 to CH_3COOH, so AQE for CH_3COOH can be calculated using the following equations: 2.

$$AQE-CH_3COOH = \frac{8 \times the\ number\ of\ evolved\ CH3COOH\ molecules}{the\ number\ of\ incident\ photons} \times 100\%$$

Eq. S2

In the following, we described the AQE determination at 450 nm for **Ce-MOF-Ru^{II}-bpy**.

1) The amounts of CH_3COOH produced were measured by applying a 450 nm band-pass filter for 6 h. The amounts of CH_3COOH molecules evolved in 6 h were 0.301 μmol.

2) The average intensity of irradiation after the 450 nm band pass filter was determined to be 3.2 mW cm^{-2} by a light meter (LI-COR Biosciences, LI-250A) at room temperature.

3) The irradiation area was controlled to be 1 cm^2.

4) The number of incident photons (N) is 1.56×10^{20} as calculated by equation (3).

$$N = \frac{E\lambda}{hc} = \frac{3.2 \times 10^{-3} \times 1 \times 3600 \times 6 \times 450 \times 10^{-9}}{6.626 \times 10^{-34} \times 3 \times 10^{8}} = 1.56 \times 10^{20} \qquad Eq.\ S3$$

5) The AQE for CH_3COOH was calculated based on *Eq. S2*.

$$AQE - CH_3COOH = \frac{8 \times the\ number\ of\ evolved\ CH3COOH\ molecules}{the\ number\ of\ incident\ photons} \times 100\%$$

$$= \frac{8 \times NA \times [CH3COOH]}{N} \times 100\%$$

$$= \frac{8 \times 6.023 \times 10^{23} \times 3.01 \times 10^{-7}}{1.56 \times 10^{20}} \times 100\% = 0.93\ \%\ in\ H_2O$$

Therefore, the AQE of **Ce-MOF-Ru^{II}-bpy** at 450 nm was 0.93% in H_2O.

N is the number of incident photons

E is the total incident energy on the photocatalyst (J)

λ is the light wavelength (m)

h is Planck's constant (J s)

c is the speed of light (m s^{-1})

N_A is Avogadro's number (mol^{-1})

[CH_3COOH] is the amounts of CH_3COOH, after 6 hours.
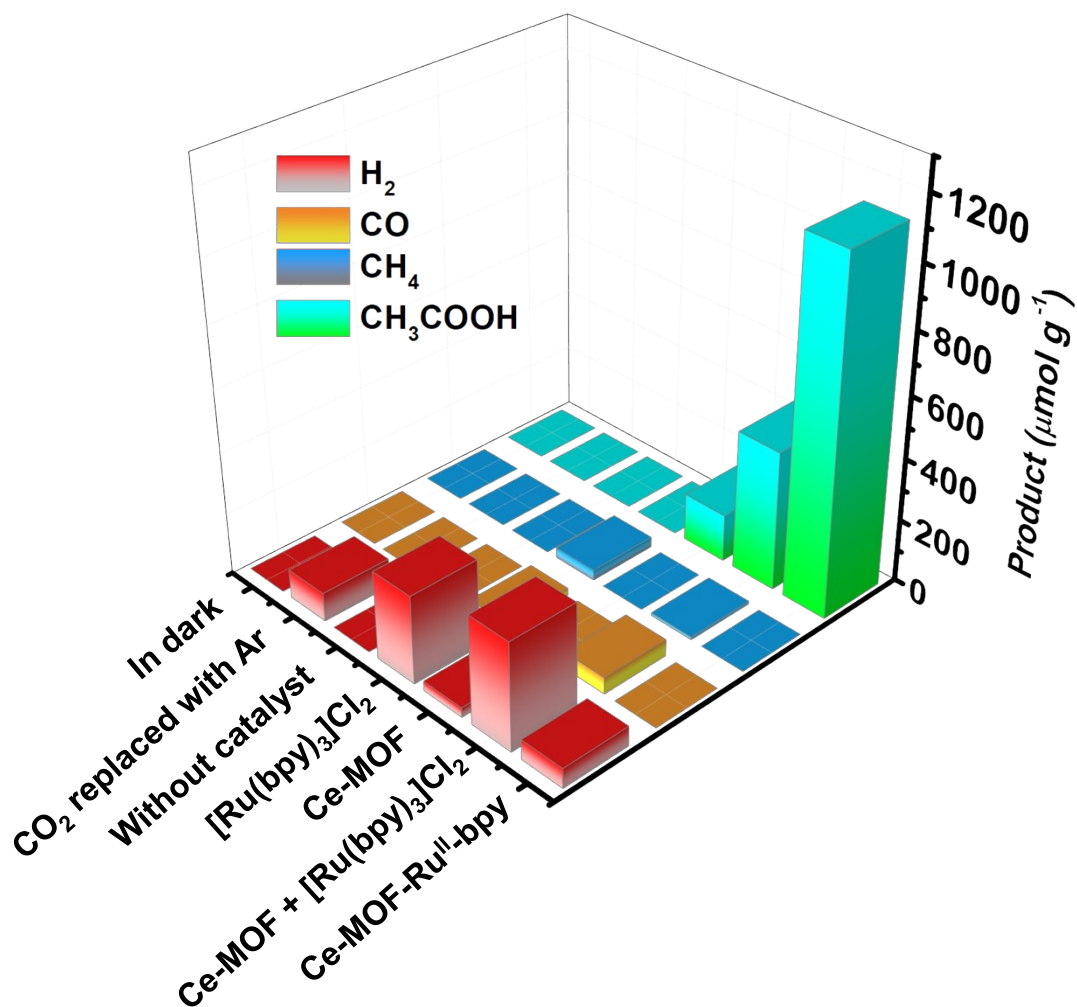
Fig. S25 Photocatalytic CO_2 reduction in water for 10 h.

Table S4. Comparison studies of photocatalytic CO_2 reduction in water.

Catalyst	Reaction condition	Products			
		H_2 ($\mu mol\ g^{-1}$)	CO ($\mu mol\ g^{-1}$)	CH_4 ($\mu mol\ g^{-1}$)	CH_3COOH ($\mu mol\ g^{-1}$)
Ce-MOF-Ru^{II}-bpy	300 W Xe lamp,>400 nm CO_2 saturated water medium	65	N.D.	N.D.	1133

Ce-MOF + [Ru(bpy)$_3$]Cl$_2$	300 W Xe lamp,>400 nm CO$_2$ saturated water medium	350	55	11	450
Ce-MOF	300 W Xe lamp,>400 nm CO$_2$ saturated water medium	32	N.D.	N.D.	152.5
[Ru(bpy)$_3$]Cl$_2$	300 W Xe lamp,>400 nm CO$_2$ saturated water medium	285	23	34	N.D.
Without catalyst	300 W Xe lamp,>400 nm CO$_2$ saturated water medium	N.D.	N.D.	N.D.	N.D.
Ce-MOF-Ru^{II}-bpy	CO$_2$ replaced with Ar	93	N.D.	N.D.	N.D.
Ce-MOF-Ru^{II}-bpy	In dark	N.D.	N.D.	N.D.	N.D.

N.D.= Not detected
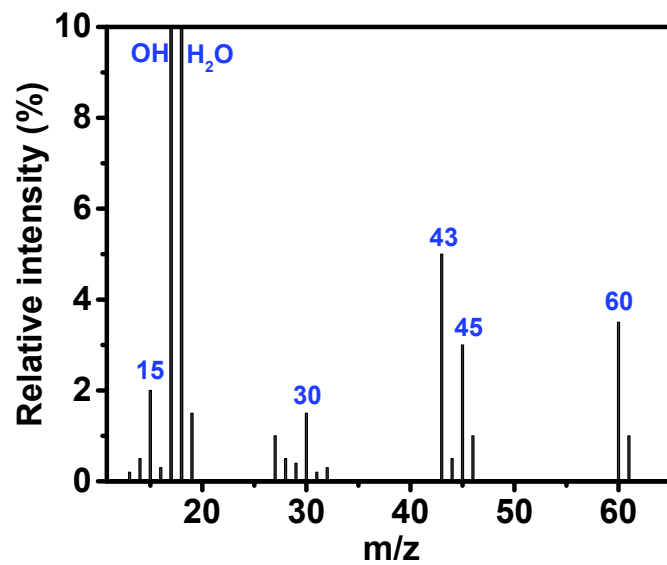
Fig. S26 Mass spectra extracted from GC-MS analysis of acetic acid product from $^{12}CO_2$ reduction over **Ce-MOF-Ru^{II}-bpy** in water.
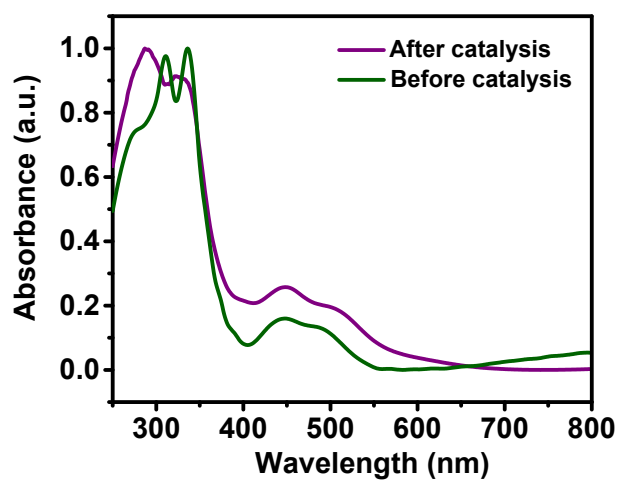
Fig. S27 UV-vis spectra of **Ce-MOF-Ru^{II}-bpy** after and before catalysis.
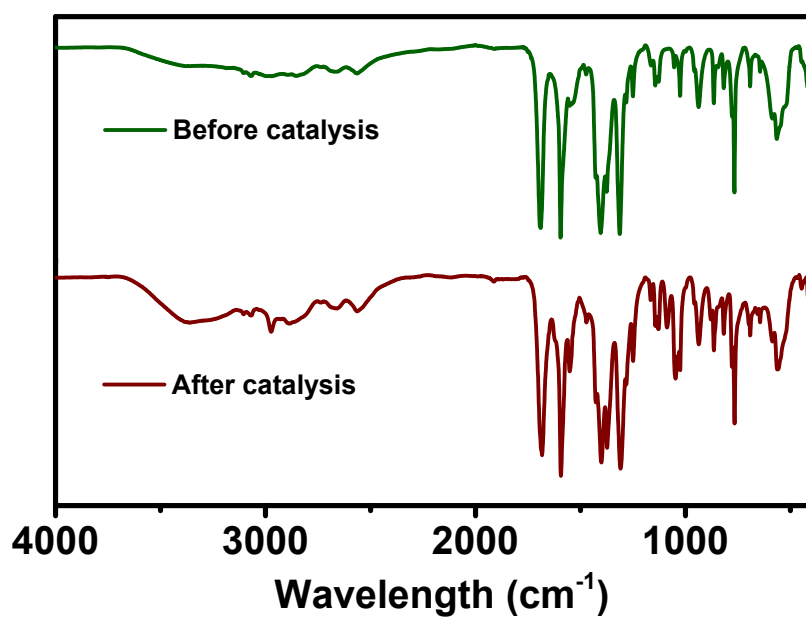
Fig. S28 FTIR spectra before and after catalysis.
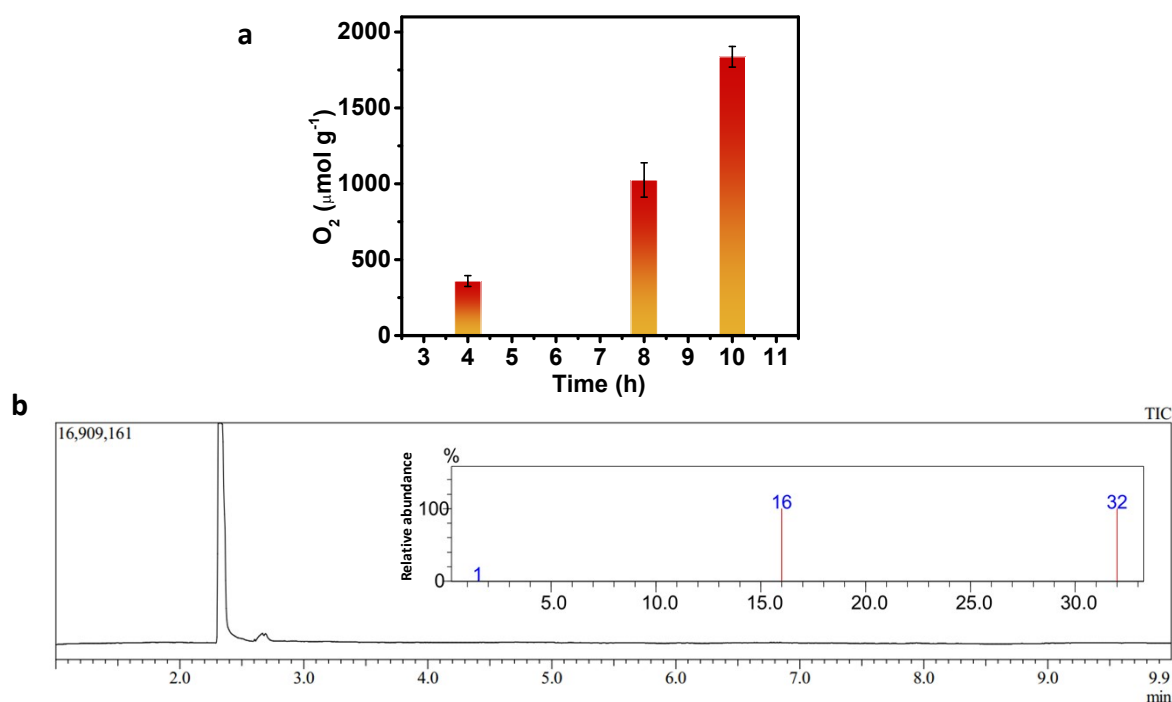
Fig. S29 (a) O_2 production (oxidation product from water oxidation) over **Ce-MOF-Ru^{II}-bpy** as a function of time of irradiation in water. (b) Gas chromatogram of O_2 production over **Ce-MOF-Ru^{II}-bpy** in water. Inset is showing the corresponding mass spectra of O_2 chromatogram.
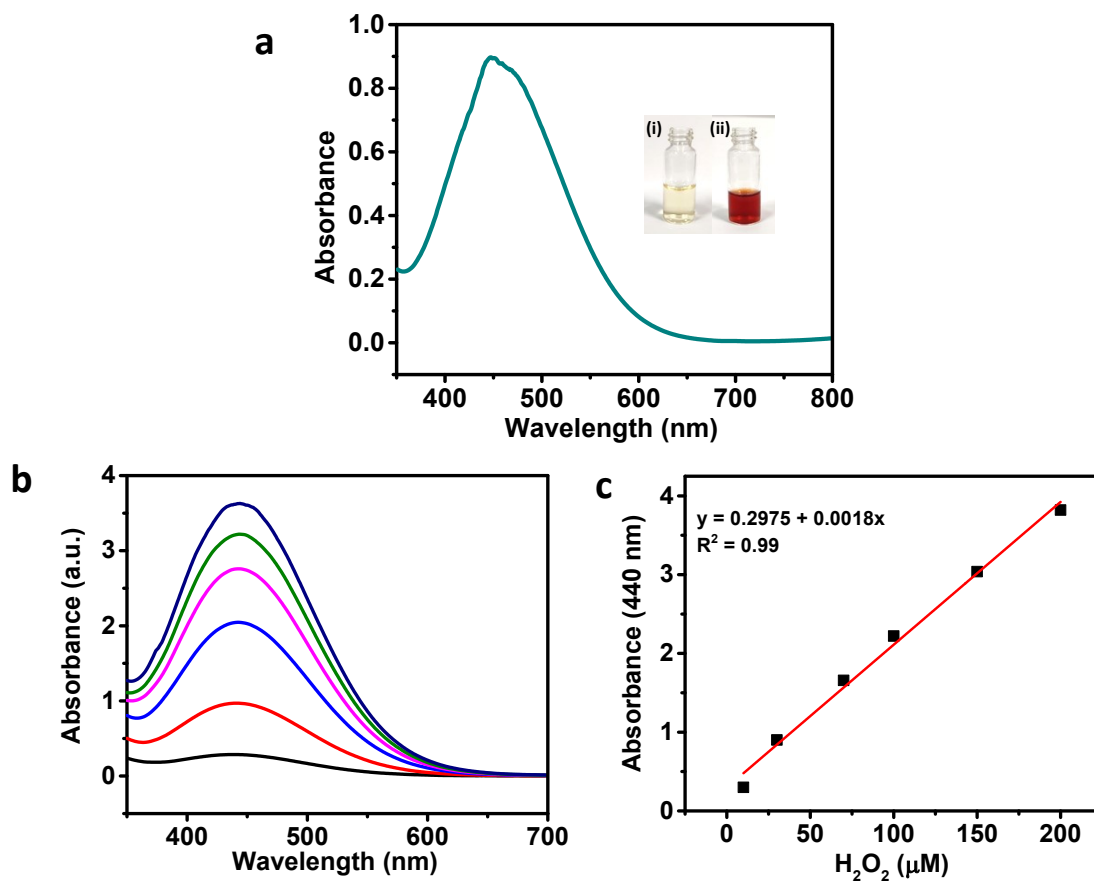
Fig. S30 (a) UV–vis spectrum of the reaction solution with addition of $FeCl_2$ and KSCN. The inset is the supernatant of the catalytic system of the photocatalytic CO_2 reduction in H_2O using **Ce-MOF-Ru^{II}-bpy** before (i) and after (ii) $FeCl_2$ /KSCN addition. (b) UV–vis spectra of a solution containing $FeCl_2$ and KSCN with the different concentration of H_2O_2. (c) Corresponding fitting of the UV-vis spectra.
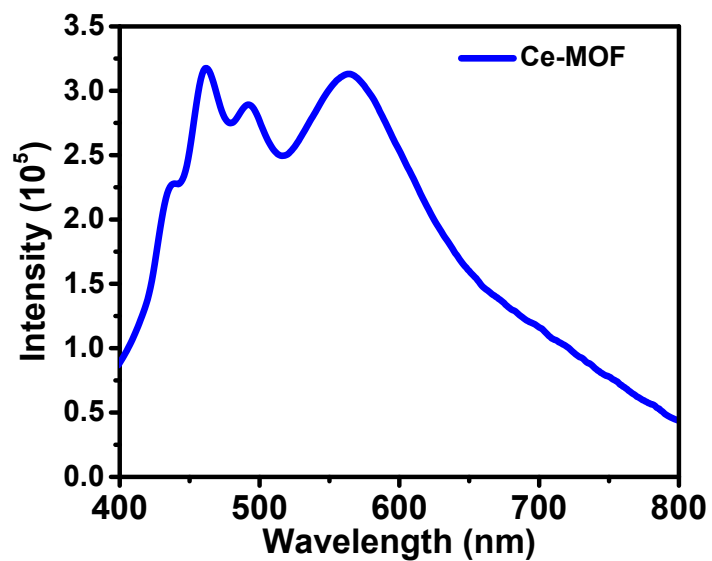
Fig. S31 Photoluminescence spectra of **Ce-MOF**. (λ_{ex} = 340 nm).
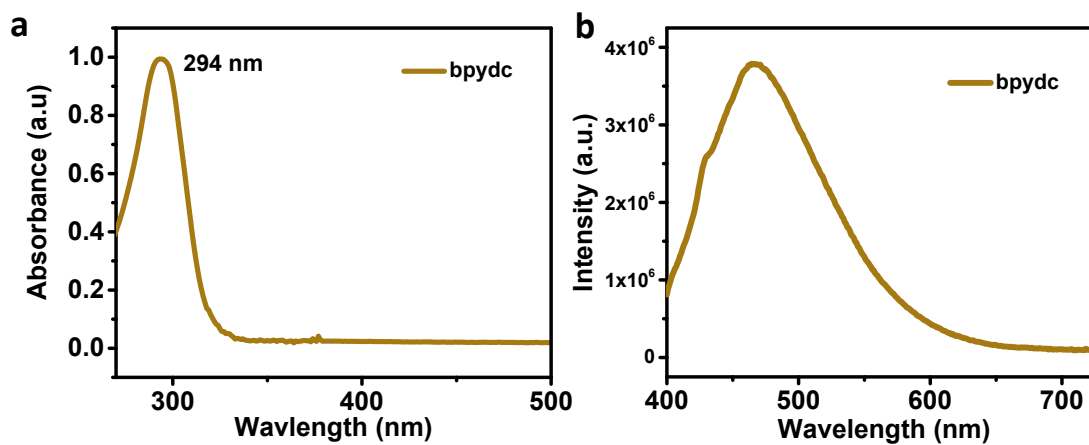
Fig. S32 (a) UV-vis spectrum of bpydc. (b) Photoluminescence spectrum of bpydc. (λ_{ex} = 300 nm).
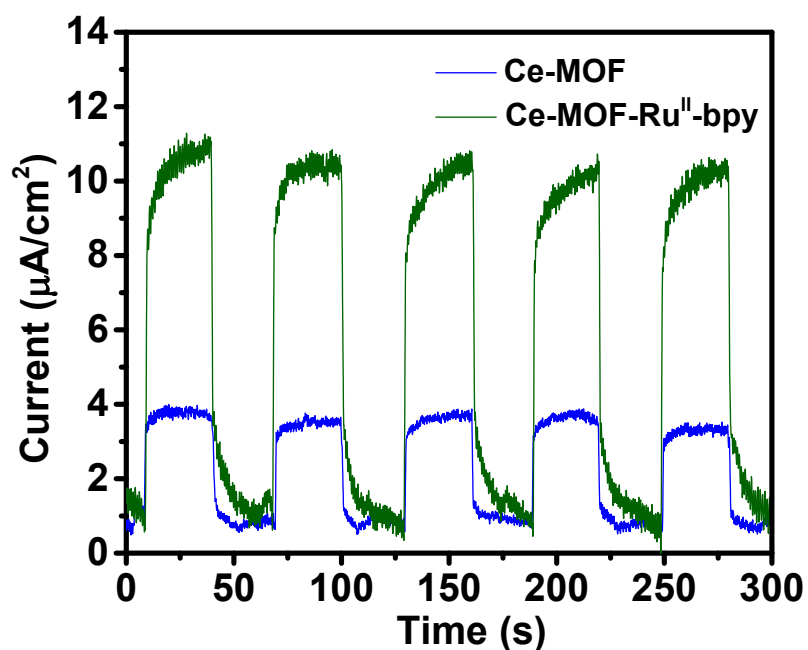
Fig. S33 Transient photocurrent responses of **Ce-MOF** and **Ce-MOF-Ru^{II}-bpy** in 0.2 M Na$_2$SO$_4$ aqueous solution under visible-light irradiation.
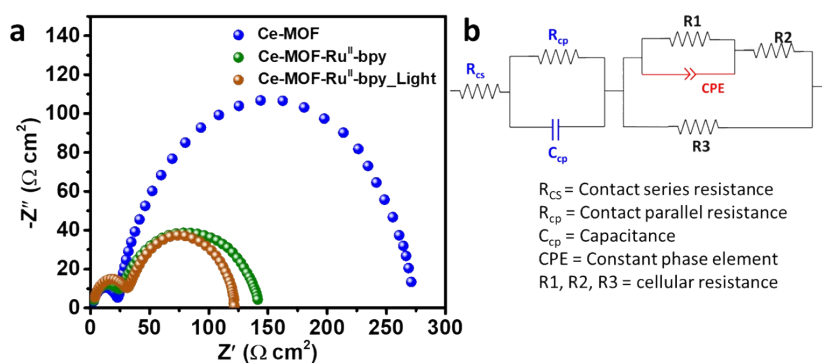
Fig. S34 (a) EIS Nyquist plot of **Ce-MOF** and **Ce-MOF-Ru^{II}-bpy**. (b) The equivalent circuit model used for fitting the impedance spectra of **Ce-MOF**, **Ce-MOF-Ru^{II}-bpy** and **Ce-MOF-Ru^{II}-bpy_Light**.
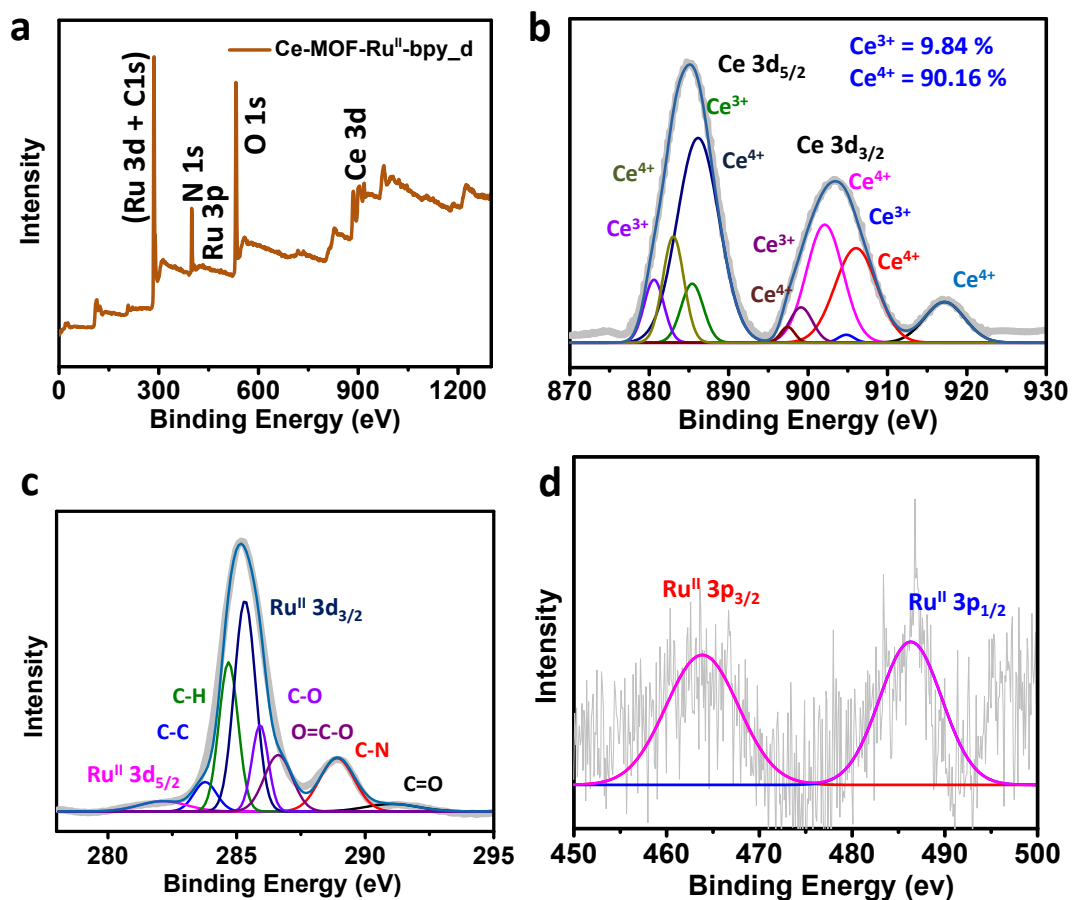
Fig. S35 (a) XPS spectra of **Ce-MOF-Ru^II-bpy_d**. (b) XPS spectrum of Ce 3d in **Ce-MOF-Ru^II-bpy_d**. (c) XPS spectra of Ru 3d and C 1s in **Ce-MOF-Ru^II-bpy_d**. (d) XPS spectra of Ru 3p in **Ce-MOF-Ru^II-bpy_d**.
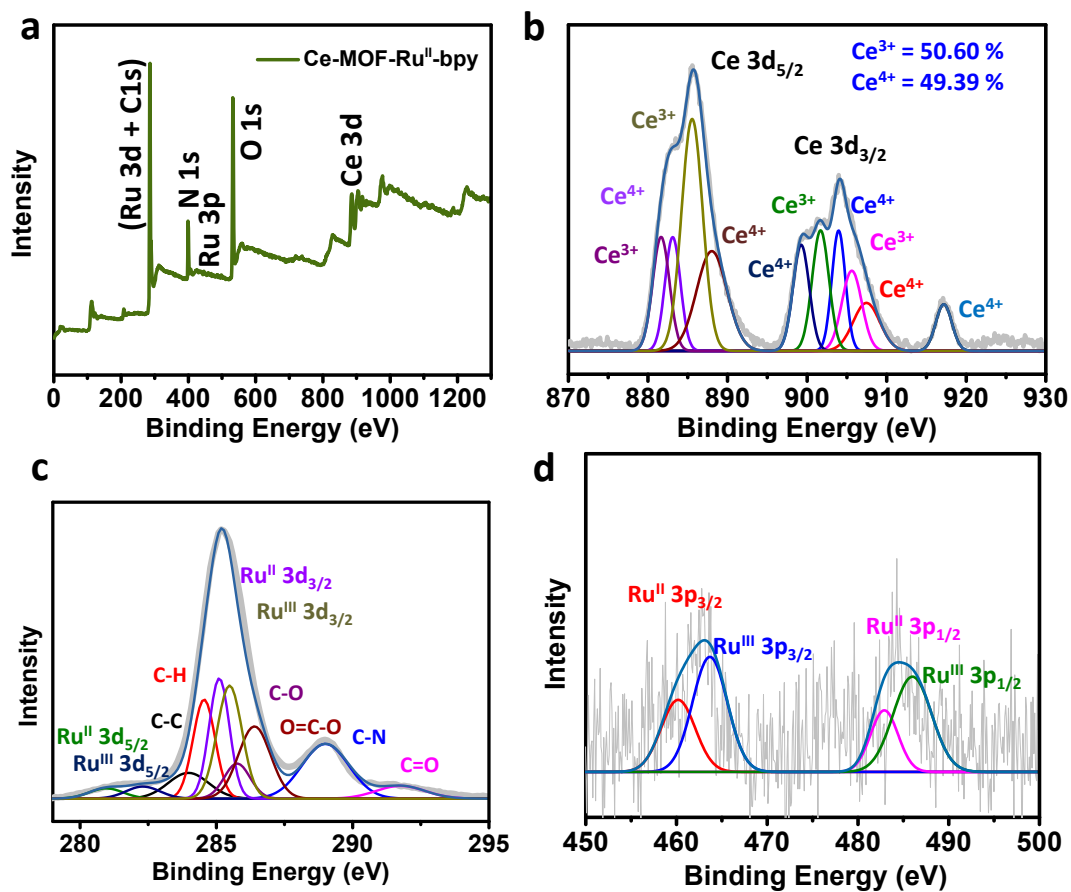
Fig. S36 (a) XPS spectra of **Ce-MOF-Ru^{II}-bpy** after LED (λ=380-780 nm) light irradiation onto **Ce-MOF-Ru^{II}-bpy_d**. (b) XPS spectrum of Ce 3d in **Ce-MOF-Ru^{II}-bpy**. (c) XPS spectra of Ru 3d and C 1s in **Ce-MOF-Ru^{II}-bpy**. (d) XPS spectra of Ru 3p in **Ce-MOF-Ru^{II}-bpy**.
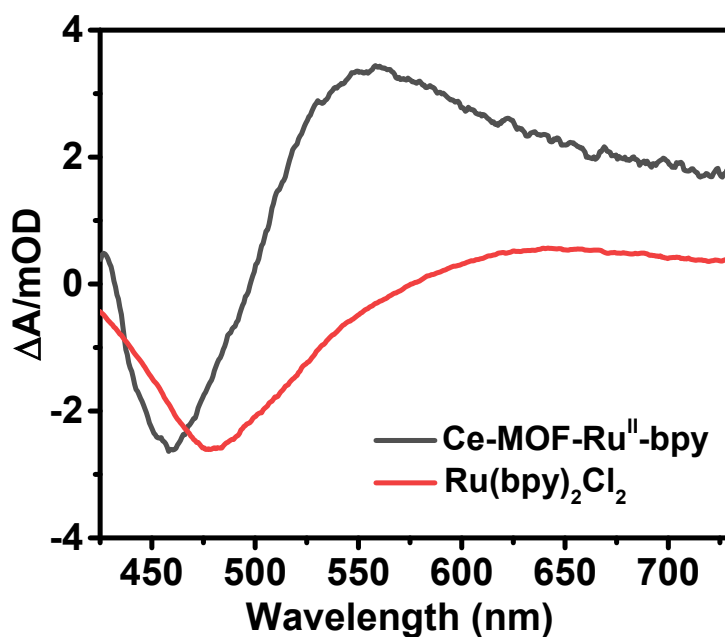
Fig. S37 Transient absorption spectra of **Ce-MOF-Ru^{II}-bpy** and [Ru(bpy)$_2$Cl$_2$] recorded at 1 ps delay.
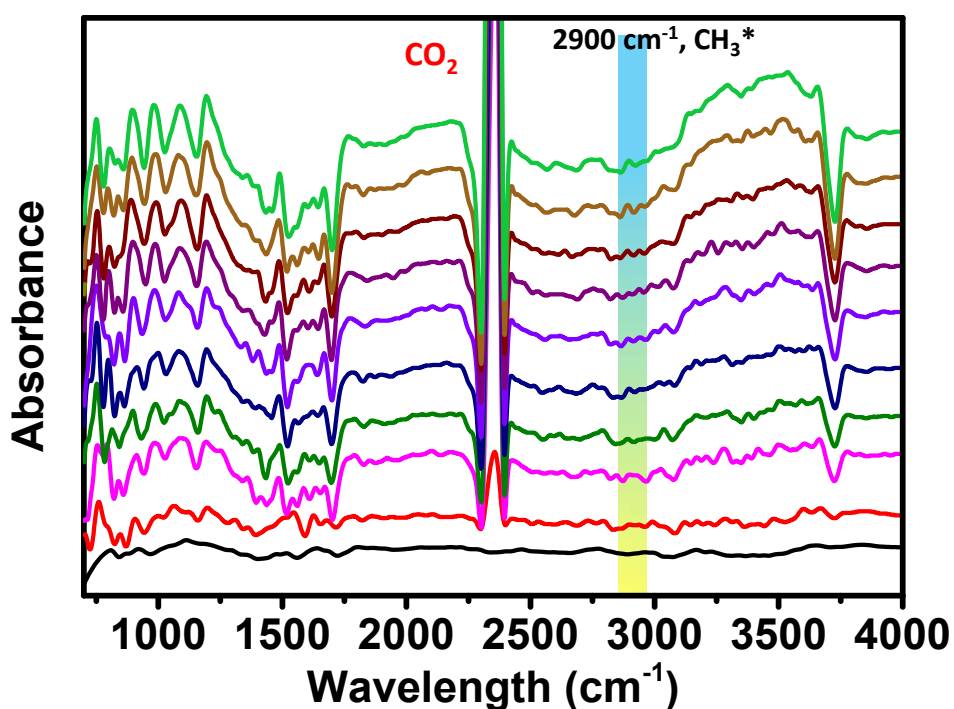
Fig. S38 Time-dependent in situ diffuse reflectance FT-IR spectra for CO$_2$ reduction in a mixture of CO$_2$ and H$_2$O vapour on **Ce-MOF-Ru^{II}-bpy** in the dark (background) and under visible light irradiation (LED lamp, l =420 nm). Irradiation time 20, 40, 60, 80, 100, 120, 140, 160 and 180 min, respectively.

In short, the possible reaction pathway for the acetic acid production from CO_2 might be followed these steps:

$$CO_2^* + e^- + H^+ \rightarrow COOH^* \qquad (1)$$

$$CO_2^* + e^- + H^+ + COOH \rightarrow COOH^* + COOH^* \qquad (2)$$

$$COOH^* + COOH^* \rightarrow HOOC - COOH^* \qquad (3)$$

$$HOOC - COOH^* + e^- + H^+ \rightarrow HOOC - CO^* + H_2O \qquad (4)$$

$$HOOC - CO^* + e^- + H^+ \rightarrow HOOC - CHO^* \qquad (5)$$

$$HOOC - CHO^* + e^- + H^+ \rightarrow HOOC - CH_2O^* \qquad (6)$$

$$HCOO - CH_2O^* + e^- + H^+ \rightarrow HOOC - CH_3 + O^* \qquad (7)$$
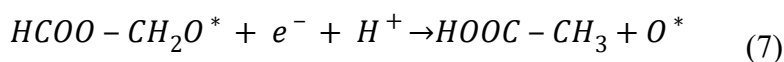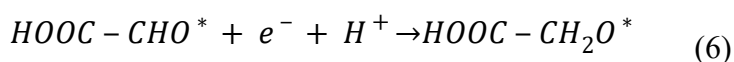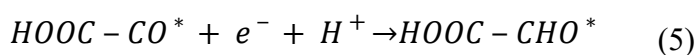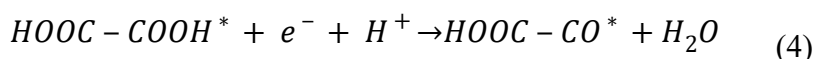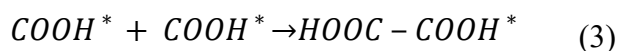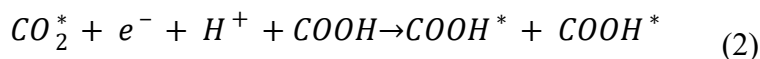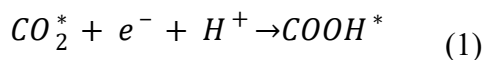
Computational Details:

Cartesian coordinates of the computed structures

Coordinates are given in standard XYZ format

Table S5: DFT-optimized geometry of $[Ru^{II}(bpydc)(bpy)_2]^{2+}$ (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ LANL2DZ (Ru) level in water solvent using PCM.

Atom	x	y	z
C	3.38832500	-2.38031600	-0.65422000
C	2.79498600	-3.63940800	-0.53018600
C	2.58700200	-1.24669200	-0.51993200
C	1.43136200	-3.72192600	-0.27973300
H	3.40295000	-4.53140200	-0.62898200
H	3.00389100	-0.25285400	-0.60912200
C	0.68079300	-2.54873600	-0.15698900
H	0.96125200	-4.69140100	-0.17765800
C	-0.76940600	-2.52593500	0.10596000
C	-1.55923400	-3.67358000	0.21231600
C	-2.63052600	-1.16820300	0.48077500
C	-2.92187200	-3.55237200	0.46234000
H	-1.12130200	-4.65663300	0.09821800
C	-3.47130100	-2.27452300	0.59976200
H	-3.02806100	-0.16684600	0.58301700
H	-3.54689700	-4.43308200	0.54697000

N	1.26987400	-1.32363400	-0.27812200
N	-1.31742900	-1.28241300	0.24315000
Ru	0.00531000	0.32375300	0.00215700
C	1.68466500	1.29517100	2.22538100
C	0.19753800	-0.33411800	3.00144000
C	2.22699200	1.43358400	3.50584900
C	0.69578700	-0.24004300	4.29611000
H	-0.60712700	-1.01569200	2.75474300
C	1.72954200	0.66033300	4.55143600
H	3.02957300	2.13666600	3.68900200
H	0.27697700	-0.86191900	5.07890500
H	2.14448700	0.76157000	5.54855100
C	-1.63363700	1.41564900	-2.19463000
C	-0.20887000	-0.24873200	-3.01223500
C	-2.16774700	1.60861200	-3.47153500
C	-0.70089400	-0.10179600	-4.30433700
H	0.56798900	-0.96741400	-2.78246300
C	-1.69862200	0.84437500	-4.53665000
H	-2.94203600	2.34691600	-3.63696600
H	-0.30515700	-0.71881500	-5.10283400
H	-2.10760300	0.98772600	-5.53106200
C	-2.05746800	2.17685700	-1.00288500
C	-1.75072600	2.48911200	1.29443900
C	-3.03607200	3.17420200	-1.02446700
C	-2.71506300	3.48990600	1.33492100
H	-1.21851300	2.18137300	2.18588100
C	-3.36958200	3.83718400	0.15362600
H	-3.53526300	3.43374600	-1.94943100
H	-2.94121300	3.97924500	2.27533500
H	-4.12852400	4.61223000	0.14593200
C	2.13690000	2.07060800	1.05345500
C	1.84181100	2.45392600	-1.23467000
C	3.15376900	3.02808800	1.09947300
C	2.84517700	3.41627400	-1.25081200
H	1.29715800	2.19028500	-2.13269700
C	3.51299100	3.70723500	-0.06174100
H	3.66261200	3.24435400	2.03029500
H	3.09034500	3.92025100	-2.17866300
H	4.30187500	4.45134400	-0.03511100
N	-0.65811500	0.48872800	-1.98047600
N	-1.42786900	1.84346500	0.15890200
N	0.67401300	0.41226600	1.98848600
N	1.49439600	1.79231400	-0.11571300
C	-4.91654200	-2.01994600	0.86641800
O	-5.39686500	-0.90805200	0.97763100
O	-5.62489200	-3.15695300	0.96970300
H	-6.55551100	-2.91526300	1.14243500
C	4.85262800	-2.28402800	-0.92150000
O	5.57844300	-3.25106400	-1.04273000
O	5.27662800	-1.01056300	-1.01208400
H	6.23760400	-1.02612500	-1.18601400

Sum of electronic and thermal Free Energies = -1956.697102 (Hartree/Particle).

From TDDFT calculation in water, λ_{abs} = 490.25 nm.

From TDDFT calculation in absence of any solvent, λ_{abs} = 457.87 nm (^{1}MLCT), 498.64 nm (^{3}MLCT).

Table S6: DFT-optimized geometry of **[Ru^{II}(bpydc$^-$)(bpy)$_2$]$^+$** (doublet), computed at the UB3LYP-D3/ 6-31G* (HCNO)/ LANL2DZ (Ru) level in water solvent using PCM. The spin density plot is also shown below. (Isovalue = 0.0004)
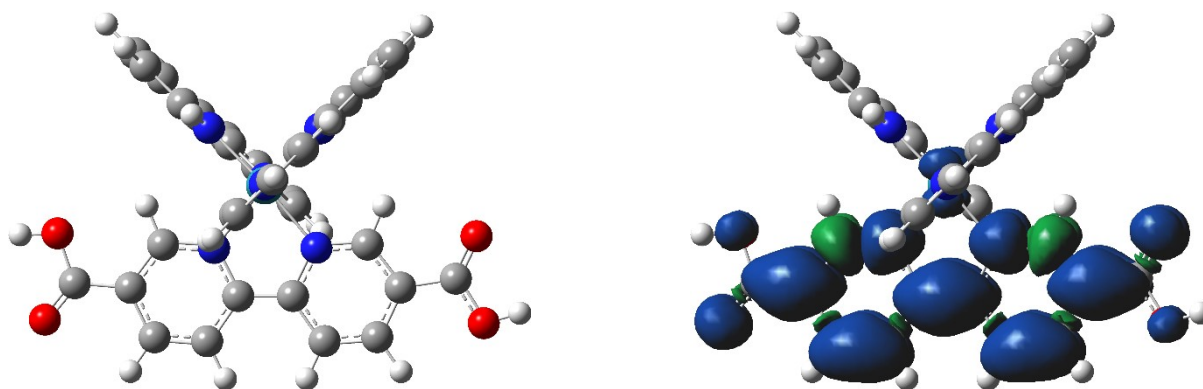
Spin Density Distribution

Atom	x	y	z
C	3.40477700	-2.35590100	-0.66437700
C	2.78042600	-3.62966700	-0.56542600
C	2.59257600	-1.22634100	-0.50406400
C	1.43359300	-3.71129400	-0.31891500
H	3.38365700	-4.52299600	-0.68620000
H	3.01552400	-0.23190500	-0.57367000
C	0.65407900	-2.52917000	-0.16171800
H	0.95818800	-4.68199400	-0.24158600
C	-0.74723200	-2.50648200	0.09458500
C	-1.56934100	-3.66166400	0.22679800
C	-2.63674700	-1.14515200	0.46170200
C	-2.91448500	-3.54065000	0.47436500
H	-1.12860900	-4.64682000	0.12977600
C	-3.49129400	-2.24610300	0.59826300
H	-3.03765000	-0.14250800	0.55295800
H	-3.53741800	-4.42220600	0.57434400
N	1.28283500	-1.29135300	-0.26822300
N	-1.33116000	-1.24835200	0.22714200
Ru	0.00622900	0.34554100	0.00344800
C	1.65052300	1.25391600	2.27638700
C	0.11037000	-0.35501300	2.98829400
C	2.17522600	1.34791000	3.56907300
C	0.58910000	-0.30414000	4.29255700
H	-0.70389100	-1.01124300	2.70635700
C	1.64135500	0.56322300	4.58745100
H	2.99337900	2.02463500	3.78176200
H	0.14298800	-0.93476200	5.05328800
H	2.04234900	0.62908800	5.59334000
C	-1.59519200	1.39208800	-2.24011500
C	-0.11947100	-0.25362900	-3.00251100
C	-2.10885300	1.55303900	-3.53061300
C	-0.58964300	-0.13797600	-4.30576100

H	0.66555100	-0.95252800	-2.74085100
C	-1.60306800	0.78269000	-4.57391500
H	-2.89648200	2.27093700	-3.72224900
H	-0.16665400	-0.76005400	-5.08646700
H	-1.99575600	0.90037600	-5.57835500
C	-2.05778100	2.16215000	-1.06887400
C	-1.80028500	2.51664200	1.22709000
C	-3.05458800	3.14105500	-1.12492500
C	-2.78339000	3.49964000	1.23432200
H	-1.27878900	2.23101600	2.13272200
C	-3.42302500	3.81600000	0.03546600
H	-3.54053800	3.37654800	-2.06351000
H	-3.03671200	3.99958800	2.16237600
H	-4.19638400	4.57609200	0.00154600
C	2.13984600	2.04519600	1.13040800
C	1.89269200	2.48552900	-1.15192100
C	3.17240500	2.98403700	1.21646500
C	2.91232100	3.43031400	-1.12908200
H	1.35924100	2.25003800	-2.06494600
C	3.56458100	3.68274200	0.07812600
H	3.66732600	3.17051100	2.16131800
H	3.18323700	3.95088400	-2.04067900
H	4.36570300	4.41203600	0.13537800
N	-0.60358200	0.49083900	-1.99118000
N	-1.44343000	1.85791400	0.10911100
N	0.62195700	0.40310500	2.00095100
N	1.51278200	1.80386600	-0.05547600
C	-4.90679400	-1.99448100	0.85741800
O	-5.42237200	-0.88640700	0.96825100
O	-5.63714200	-3.13675100	0.96971500
H	-6.55776100	-2.86262000	1.13941400
C	4.83900200	-2.25853800	-0.92276800
O	5.59154000	-3.21517300	-1.06827200
O	5.29166500	-0.97541800	-0.99125100
H	6.24996000	-1.02788400	-1.16429800

Sum of electronic and thermal Free Energies = -1956.828429 (Hartree/Particle).

Table S7: DFT-optimized geometry of **f-[Ce^{IV}(H$_2$O)-Ce^{IV}(H$_2$O)]** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z

Ce	-1	1.40782100	-2.17451800	-0.55217700
Ce	0	-1.02480700	1.85239900	1.92778900
Ce	-1	-1.73336600	-1.66311500	1.53850700
Ce	-1	2.17276200	1.56477300	-0.07969800
Ce	-1	-1.23134100	0.44504300	-1.38659400
Ce	0	1.68060800	-0.69203300	2.94594200
O	-1	-4.65566700	13.14812100	-4.43658400
C	-1	-4.15961900	10.82086000	-2.81251100
C	-1	-3.89386100	9.62509300	-2.15460200
O	-1	-6.00970700	-9.95306200	-7.78032200
C	-1	-3.96036600	-8.32228100	-6.65139200
C	-1	-3.10575800	-7.41672800	-6.03651200
O	-1	14.15469100	-3.97575800	0.41883100

C	-1	11.31904800	-4.18076000	0.27317100
C	-1	9.93230700	-4.13368000	0.30503900
O	-1	14.82196700	0.48136600	0.63767200
C	-1	12.26386900	1.05185700	1.47822400
O	-1	-6.85969800	1.06761400	12.74743900
C	-1	-4.79624400	0.57742200	10.83699500
C	-1	-3.90872900	0.27480300	9.81176800
O	-1	-9.16791800	-8.65645500	-7.32400800
C	-1	-7.71252000	-6.44277400	-6.20194000
C	-1	-6.98884300	-5.45966200	-5.53810600
C	-1	-2.25382600	9.35183500	-6.25480200
C	-1	-1.94594000	8.14803600	-5.63617000
O	-1	-2.36074200	13.62624200	-2.72855100
C	-1	-1.17719400	11.52066100	-1.39405800
C	-1	12.21595800	-0.77347500	-1.42206800
C	-1	10.84826100	-0.53758000	-1.36026400
O	-1	-7.60508200	-11.21613200	-5.13904900
C	-1	-6.24108300	-9.23477700	-3.61115800
C	-1	-5.48999400	-8.29842300	-2.91329000
O	-1	-10.02701100	0.51759600	12.17236200
C	-1	-8.75211200	-0.08068600	9.64519000
C	-1	-7.92061500	-0.28469500	8.55089800
O	-1	14.44286000	-3.31575100	-2.78597600
C	-1	11.73239500	-2.71765900	-2.74372100
O	-1	-5.64909300	-12.26785700	-5.54102100
C	-1	-4.20009000	-10.41193800	-4.06789100
O	-1	-9.81519800	2.71410600	11.71807700
C	-1	-8.03759500	2.21194400	9.64249500
O	-1	-1.33958200	13.11283300	-4.67725000
C	-1	-0.07862800	10.87526000	-3.42821700
C	-1	0.35192000	9.72694100	-2.77671100
O	-1	15.00885800	-1.31098000	1.99629000
C	-1	12.23332900	-1.00799900	2.70886900
C	-1	10.86924100	-0.81514700	2.89565100
C	-1	0.09890800	9.69156300	-6.58455200
O	-1	-10.10325900	-9.04884100	-5.31272200
C	-1	-8.76627900	-6.95426500	-4.10718900
O	-1	-7.64278800	-1.02685800	12.44937400
C	-1	-5.66588300	-1.65029000	10.61947800
O	-1	14.04639900	-4.00959300	2.67465100
C	-1	11.29069600	-4.29194700	2.67049000
O	-1	-5.55606300	11.83040400	-6.02622000
C	-1	-5.20883800	9.53144100	-4.54375100
O	-1	-6.77312600	-8.18364200	-8.95933300
C	-1	-4.80807600	-6.50651000	-7.97155000
O	-1	0.18084000	-4.28369800	-0.51702000
C	-1	-1.34773000	-6.25530100	-1.91055900
O	-1	-2.83872200	1.34768600	3.40885900
C	-1	-4.38116200	1.36223300	5.77259100
O	-1	0.08677400	4.07661300	1.84425100
C	-1	1.80764000	6.42085700	-0.34677300
C	-1	1.55112200	7.64046400	-0.95987500
O	-1	3.59118600	-1.64707900	-1.51747700
C	-1	6.38972400	-2.06341800	-1.73521900
O	-1	-3.47313400	-0.77581500	3.00211900
C	-1	-5.58795300	-0.50216900	4.87006600
C	-1	-6.47016400	-0.37908000	5.93650400
O	-1	2.00700800	3.82444600	0.69474200
C	-1	-0.37076600	6.56912300	0.64810200
O	-1	3.91815400	0.57651600	-1.37867400

C	-1	6.63189200	0.31331000	-1.93681200
C	-1	8.00236100	0.11291600	-2.03188500
O	-1	-1.52591500	-3.98094500	0.92206500
C	-1	-2.99034100	-6.04582700	-0.17681100
C	-1	-3.75626300	-6.97951400	-0.85971600
O	-1	-0.85209900	-1.00743700	-3.31288800
C	-1	-2.23393400	-2.94092800	-4.81423000
O	-1	3.24576200	-2.49736100	2.73092100
C	-1	6.00521400	-3.03639700	2.66120500
O	0	1.48315400	0.79335900	5.03688900
O	-1	-2.60160700	2.42912600	-1.35267400
C	-1	-3.34339400	4.91738600	-2.41838600
O	-1	-2.52182200	3.29073300	0.72707300
C	-1	-3.58691100	5.73507100	-0.17936200
C	-1	-3.94138000	6.96430400	-0.72350300
O	-1	0.77349800	-2.49027500	-2.83138300
C	-1	-0.34284000	-4.39442000	-4.55520400
C	-1	-1.04650700	-5.35073900	-5.27621500
O	-1	2.98018200	-3.45769500	0.70908400
C	-1	5.61900400	-4.37001000	0.70262200
C	-1	6.98638800	-4.60503400	0.65837700
O	0	-0.45060100	2.68574200	4.38922700
O	-1	-3.57309100	-2.12548500	0.03093900
C	-1	-5.23214400	-3.81515100	-1.45779900
O	-1	1.71694900	2.82766000	-2.13276600
C	-1	1.13564900	5.28632700	-3.48315800
O	-1	4.12262500	1.67009600	1.31893900
C	-1	6.65733100	0.22155800	3.49563500
C	-1	8.03810100	0.05767300	3.50157200
O	-1	-1.36929200	-2.73880800	3.69554100
C	-1	-2.83977000	-2.35274000	6.03134600
O	-1	-3.30639400	-0.74432200	-1.72808300
C	-1	-5.17338400	-2.21648600	-3.24224900
C	-1	-5.97637600	-3.08418800	-3.97350200
O	-1	0.52308200	-1.97352000	4.65256100
C	-1	-0.93725400	-1.24516700	6.97648000
C	-1	-1.73737100	-0.90972000	8.06245200
O	-1	3.85308100	0.36062600	3.13197800
C	-1	6.88216500	1.24572700	1.33953000
O	-1	-0.18590500	1.94154700	-2.95287400
C	-1	-0.73038200	4.16017400	-4.48174800
C	-1	-1.04595100	5.35238900	-5.11658000
O	-1	2.12856400	-0.50635200	0.80921000
O	-1	0.00474000	1.77419800	-0.01929500
O	-1	-0.45639600	-0.18018800	2.66108600
O	-1	-0.67374900	-1.50969600	-0.43467700
O	-1	0.59536300	-2.42169800	1.71551600
O	-1	1.18767200	-0.01703800	-1.58674100
O	-1	1.40475900	1.58589000	2.28182200
O	-1	-2.08527300	0.38340100	0.69693500
C	-1	-4.98928700	12.04045700	-4.82430100
C	-1	-4.81113900	10.78430600	-4.04891300
C	-1	-4.29190800	8.41868800	-2.75178100
C	-1	-5.90619700	-8.78762600	-8.12007900
C	-1	-4.85752200	-7.86328100	-7.61904300
C	-1	-3.16937300	-6.06713000	-6.42123200
C	-1	13.50242700	-4.08210900	1.44215400
C	-1	12.02539700	-4.23095500	1.47668000
C	-1	9.28886000	-4.14856800	1.55303400
C	-1	14.35608100	-0.37377100	1.57042000

C	-1	12.95001700	-0.07880800	1.95091900
C	-1	10.25783500	0.31194100	2.32593000
C	-1	-6.75486600	-0.03710900	12.24072400
C	-1	-5.70384700	-0.39923300	11.25498400
C	-1	-3.96655200	-0.99584800	9.21877400
C	-1	-9.30496900	-8.36016700	-6.14808600
C	-1	-8.61078400	-7.22989400	-5.47601000
C	-1	-7.17895900	-5.29072300	-4.15839300
C	-1	-1.21704400	10.15415200	-6.73669200
C	-1	-0.59674900	7.77475700	-5.52521100
C	-1	-1.51604400	12.90051000	-3.49075400
C	-1	-0.88652300	11.78467000	-2.74045900
C	-1	-0.03937500	9.52587900	-1.44312200
C	-1	12.68051200	-1.89282900	-2.11710700
C	-1	9.97737200	-1.42726800	-2.00951000
C	-1	-6.39673100	-11.28575000	-5.00125700
C	-1	-5.59201200	-10.31672300	-4.21222100
C	-1	-4.09899000	-8.47947900	-2.82919300
C	-1	-9.60498600	1.41298800	11.45522200
C	-1	-8.81222900	1.19394300	10.21895100
C	-1	-7.16834400	0.79296400	8.05439300
C	-1	-0.96652100	-4.56795800	-0.05583800
C	-1	-1.76146600	-5.65178900	-0.71589700
C	-1	-3.27148400	-7.50163000	-2.06855200
C	-1	-3.54498700	0.31317900	3.63818600
C	-1	-4.52339700	0.39462000	4.76700400
C	-1	-6.24425600	0.62032600	6.89608900
C	-1	0.98356000	4.49489000	1.05680100
C	-1	0.81960600	5.85387700	0.46300000
C	-1	0.31107300	8.26095100	-0.74271600
C	-1	4.32562000	-0.61535400	-1.54835700
C	-1	5.79613700	-0.79390800	-1.76331600
C	-1	8.50563900	-1.19511200	-1.95530600
C	-1	-0.29619000	-2.13857200	-3.42927100
C	-1	-0.95006500	-3.16193700	-4.29726700
C	-1	-2.34428800	-5.04758900	-5.71792200
C	-1	3.67320700	-3.15045400	1.72817100
C	-1	5.10966900	-3.54917700	1.71292900
C	-1	7.80923300	-4.00436400	1.62440000
C	-1	-2.77234600	3.36621000	-0.51581900
C	-1	-3.26152900	4.68201500	-1.03853600
C	-1	-3.96065800	7.10998200	-2.11923300
C	-1	-3.82390400	-1.75139700	-1.15550100
C	-1	-4.77215900	-2.58819700	-1.95627400
C	-1	-6.36028700	-4.30516100	-3.39709600
C	-1	0.67033700	2.87377400	-2.84807300
C	-1	0.37445500	4.11860700	-3.62666100
C	-1	-0.24360200	6.47854100	-4.88146300
C	-1	4.56925000	0.96499700	2.27667100
C	-1	6.05305800	0.82079100	2.38745600
C	-1	8.78057500	0.49933600	2.39496400
C	-1	-0.72192600	-2.26074200	4.67217300
C	-1	-1.49451000	-1.96743000	5.91879900
C	-1	-3.07378600	-1.33701300	8.07693900
H	-1	1.46660000	0.03353500	-2.51525900
H	-1	1.85025800	2.33825200	2.70119900
H	-1	0.63445700	-3.32259300	2.07497200
C	-1	14.13936200	-2.18251800	-2.12402400
O	-1	14.98146700	-1.47962000	-1.59283800
H	-1	15.40809600	-3.44398100	-2.71574400

H	-1	-7.57380100	-8.74279300	-9.01284000
H	-1	-6.24833600	-12.83648900	-6.06097900
H	-1	-10.45549700	-9.81365600	-5.80685200
H	-1	15.64666700	0.10507000	0.27437100
H	-1	-2.94180900	14.12939300	-3.33276200
C	-1	-1.55762300	11.46472800	-7.34964700
O	-1	-2.69515700	11.88292700	-7.47295500
O	-1	-0.47316900	12.14205500	-7.77453400
H	-1	-0.78554100	12.99471700	-8.13255600
H	-1	-5.56366100	12.68396800	-6.50013100
H	-1	-10.30166800	2.77086000	12.56352100
H	-1	-8.44096600	-0.63215400	12.86049800
H	-1	14.95222500	-3.65815700	2.57354100
H	-1	0.10509500	-0.95700800	6.94355200
H	-1	-1.32702500	-0.35372600	8.89827500
H	-1	-3.30132100	-2.90903600	5.22134900
H	-1	-3.21747000	1.02426200	9.44400600
H	-1	-4.81721300	1.56046600	11.29512800
H	-1	-6.35104600	-2.43555900	10.92535000
H	-1	5.62933800	-2.40512200	3.46027000
H	-1	7.41265900	-5.23792600	-0.11155600
H	-1	4.94824000	-4.79549700	-0.03588300
H	-1	11.80550200	-4.35788000	3.62509900
H	-1	11.86562200	-4.13770000	-0.65999700
H	-1	9.36299500	-4.01182800	-0.60976600
H	-1	5.76332200	-2.94101000	-1.61142100
H	-1	12.05636500	-3.59249300	-3.30088000
H	-1	12.92794800	-0.11957900	-0.93329200
H	-1	10.45587300	0.29555900	-0.78763400
H	-1	8.67308800	0.95309800	-2.16994000
H	-1	6.20375200	1.30819300	-1.98692800
H	-1	2.00344400	5.27949400	-2.83191200
H	-1	0.93105500	10.28542300	-6.95299300
H	-1	-3.27671800	9.68884300	-6.36422400
H	-1	-2.72753500	7.51902100	-5.22286400
H	-1	-1.89741500	5.41424700	-5.78454100
H	-1	-1.32787300	3.26773200	-4.62890300
H	-1	-3.55733300	5.58366700	0.89389000
H	-1	-4.20699600	7.79361200	-0.07803300
H	-1	-3.10694200	4.11397300	-3.10819400
H	-1	-5.74252400	9.46407000	-5.48793800
H	-1	-3.84542200	11.77310400	-2.40171200
H	-1	-3.33850900	9.62336300	-1.22358300
H	-1	-3.55851200	2.07111500	5.71766600
H	-1	-5.72849600	-1.26199500	4.10911100
H	-1	-7.33276000	-1.03218400	6.00718200
H	-1	-8.05503700	3.21266500	10.06577400
H	-1	-9.32612700	-0.89328400	10.07715100
H	-1	-7.82617800	-1.27325600	8.11751600
H	-1	0.65627600	-4.59053900	-4.18170000
H	-1	-0.60128100	-6.31483800	-5.49325400
H	-1	-2.46075100	-7.73187000	-5.22327500
H	-1	-3.97796600	-9.36584800	-6.36512200
H	-1	-5.47278600	-6.11773200	-8.73817000
H	-1	-2.72097500	-1.98836100	-4.63271800
H	-1	-0.39374400	-5.97568100	-2.34720800
H	-1	-4.71150600	-7.30356200	-0.46341700
H	-1	-3.33025400	-5.61311000	0.75687500
H	-1	-5.96249000	-7.42788400	-2.46996500
H	-1	-7.31511100	-9.13866200	-3.71254600

Atom		x	y	z
H	-1	-3.66156300	-11.24097500	-4.51940200
H	-1	-4.84883700	-1.26773200	-3.65490600
H	-1	-6.30648300	-2.81645400	-4.97069500
H	-1	-4.94040200	-4.12506100	-0.45999300
H	-1	-9.47582800	-7.52520800	-3.51456700
H	-1	-7.57331700	-6.62732800	-7.25998500
H	-1	-6.24703900	-4.87325200	-6.06818200
H	-1	6.43592800	1.71202100	0.46718900
H	-1	12.79430100	1.81473200	0.91487100
H	-1	12.73779000	-1.88544300	3.09590800
H	-1	10.27858000	-1.56280800	3.41199400
H	-1	8.53150900	-0.39550700	4.35384000
H	-1	6.04839700	-0.10891300	4.33028200
H	-1	2.29508400	8.10456000	-1.59716100
H	-1	2.74531300	5.89809800	-0.49995000
H	-1	-1.14775300	6.14773700	1.27788800
H	-1	0.90988500	8.96435200	-3.30967500
H	-1	0.16179900	11.05958900	-4.46753800
H	-1	-1.78012700	12.21857500	-0.81963500
N	-1	-2.07208700	-7.15828000	-2.57801500
N	-1	-3.46310400	-9.51908500	-3.40320500
N	-1	-2.92071300	-3.84811100	-5.50885600
N	-1	-3.99456700	-5.62419100	-7.39132900
N	-1	-6.00115600	-4.65811200	-2.14717700
N	-1	-8.07020200	-6.02137700	-3.45702100
N	-1	10.95818400	1.24841500	1.65216800
N	-1	8.20529800	1.09338700	1.33011000
N	-1	-0.77639100	10.42134900	-0.75585200
N	-1	-0.62972600	7.74191700	0.07006000
N	-1	-5.20524400	1.47682200	6.81378300
N	-1	-7.23496600	2.02528400	8.59619400
N	-1	-3.61048600	-2.07117100	7.08190100
N	-1	-4.83055700	-1.94779100	9.62439200
N	-1	7.32065300	-3.25120400	2.62904600
N	-1	9.95913200	-4.24607700	2.71882000
N	-1	7.70563700	-2.27236700	-1.82761800
N	-1	10.41535300	-2.50400300	-2.69194400
N	-1	0.41229700	8.53735800	-5.98994500
N	-1	0.84602900	6.44191300	-4.08942400
N	-1	-3.67916300	6.09066000	-2.95542800
N	-1	-4.95626400	8.37834400	-3.92500500
H	0	1.14638800	0.27311500	5.78370900
H	0	0.82047200	1.51041300	4.89474900
H	0	-1.24698300	2.65361000	4.94969400
H	0	-0.16136900	3.61698500	4.37350700

Sum of electronic and thermal Free Energies = -13200.795160 (Hartree/Particle).

Table S8: DFT-optimized geometry of **f-[Ce^{IV}(H$_2$O)-Ce^{III}]$^-$** (doublet), computed at the UB3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.41621700	-2.16593500	-0.53072900
Ce	0	-0.96144000	1.78918700	1.98011900
Ce	-1	-1.73017800	-1.66435500	1.55448200

Ce	-1	2.17618600	1.57263800	-0.04482200
Ce	-1	-1.22381300	0.45349200	-1.36286500
Ce	0	1.73159400	-0.70252800	3.06749600
O	-1	-4.65458800	13.16247900	-4.38074100
C	-1	-4.15974500	10.83065700	-2.76285400
C	-1	-3.89420900	9.63311200	-2.10809700
O	-1	-5.97693400	-9.92951000	-7.79982500
C	-1	-3.93183700	-8.30014300	-6.66119600
C	-1	-3.07955900	-7.39563200	-6.04156800
O	-1	14.16276300	-3.95695200	0.46325000
C	-1	11.32767100	-4.16444700	0.31058300
C	-1	9.94081200	-4.11890900	0.33948500
O	-1	14.82487900	0.50015600	0.69754400
C	-1	12.26430700	1.06534800	1.53413200
O	-1	-6.88448100	1.02590100	12.76038100
C	-1	-4.81623800	0.54384500	10.85304900
C	-1	-3.92611000	0.24536300	9.82887500
O	-1	-9.13751500	-8.63762500	-7.34654500
C	-1	-7.68695700	-6.42595700	-6.21428700
C	-1	-6.96580000	-5.44417900	-5.54575500
C	-1	-2.24470300	9.37440900	-6.20543900
C	-1	-1.93694300	8.16899900	-5.58989100
O	-1	-2.36399900	13.63763200	-2.66607200
C	-1	-1.18124100	11.52911200	-1.33552600
C	-1	12.22480800	-0.75093500	-1.37196100
C	-1	10.85673100	-0.51665800	-1.31249000
O	-1	-7.57690100	-11.20250900	-5.16610800
C	-1	-6.21840700	-9.22453300	-3.62896300
C	-1	-5.46986400	-8.28958900	-2.92648200
O	-1	-10.04992000	0.47439300	12.17647600
C	-1	-8.76873300	-0.11464100	9.65031200
C	-1	-7.93457100	-0.31435600	8.55725600
O	-1	14.45742300	-3.28660600	-2.73882000
C	-1	11.74624600	-2.69147100	-2.70077800
O	-1	-5.61891600	-12.25093400	-5.56697900
C	-1	-4.17516300	-10.39813200	-4.08479600
O	-1	-9.83938900	2.67253400	11.72954800
C	-1	-8.05661200	2.17872800	9.65639900
O	-1	-1.33793700	13.13139500	-4.61407200
C	-1	-0.07744200	10.89123200	-3.36922300
C	-1	0.35284700	9.74132600	-2.72035000
O	-1	15.01059900	-1.29624200	2.05095800
C	-1	12.23316500	-0.99838400	2.75825000
C	-1	10.86846100	-0.80753800	2.94257100
C	-1	0.10840700	9.71761700	-6.52884300
O	-1	-10.07695100	-9.03728500	-5.33860300
C	-1	-8.74487300	-6.94510500	-4.12351900
O	-1	-7.66470600	-1.06844100	12.45400300
C	-1	-5.68305200	-1.68407800	10.62660700
O	-1	14.04945000	-3.99796800	2.71870400
C	-1	11.29406000	-4.28317400	2.70747300
O	-1	-5.55003800	11.84881400	-5.97651300
C	-1	-5.20372900	9.54557900	-4.50047300
O	-1	-6.73956000	-8.15719900	-8.97500100
C	-1	-4.77848600	-6.48112700	-7.97756200
O	-1	0.19137500	-4.27649500	-0.50492900
C	-1	-1.33200100	-6.24531100	-1.90806200
O	-1	-2.84290000	1.33935800	3.43187000
C	-1	-4.39060100	1.34494200	5.79232400
O	-1	0.08310600	4.07636400	1.88248000

C	-1	1.80657700	6.42916000	-0.29751400
C	-1	1.55015700	7.65041600	-0.90737000
O	-1	3.60119200	-1.63320900	-1.48946700
C	-1	6.40064600	-2.04595100	-1.70222800
O	-1	-3.47415300	-0.78345500	3.01696300
C	-1	-5.59343700	-0.51786700	4.88100700
C	-1	-6.47816500	-0.39903900	5.94584200
O	-1	2.00635100	3.82972300	0.73634700
C	-1	-0.37420800	6.57204300	0.69292700
O	-1	3.92551900	0.59028200	-1.34297000
C	-1	6.64077500	0.33164800	-1.89583400
C	-1	8.01166300	0.13297800	-1.98845800
O	-1	-1.51892400	-3.98003000	0.93126400
C	-1	-2.97871200	-6.04298000	-0.17735800
C	-1	-3.74212400	-6.97531800	-0.86490100
O	-1	-0.83873300	-0.99256300	-3.29284000
C	-1	-2.21516500	-2.92278000	-4.80332300
O	-1	3.24712400	-2.49714200	2.75542700
C	-1	6.00730000	-3.03310100	2.69025400
O	-1	-2.59621700	2.43601900	-1.32580300
C	-1	-3.33822300	4.92683000	-2.38538300
O	-1	-2.52200100	3.29118500	0.75680400
C	-1	-3.58761400	5.73724100	-0.14436200
C	-1	-3.94214900	6.96780500	-0.68544600
O	-1	0.78734100	-2.47521300	-2.81232900
C	-1	-0.32313500	-4.37510900	-4.54460500
C	-1	-1.02418300	-5.32989500	-5.27018500
O	-1	2.98709400	-3.45142800	0.73003700
C	-1	5.62687900	-4.36097100	0.72664300
C	-1	6.99460400	-4.59443200	0.68473200
O	0	-0.62822700	2.90851800	4.35947100
O	-1	-3.56603800	-2.12391500	0.04136200
C	-1	-5.21997400	-3.81063400	-1.45638600
O	-1	1.72365300	2.84148600	-2.09494800
C	-1	1.14280800	5.30376500	-3.43893700
O	-1	4.12279600	1.67561100	1.35850800
C	-1	6.65413200	0.22290100	3.53634200
C	-1	8.03505700	0.06043400	3.54486600
O	-1	-1.36981100	-2.74642400	3.70895900
C	-1	-2.84592800	-2.36920800	6.04265400
O	-1	-3.29684500	-0.73696400	-1.71273200
C	-1	-5.15888900	-2.20632400	-3.23568500
C	-1	-5.95933000	-3.07256700	-3.97145200
O	-1	0.51962600	-1.98214300	4.67264600
C	-1	-0.94669600	-1.26262400	6.99552000
C	-1	-1.74959700	-0.93141400	8.08073700
O	-1	3.85054300	0.36016900	3.16682400
C	-1	6.88272600	1.25405400	1.38396500
O	-1	-0.17642500	1.95596600	-2.92209400
C	-1	-0.71980000	4.17880600	-4.44523500
C	-1	-1.03519400	5.37267500	-5.07703700
O	-1	2.13213600	-0.50129900	0.83752100
O	-1	0.00778500	1.77966700	0.01136300
O	-1	-0.45725400	-0.18366200	2.68455800
O	-1	-0.66631000	-1.50365600	-0.41582200
O	-1	0.59896300	-2.42103800	1.73434800
O	-1	1.19613500	-0.00545900	-1.55902400
O	-1	1.40286600	1.58546200	2.31501400
O	-1	-2.08228200	0.38438300	0.71852200
C	-1	-4.98617700	12.05568900	-4.77267200

C	-1	-4.80845200	10.79730000	-4.00082400
C	-1	-4.28965300	8.42817100	-2.70994300
C	-1	-5.87388300	-8.76290700	-8.13569800
C	-1	-4.82730200	-7.83904700	-7.62941800
C	-1	-3.14372400	-6.04490200	-6.42220200
C	-1	13.50831800	-4.06718700	1.48476800
C	-1	12.03137200	-4.21767800	1.51551100
C	-1	9.29458600	-4.13837700	1.58598000
C	-1	14.35779800	-0.35838400	1.62656100
C	-1	12.95057700	-0.06607700	2.00482400
C	-1	10.25715300	0.32069400	2.37501200
C	-1	-6.77735700	-0.07712000	12.25044700
C	-1	-5.72375200	-0.43506000	11.26593900
C	-1	-3.98127200	-1.02348400	9.23177700
C	-1	-9.27751300	-8.34516600	-6.17001100
C	-1	-8.58602100	-7.21628300	-5.49284300
C	-1	-7.15918400	-5.27976100	-4.16595100
C	-1	-1.20768300	10.17931000	-6.68248700
C	-1	-0.58761400	7.79677900	-5.47707300
C	-1	-1.51683400	12.91517200	-3.42864600
C	-1	-0.88782900	11.79764100	-2.68043700
C	-1	-0.04122600	9.53567900	-1.38828000
C	-1	12.69209200	-1.86762100	-2.06945700
C	-1	9.98823200	-1.40521300	-1.96647100
C	-1	-6.36879100	-11.27130100	-5.02582300
C	-1	-5.56685700	-10.30391500	-4.23195200
C	-1	-4.07886500	-8.46946100	-2.83983000
C	-1	-9.62722600	1.37246600	11.46309200
C	-1	-8.83147000	1.15812100	10.22792500
C	-1	-7.18231800	0.76563600	8.06581800
C	-1	-0.95671800	-4.56339200	-0.04721500
C	-1	-1.74904700	-5.64597600	-0.71244800
C	-1	-3.25409000	-7.49313900	-2.07427500
C	-1	-3.54851900	0.30341700	3.65623200
C	-1	-4.52959200	0.38034600	4.78314500
C	-1	-6.25545500	0.59759000	6.90905600
C	-1	0.98140000	4.49787300	1.09816300
C	-1	0.81730500	5.85860200	0.50822900
C	-1	0.30897500	8.26893000	-0.69105400
C	-1	4.33461200	-0.60062800	-1.51546700
C	-1	5.80579400	-0.77697700	-1.72768300
C	-1	8.51613800	-1.17475900	-1.91484500
C	-1	-0.28137200	-2.12275200	-3.41151300
C	-1	-0.93222600	-3.14407100	-4.28417300
C	-1	-2.32128700	-5.02671300	-5.71385200
C	-1	3.67750900	-3.14665500	1.75163100
C	-1	5.11442100	-3.54383900	1.73836900
C	-1	7.81465200	-3.99593600	1.65447600
C	-1	-2.76981700	3.37029500	-0.48640500
C	-1	-3.25920400	4.68722200	-1.00609600
C	-1	-3.95845200	7.11783600	-2.08075300
C	-1	-3.81457800	-1.74637400	-1.14446700
C	-1	-4.76015800	-2.58164500	-1.94998200
C	-1	-6.34325400	-4.29573900	-3.39973500
C	-1	0.67860000	2.88875000	-2.81245500
C	-1	0.38316100	4.13570900	-3.58780400
C	-1	-0.23455300	6.49891900	-4.83659500
C	-1	4.56800500	0.96798900	2.31502500
C	-1	6.05171900	0.82497500	2.42869200
C	-1	8.77954700	0.50633500	2.44131600

C	-1	-0.72513900	-2.27074900	4.68852500
C	-1	-1.50082300	-1.98215000	5.93433400
C	-1	-3.08559200	-1.36014000	8.09088600
H	-1	1.47708900	0.04831400	-2.48674900
H	-1	1.84663100	2.33704900	2.73779200
H	-1	0.63817200	-3.32304400	2.09107600
C	-1	14.15125600	-2.15577000	-2.07400700
O	-1	14.99143100	-1.45366500	-1.53873200
H	-1	15.42263400	-3.41405200	-2.66682300
H	-1	-7.53952700	-8.71701200	-9.03205600
H	-1	-6.21639500	-12.81855600	-6.09005900
H	-1	-10.42728000	-9.80091200	-5.83591500
H	-1	15.65078400	0.12585900	0.33491800
H	-1	-2.94423600	14.14207000	-3.27000800
C	-1	-1.54826100	11.49144600	-7.29210000
O	-1	-2.68595200	11.90884500	-7.41664900
O	-1	-0.46356600	12.17122900	-7.71242800
H	-1	-0.77602800	13.02468300	-8.06847800
H	-1	-5.55746800	12.70385000	-6.44776600
H	-1	-10.32781200	2.72613300	12.57407100
H	-1	-8.46421600	-0.67585800	12.86456800
H	-1	14.95513100	-3.64527400	2.62072900
H	-1	0.09542300	-0.97328000	6.96583400
H	-1	-1.34170700	-0.37761500	8.91921600
H	-1	-3.30507900	-2.92344300	5.22988500
H	-1	-3.23481300	0.99668900	9.46501400
H	-1	-4.83926300	1.52542500	11.31421000
H	-1	-6.36807700	-2.47101500	10.92848000
H	-1	5.62897200	-2.40472300	3.49044600
H	-1	7.42326200	-5.22446400	-0.08622000
H	-1	4.95821800	-4.78483900	-0.01469500
H	-1	11.80679400	-4.35156200	3.66302300
H	-1	11.87628900	-4.11789400	-0.62121600
H	-1	9.37342500	-3.99478300	-0.57621000
H	-1	5.77488700	-2.92457700	-1.58258500
H	-1	12.07238000	-3.56421800	-3.25994400
H	-1	12.93501600	-0.09783400	-0.87954400
H	-1	10.46218800	0.31427500	-0.73813500
H	-1	8.68181700	0.97428600	-2.12237500
H	-1	6.21170700	1.32623600	-1.94379600
H	-1	2.00914700	5.29579500	-2.78576900
H	-1	0.94075600	10.31349300	-6.89355300
H	-1	-3.26769900	9.71069500	-6.31610200
H	-1	-2.71880300	7.53787900	-5.18031200
H	-1	-1.88522200	5.43574000	-5.74671100
H	-1	-1.31602400	3.28620900	-4.59652300
H	-1	-3.56028300	5.58250700	0.92847400
H	-1	-4.21008100	7.79481000	-0.03798100
H	-1	-3.09938300	4.12582900	-3.07717100
H	-1	-5.73522700	9.48061200	-5.44606300
H	-1	-3.84746700	11.78193700	-2.34837100
H	-1	-3.34094500	9.62904300	-1.17584400
H	-1	-3.56854000	2.05504900	5.74069700
H	-1	-5.73147800	-1.27545200	4.11736300
H	-1	-7.34023200	-1.05325800	6.01253700
H	-1	-8.07605100	3.17809900	10.08276900
H	-1	-9.34286300	-0.92918600	10.07843600
H	-1	-7.83812700	-1.30145400	8.12099400
H	-1	0.67534500	-4.57135600	-4.16947400
H	-1	-0.57746200	-6.29284500	-5.48924200

H	-1	-2.43604700	-7.71265000	-5.22787500
H	-1	-3.94898600	-9.34461900	-6.37823600
H	-1	-5.44188300	-6.09064000	-8.74445200
H	-1	-2.70360900	-1.97129300	-4.61992400
H	-1	-0.37733200	-5.96333200	-2.34169100
H	-1	-4.69791400	-7.30160000	-0.47176400
H	-1	-3.32117100	-5.61354300	0.75691200
H	-1	-5.94426600	-7.42093500	-2.48149600
H	-1	-7.29230400	-9.12921900	-3.73246000
H	-1	-3.63475700	-11.22519100	-4.53769100
H	-1	-4.83441100	-1.25594600	-3.64464000
H	-1	-6.28748100	-2.80205200	-4.96854100
H	-1	-4.93014500	-4.12336600	-0.45890200
H	-1	-9.45514900	-7.51864000	-3.53428100
H	-1	-7.54518800	-6.60705100	-7.27259000
H	-1	-6.22342200	-4.85533900	-6.07232600
H	-1	6.43795800	1.72261500	0.51208800
H	-1	12.79520000	1.83053700	0.97436300
H	-1	12.73767700	-1.87651000	3.14367200
H	-1	10.27742700	-1.55742600	3.45524500
H	-1	8.52702800	-0.39490000	4.39681600
H	-1	6.04367500	-0.11081600	4.36858100
H	-1	2.29506000	8.11728000	-1.54152700
H	-1	2.74513900	5.90785900	-0.45022200
H	-1	-1.15216300	6.14787800	1.31964500
H	-1	0.91280200	8.98099200	-3.25444600
H	-1	0.16512000	11.07906700	-4.40742000
H	-1	-1.78619100	12.22459600	-0.76027500
N	-1	-2.05391400	-7.14694700	-2.57996600
N	-1	-3.44060400	-9.50660200	-3.41566400
N	-1	-2.89943400	-3.82849600	-5.50232600
N	-1	-3.96720500	-5.59978500	-7.39275800
N	-1	-5.98655500	-4.65222900	-2.15012400
N	-1	-8.05123100	-6.01353600	-3.46887100
N	-1	10.95803000	1.26000300	1.70575900
N	-1	8.20603600	1.10312100	1.37703800
N	-1	-0.78071800	10.42822400	-0.69986600
N	-1	-0.63309800	7.74637200	0.11797900
N	-1	-5.21713000	1.45538700	6.83179300
N	-1	-7.25144400	1.99618300	8.61132300
N	-1	-3.61929100	-2.09173500	7.09235200
N	-1	-4.84518700	-1.97759100	9.63247100
N	-1	7.32303200	-3.24643600	2.66037500
N	-1	9.96234500	-4.23884200	2.75295700
N	-1	7.71698000	-2.25324100	-1.79232700
N	-1	10.42886900	-2.47934700	-2.65128900
N	-1	0.42167200	8.56188000	-5.93715000
N	-1	0.85333700	6.46094400	-4.04223000
N	-1	-3.67401600	6.10143000	-2.91950100
N	-1	-4.95133600	8.39081200	-3.88477600
H	0	-1.51909400	2.93910400	4.74876200
H	0	-0.40921000	3.82648500	4.11597900

Sum of electronic and thermal Free Energies = -13124.531525 (Hartree/Particle).

Table S9: DFT-optimized geometry of **f-[Ce^{IV}-Ce^{III}]$^{2-}$** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.41128600	-2.14785900	-0.52059700
Ce	0	-0.99091700	1.81208700	1.98413300
Ce	-1	-1.73378400	-1.65974300	1.56972900
Ce	-1	2.17831600	1.58457200	-0.00018200
Ce	-1	-1.22395100	0.48402700	-1.32791700
Ce	0	1.66766000	-0.71568200	2.95334200
O	-1	-4.63151500	13.22687300	-4.22726000
C	-1	-4.14075200	10.87924100	-2.63114100
C	-1	-3.87734200	9.67518600	-1.98755900
O	-1	-5.99760600	-9.82993300	-7.85991000
C	-1	-3.94927200	-8.21500900	-6.70662100
C	-1	-3.09519700	-7.31787200	-6.07879900
O	-1	14.15464300	-3.97181500	0.45432800
C	-1	11.31914100	-4.17259200	0.30028300
C	-1	9.93237600	-4.12473500	0.32986900
O	-1	14.82512700	0.48168700	0.72978300
C	-1	12.26576100	1.04388400	1.57205900
O	-1	-6.88112900	0.93617000	12.80109600
C	-1	-4.81411900	0.46794600	10.88898700
C	-1	-3.92472800	0.17730600	9.86192200
O	-1	-9.15569000	-8.53640500	-7.39407900
C	-1	-7.70080400	-6.33803700	-6.24165200
C	-1	-6.97769800	-5.36384200	-5.56418900
C	-1	-2.22902800	9.45138100	-6.08743700
C	-1	-1.92341600	8.23974600	-5.48314100
O	-1	-2.33974700	13.68184000	-2.50869600
C	-1	-1.16070200	11.55887700	-1.19796700
C	-1	12.22236700	-0.74531800	-1.35073100
C	-1	10.85473900	-0.50904700	-1.28883100
O	-1	-7.59949600	-11.12429200	-5.23779700
C	-1	-6.23704200	-9.16318500	-3.68264800
C	-1	-5.48663300	-8.23619000	-2.97167700
O	-1	-10.04769300	0.39600800	12.21270700
C	-1	-8.76804600	-0.17198500	9.68095000
C	-1	-7.93444800	-0.36311900	8.58593200
O	-1	14.45000400	-3.27238000	-2.74144900
C	-1	11.73994900	-2.67256000	-2.69737900
O	-1	-5.64354300	-12.17261200	-5.64873700
C	-1	-4.19607400	-10.33632400	-4.14972400
O	-1	-9.83313200	2.59780000	11.78612500
C	-1	-8.05164000	2.11989600	9.70815200
O	-1	-1.31496800	13.19175900	-4.46149700
C	-1	-0.05844800	10.93780800	-3.23769800
C	-1	0.36980300	9.78113700	-2.59959000
O	-1	15.00772500	-1.32752000	2.06646000
C	-1	12.23097400	-1.03104100	2.77700900
C	-1	10.86666000	-0.83936300	2.96335000
C	-1	0.12466300	9.79317500	-6.40809200
O	-1	-10.09552500	-8.95289800	-5.38974700
C	-1	-8.75932700	-6.87455900	-4.15558300
O	-1	-7.66532100	-1.15378200	12.47547300
C	-1	-5.68513600	-1.75616000	10.64207500
O	-1	14.04164200	-4.03351700	2.70932600
C	-1	11.28572300	-4.31346100	2.69597600
O	-1	-5.52969400	11.92972500	-5.83496400
C	-1	-5.18743600	9.61226900	-4.38039500
O	-1	-6.75712200	-8.04538900	-9.01846900

C	-1	-4.79274800	-6.38229600	-8.00591500
O	-1	0.18251600	-4.25628500	-0.51411800
C	-1	-1.34478000	-6.20916600	-1.93514500
O	-1	-2.84062400	1.32859800	3.47492200
C	-1	-4.38788500	1.31511900	5.83556900
O	-1	0.09042300	4.07419300	1.95041300
C	-1	1.81775900	6.44395500	-0.20782400
C	-1	1.56351600	7.67128500	-0.80628800
O	-1	3.59709600	-1.61036100	-1.47477100
C	-1	6.39573700	-2.02634000	-1.69187700
O	-1	-3.47587600	-0.78918300	3.04066900
C	-1	-5.59433300	-0.53693000	4.90751100
C	-1	-6.47865300	-0.42632100	5.97356900
O	-1	2.01283000	3.83466200	0.80184300
C	-1	-0.36258400	6.58172500	0.78431300
O	-1	3.92560600	0.61108000	-1.30774400
C	-1	6.64027700	0.35249800	-1.86349100
C	-1	8.01077500	0.15213600	-1.95821100
O	-1	-1.52697000	-3.96995000	0.92510000
C	-1	-2.99081200	-6.01980600	-0.20232800
C	-1	-3.75608300	-6.94430700	-0.89833500
O	-1	-0.84191600	-0.94474300	-3.27128300
C	-1	-2.22223200	-2.85830600	-4.79932800
O	-1	3.24215500	-2.51289600	2.76197400
C	-1	6.00130500	-3.05341200	2.69134400
O	-1	-2.59267400	2.46873700	-1.27223500
C	-1	-3.33020000	4.97064500	-2.30854600
O	-1	-2.51659200	3.30442700	0.81820600
C	-1	-3.57769000	5.76072000	-0.06006500
C	-1	-3.93001800	6.99690400	-0.58965700
O	-1	0.78144700	-2.43481400	-2.80484200
C	-1	-0.33287500	-4.31650000	-4.55443700
C	-1	-1.03583100	-5.26321200	-5.28869900
O	-1	2.97998400	-3.44792300	0.72791000
C	-1	5.61806400	-4.36231800	0.71558600
C	-1	6.98534300	-4.59793400	0.67125400
O	-1	-3.57075600	-2.10184700	0.05278700
C	-1	-5.22811800	-3.77152300	-1.46019000
O	-1	1.72782000	2.87325000	-2.03840700
C	-1	1.15134500	5.34895800	-3.35941300
O	-1	4.12537400	1.67094100	1.40364200
C	-1	6.65436800	0.19339600	3.56744200
C	-1	8.03498700	0.02827900	3.57419800
O	-1	-1.37509400	-2.76241600	3.71406800
C	-1	-2.85008800	-2.40408200	6.05143200
O	-1	-3.29929000	-0.69920800	-1.68841300
C	-1	-5.16434100	-2.15091300	-3.22456000
C	-1	-5.96652700	-3.00880300	-3.96816900
O	-1	0.51593800	-2.01057200	4.68443400
C	-1	-0.94862700	-1.30992200	7.01415000
C	-1	-1.75071900	-0.98728400	8.10254200
O	-1	3.85094400	0.33933100	3.19977900
C	-1	6.88451700	1.24402000	1.42466800
O	-1	-0.17405400	1.99898200	-2.87336400
C	-1	-0.71353600	4.23685200	-4.37573700
C	-1	-1.02680600	5.43711100	-4.99639100
O	-1	2.13052400	-0.49734300	0.86288700
O	-1	0.01036900	1.79498200	0.05846600
O	-1	-0.45785200	-0.19186900	2.71319500
O	-1	-0.66994600	-1.48279800	-0.39914900

O	-1	0.59396700	-2.42238800	1.74214800
O	-1	1.19507000	0.02245400	-1.52878300
O	-1	1.40548100	1.57701500	2.35977400
O	-1	-2.08229600	0.39736500	0.75291900
C	-1	-4.96524000	12.12438300	-4.62936600
C	-1	-4.78973400	10.85856700	-3.86924400
C	-1	-4.27514100	8.47661300	-2.60046800
C	-1	-5.89243300	-8.66046400	-8.18497800
C	-1	-4.84404000	-7.74328900	-7.67035800
C	-1	-3.15690400	-5.96355500	-6.44689000
C	-1	13.50017000	-4.09028900	1.47490500
C	-1	12.02294900	-4.23829900	1.50453300
C	-1	9.28632800	-4.15454500	1.57625300
C	-1	14.35660400	-0.38455100	1.65089500
C	-1	12.94999700	-0.09313500	2.03211700
C	-1	10.25736400	0.29521800	2.40638400
C	-1	-6.77615400	-0.16227600	12.28094300
C	-1	-5.72339000	-0.51304500	11.29296100
C	-1	-3.98236500	-1.08584800	9.25310300
C	-1	-9.29493700	-8.25459900	-6.21485900
C	-1	-8.60121900	-7.13333200	-5.52739100
C	-1	-7.17053700	-5.21185700	-4.18288300
C	-1	-1.19058900	10.25873000	-6.55720200
C	-1	-0.57476600	7.86397600	-5.37403300
C	-1	-1.49406600	12.96489600	-3.27809200
C	-1	-0.86702100	11.83930800	-2.54038900
C	-1	-0.02442400	9.56389300	-1.26940700
C	-1	12.68744200	-1.85636400	-2.05863200
C	-1	9.98446800	-1.38988100	-1.95085300
C	-1	-6.39149100	-11.19663700	-5.09838400
C	-1	-5.58761500	-10.23814700	-4.29573600
C	-1	-4.09595600	-8.41945300	-2.88695900
C	-1	-9.62344500	1.29986200	11.50759500
C	-1	-8.82830500	1.09548500	10.27034300
C	-1	-7.18026200	0.71997300	8.10437900
C	-1	-0.96603400	-4.54526600	-0.05886500
C	-1	-1.76049800	-5.62015800	-0.73394900
C	-1	-3.26922600	-7.45181000	-2.11254700
C	-1	-3.54808400	0.29186400	3.69011800
C	-1	-4.52878700	0.36014400	4.81781000
C	-1	-6.25391500	0.56092200	6.94593400
C	-1	0.98918500	4.50143800	1.17006200
C	-1	0.82758100	5.86781900	0.59281700
C	-1	0.32353000	8.29008400	-0.58401400
C	-1	4.33244100	-0.57895400	-1.49134000
C	-1	5.80325300	-0.75607600	-1.70546000
C	-1	8.51281700	-1.15716700	-1.89681400
C	-1	-0.28670700	-2.07482200	-3.40053100
C	-1	-0.93962100	-3.08679500	-4.28249500
C	-1	-2.33244300	-4.95351000	-5.72929300
C	-1	3.67113100	-3.15390700	1.75214100
C	-1	5.10730900	-3.55363800	1.73493600
C	-1	7.80667500	-4.00998200	1.64634600
C	-1	-2.76435100	3.39555300	-0.42418300
C	-1	-3.25136700	4.71812700	-0.93155900
C	-1	-3.94628000	7.15988700	-1.98351000
C	-1	-3.81881200	-1.71286900	-1.12942500
C	-1	-4.76609100	-2.53887500	-1.94246600
C	-1	-6.35263700	-4.23650100	-3.40773800
C	-1	0.68273300	2.92911400	-2.75524700

C	-1	0.38949000	4.18375200	-3.51895200
C	-1	-0.22402100	6.55958100	-4.74567500
C	-1	4.56942400	0.95365900	2.35347400
C	-1	6.05288900	0.80683300	2.46553400
C	-1	8.78011900	0.48299500	2.47468600
C	-1	-0.72935600	-2.29702800	4.69786900
C	-1	-1.50428100	-2.01854500	5.94644700
C	-1	-3.08751200	-1.41359000	8.10897200
H	-1	1.47596800	0.08429400	-2.45602500
H	-1	1.85069500	2.32384300	2.78939600
H	-1	0.63154200	-3.32776500	2.09052300
C	-1	14.14606500	-2.14718200	-2.06612800
O	-1	14.98764300	-1.45163600	-1.52453100
H	-1	15.41498600	-3.40228900	-2.67082000
H	-1	-7.55814400	-8.60315400	-9.08055600
H	-1	-6.24217300	-12.73424700	-6.17694000
H	-1	-10.44736500	-9.71123000	-5.89404600
H	-1	15.65027000	0.10922400	0.36354900
H	-1	-2.91914500	14.19293400	-3.10782200
C	-1	-1.52881800	11.57709100	-7.15456500
O	-1	-2.66575000	11.99775100	-7.27502700
O	-1	-0.44292800	12.25871300	-7.56878300
H	-1	-0.75385600	13.11601200	-7.91685100
H	-1	-5.53560600	12.78910300	-6.29827200
H	-1	-10.32130900	2.64448200	12.63120100
H	-1	-8.46402500	-0.76352800	12.88981000
H	-1	14.94796500	-3.68162300	2.61445100
H	-1	0.09402500	-1.02226100	6.98694900
H	-1	-1.34165200	-0.44204000	8.94603900
H	-1	-3.31041400	-2.94990400	5.23365000
H	-1	-3.23209100	0.93068000	9.50490700
H	-1	-4.83523100	1.44525400	11.35922700
H	-1	-6.37157800	-2.54457900	10.93677300
H	-1	5.62429100	-2.43177100	3.49739500
H	-1	7.41269000	-5.22159600	-0.10558400
H	-1	4.94848400	-4.77804900	-0.02952100
H	-1	11.79849200	-4.39165800	3.65075500
H	-1	11.86768500	-4.11843200	-0.63114900
H	-1	9.36506300	-3.99107000	-0.58452800
H	-1	5.76835800	-2.90486800	-1.58026200
H	-1	12.06435500	-3.54069500	-3.26467100
H	-1	12.93387900	-0.09813400	-0.85241700
H	-1	10.46184900	0.31726200	-0.70672800
H	-1	8.68247700	0.99339600	-2.08445500
H	-1	6.21306000	1.34828800	-1.90215300
H	-1	2.01778100	5.33331800	-2.70651100
H	-1	0.95806100	10.39085100	-6.76742300
H	-1	-3.25141400	9.79058600	-6.19478400
H	-1	-2.70638400	7.60631900	-5.07927900
H	-1	-1.87683100	5.50796500	-5.66529000
H	-1	-1.31145300	3.34680900	-4.53517800
H	-1	-3.55046400	5.59600000	1.01128600
H	-1	-4.19629100	7.81837200	0.06549500
H	-1	-3.09297800	4.17564400	-3.00777100
H	-1	-5.71921700	9.55705900	-5.32644500
H	-1	-3.82662500	11.82605300	-2.20792100
H	-1	-3.32392500	9.66144500	-1.05548900
H	-1	-3.56454000	2.02392900	5.79113400
H	-1	-5.73392100	-1.28714600	4.13690600
H	-1	-7.34193000	-1.07951900	6.03436400

H	-1	-8.06913700	3.11530800	10.14376700
H	-1	-9.34362400	-0.98938700	10.10161800
H	-1	-7.83992400	-1.34631200	8.14052400
H	-1	0.66530200	-4.51808100	-4.18133100
H	-1	-0.59094800	-6.22492400	-5.51675300
H	-1	-2.45213900	-7.64361600	-5.26820200
H	-1	-3.96832400	-9.26202900	-6.43334700
H	-1	-5.45554600	-5.98348200	-8.76902800
H	-1	-2.70886500	-1.90765000	-4.60702700
H	-1	-0.38966100	-5.92496400	-2.36632300
H	-1	-4.71241300	-7.27243200	-0.50805700
H	-1	-3.33230600	-5.59840700	0.73594700
H	-1	-5.95933200	-7.37081200	-2.51857000
H	-1	-7.31077800	-9.06491000	-3.78505400
H	-1	-3.65729300	-11.16015700	-4.61036500
H	-1	-4.83815900	-1.19739300	-3.62475200
H	-1	-6.29434400	-2.72845000	-4.96264600
H	-1	-4.93870200	-4.09402500	-0.46570300
H	-1	-9.47057400	-7.45220200	-3.57155000
H	-1	-7.55955800	-6.50958000	-7.30161400
H	-1	-6.23431400	-4.77153600	-6.08542200
H	-1	6.44047500	1.72146900	0.55725500
H	-1	12.79798800	1.81323300	1.01930300
H	-1	12.73390900	-1.91364300	3.15418100
H	-1	10.27431400	-1.59286600	3.46916400
H	-1	8.52625300	-0.43584800	4.42180000
H	-1	6.04343200	-0.14687900	4.39667000
H	-1	2.30918000	8.14261400	-1.43623400
H	-1	2.75531700	5.92234000	-0.36553300
H	-1	-1.14122300	6.15322400	1.40722100
H	-1	0.92824500	9.02474000	-3.14081400
H	-1	0.18428600	11.13480200	-4.27415600
H	-1	-1.76425200	12.25012800	-0.61618300
N	-1	-2.06849300	-7.10318800	-2.61523700
N	-1	-3.45973500	-9.45240300	-3.47250100
N	-1	-2.90831400	-3.75622700	-5.50656400
N	-1	-3.97971900	-5.50792600	-7.41312300
N	-1	-5.99639100	-4.60522200	-2.16155100
N	-1	-8.06383400	-5.95039200	-3.49246400
N	-1	10.95988000	1.23937700	1.74573100
N	-1	8.20754100	1.09068700	1.41609200
N	-1	-0.76212800	10.45140000	-0.57261200
N	-1	-0.61938000	7.76181300	0.22032100
N	-1	-5.21403100	1.41749200	6.87639800
N	-1	-7.24699500	1.94553900	8.66127600
N	-1	-3.62275000	-2.13490300	7.10380300
N	-1	-4.84799200	-2.04201200	9.64510400
N	-1	7.31663100	-3.26891900	2.65924000
N	-1	9.95409900	-4.26706500	2.74212200
N	-1	7.71166700	-2.23524300	-1.78414200
N	-1	10.42297900	-2.45844500	-2.64567700
N	-1	0.43586900	8.63142300	-5.82719300
N	-1	0.86393300	6.51221500	-3.95190300
N	-1	-3.66388900	6.15077000	-2.83169400
N	-1	-4.93709400	8.45137800	-3.77547200

Sum of electronic and thermal Free Energies = -13048.202180 (Hartree/Particle).

Table S10: DFT-optimized geometry of **f-[Ce^{IV}(CO$_2$$^-$)-Ce^{III}]$^{2-}$** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.38811600	-2.19317400	-0.55059900
Ce	0	-0.98494500	1.82759600	1.88254200
Ce	-1	-1.74588000	-1.64740800	1.54226900
Ce	-1	2.17599600	1.54515200	-0.10810700
Ce	-1	-1.23735000	0.43544600	-1.39986800
Ce	0	1.66453200	-0.69413000	2.89087700
O	-1	-4.59325800	13.13475900	-4.54011400
C	-1	-4.10762200	10.81707700	-2.89928200
C	-1	-3.84756500	9.62482200	-2.23277700
O	-1	-6.08920600	-9.98290300	-7.70469500
C	-1	-4.02811000	-8.35562000	-6.59223500
C	-1	-3.16699400	-7.45043800	-5.98595000
O	-1	14.12610400	-4.06174600	0.40938800
C	-1	11.28902600	-4.25120000	0.27080600
C	-1	9.90265000	-4.19573700	0.30500700
O	-1	14.81990500	0.39292300	0.59288700
C	-1	12.26686700	0.98481700	1.43402500
O	-1	-6.83384900	1.19878700	12.73991500
C	-1	-4.77710100	0.68193500	10.82926600
C	-1	-3.89341300	0.36630100	9.80465800
O	-1	-9.23885700	-8.66433300	-7.25216400
C	-1	-7.76829200	-6.45074300	-6.14986300
C	-1	-7.03755300	-5.46686400	-5.49496300
C	-1	-2.21730900	9.31068200	-6.33394900
C	-1	-1.91525000	8.10984800	-5.70674100
O	-1	-2.29218400	13.61240700	-2.84024300
C	-1	-1.11833700	11.51015100	-1.49201000
C	-1	12.20250300	-0.86226500	-1.45214400
C	-1	10.83633800	-0.61788000	-1.38948700
O	-1	-7.68669900	-11.21640600	-5.05076000
C	-1	-6.30808700	-9.23150100	-3.54069800
C	-1	-5.55014200	-8.29427800	-2.85146100
O	-1	-10.00546600	0.66300500	12.17520800
C	-1	-8.73911600	0.03799500	9.65020700
C	-1	-7.91100500	-0.17923100	8.55589200
O	-1	14.41176500	-3.42789900	-2.80091900
C	-1	11.70493800	-2.81359800	-2.75796900
O	-1	-5.73770500	-12.28263100	-5.44848700
C	-1	-4.27493400	-10.42407300	-3.99239100
O	-1	-9.78169600	2.85470700	11.70375100
C	-1	-8.01119200	2.32630400	9.62861600
O	-1	-1.27792200	13.07816700	-4.78694400
C	-1	-0.02761500	10.84281800	-3.52331100
C	-1	0.39749500	9.69699200	-2.86389200
O	-1	14.99899500	-1.39007700	1.96478800
C	-1	12.22670900	-1.06538000	2.68042200
C	-1	10.86414900	-0.86310300	2.86837500
C	-1	0.13671400	9.63406600	-6.67085300
O	-1	-10.17248100	-9.03587100	-5.23612700
C	-1	-8.82086400	-6.94005000	-4.04922400
O	-1	-7.62978300	-0.89326300	12.45937600
C	-1	-5.66020200	-1.54222700	10.63045700
O	-1	14.02209900	-4.07774100	2.66560700

C	-1	11.26478600	-4.34393400	2.66895500
O	-1	-5.50451400	11.81026800	-6.11788900
C	-1	-5.16781300	9.52067600	-4.61858200
O	-1	-6.84459100	-8.21807200	-8.89570000
C	-1	-4.86779400	-6.54502400	-7.92457300
O	-1	0.14884900	-4.29475700	-0.49694100
C	-1	-1.39399900	-6.26792500	-1.87241000
O	-1	-2.82990200	1.38419700	3.39158600
C	-1	-4.36749500	1.42565400	5.75821900
O	-1	0.10844600	4.08372000	1.80059300
C	-1	1.83865400	6.40104400	-0.41160800
C	-1	1.58806500	7.61742600	-1.03350700
O	-1	3.57258900	-1.68591100	-1.52412900
C	-1	6.36820500	-2.12032800	-1.74411700
O	-1	-3.47750200	-0.73875600	3.00240400
C	-1	-5.58697500	-0.43845800	4.87230400
C	-1	-6.46632900	-0.30206300	5.93948300
O	-1	2.02486300	3.81152300	0.64931900
C	-1	-0.33686500	6.56968000	0.58633500
O	-1	3.91285800	0.53672300	-1.40294200
C	-1	6.62388700	0.25333000	-1.96432500
C	-1	7.99296600	0.04417400	-2.06052700
O	-1	-1.55324000	-3.97103100	0.94311300
C	-1	-3.03190600	-6.03559600	-0.13712500
C	-1	-3.80463900	-6.96995000	-0.81139000
O	-1	-0.87043400	-1.03390200	-3.31574000
C	-1	-2.26654600	-2.97064400	-4.79958100
O	-1	3.23052300	-2.50150800	2.73091400
C	-1	5.98674000	-3.05748000	2.66034700
O	-1	-2.59588900	2.42771400	-1.37842500
C	-1	-3.32520300	4.91208900	-2.46167000
O	-1	-2.50690100	3.30454700	0.69456200
C	-1	-3.55947800	5.74824000	-0.22848700
C	-1	-3.90782200	6.97534800	-0.78131000
O	-1	0.74740000	-2.52253900	-2.82607800
C	-1	-0.38348500	-4.43319700	-4.53313500
C	-1	-1.09417200	-5.39083800	-5.24545400
O	-1	2.95542000	-3.47588000	0.71737500
C	-1	5.58883500	-4.40369900	0.71276000
C	-1	6.95472900	-4.64707800	0.66765500
O	-1	-3.59127800	-2.11043000	0.04181600
C	-1	-5.26314800	-3.80162900	-1.43075400
O	-1	1.72337300	2.79492700	-2.16992800
C	-1	1.15379900	5.24659600	-3.53792600
O	-1	4.12907600	1.64959100	1.28583600
C	-1	6.65958200	0.20285800	3.46860400
C	-1	8.03937800	0.03091900	3.47311100
O	-1	-1.38384500	-2.70870400	3.70670300
C	-1	-2.84737400	-2.29622400	6.04234300
O	-1	-3.31998600	-0.74431500	-1.72821800
C	-1	-5.19857400	-2.21699000	-3.22747200
C	-1	-6.00808500	-3.08551400	-3.95051600
O	-1	0.51508500	-1.94707400	4.65414800
C	-1	-0.93653100	-1.19266600	6.97529400
C	-1	-1.73251000	-0.84425500	8.06022500
O	-1	3.85512000	0.35582100	3.10969400
C	-1	6.88612500	1.20921800	1.30430800
O	-1	-0.18625800	1.91377400	-2.97954400
C	-1	-0.72077600	4.12383700	-4.52426100
C	-1	-1.03061700	5.31300800	-5.16756500

O	-1	2.12109400	-0.51914100	0.79662100
O	-1	0.00913200	1.76767600	-0.04511600
O	-1	-0.45779900	-0.16353100	2.65085000
O	-1	-0.68930300	-1.51524200	-0.43412800
O	-1	0.57888200	-2.41834200	1.72047700
O	-1	1.17854100	-0.04236600	-1.60117400
O	-1	1.41289300	1.58859200	2.25458000
O	-1	-2.08747300	0.39462200	0.68576800
C	-1	-4.93413000	12.02614800	-4.91871200
C	-1	-4.76180100	10.77492200	-4.13410100
C	-1	-4.25385600	8.41625600	-2.81995200
C	-1	-5.97954800	-8.82071900	-8.05354400
C	-1	-4.92448400	-7.89875300	-7.56161900
C	-1	-3.22346800	-6.10346300	-6.38084200
C	-1	13.47526400	-4.15645800	1.43475900
C	-1	11.99745800	-4.29636200	1.47328900
C	-1	9.26160800	-4.19733000	1.55432700
C	-1	14.35087300	-0.45232600	1.53304200
C	-1	12.94731900	-0.14621900	1.91400800
C	-1	10.25822200	0.26317800	2.29125200
C	-1	-6.73649500	0.08963600	12.24144800
C	-1	-5.68957600	-0.28615900	11.25646300
C	-1	-3.95985400	-0.90847400	9.22149900
C	-1	-9.37183300	-8.35828700	-6.07827500
C	-1	-8.66970600	-7.22701700	-5.41619900
C	-1	-7.22393400	-5.28629500	-4.11621400
C	-1	-1.17680600	10.10319900	-6.82396500
C	-1	-0.56805100	7.72951100	-5.59555500
C	-1	-1.45326600	12.87593700	-3.59852100
C	-1	-0.82880100	11.76217400	-2.84095000
C	-1	0.00768000	9.50840700	-1.52804800
C	-1	12.65911200	-1.98959500	-2.13951500
C	-1	9.95896500	-1.50736400	-2.03022600
C	-1	-6.47850500	-11.29206500	-4.91478700
C	-1	-5.66655800	-10.32179100	-4.13473900
C	-1	-4.16005700	-8.48285100	-2.76868500
C	-1	-9.57963000	1.55041000	11.45043300
C	-1	-8.79062700	1.31729300	10.21433300
C	-1	-7.15342300	0.89017500	8.04971100
C	-1	-0.99923000	-4.56875600	-0.03137300
C	-1	-1.80181900	-5.65290200	-0.68159000
C	-1	-3.32532900	-7.50410600	-2.01714300
C	-1	-3.54172400	0.35546600	3.63027400
C	-1	-4.51739000	0.45125200	4.76033100
C	-1	-6.23266500	0.70328800	6.89096600
C	-1	1.00610000	4.49070800	1.00823200
C	-1	0.84892800	5.84606600	0.40438800
C	-1	0.35210500	8.24682100	-0.81868500
C	-1	4.31299200	-0.65878800	-1.56431000
C	-1	5.78200800	-0.84760600	-1.78075500
C	-1	8.48872700	-1.26616400	-1.97493900
C	-1	-0.32138800	-2.16914100	-3.42455600
C	-1	-0.98296800	-3.19523800	-4.28344000
C	-1	-2.39103100	-5.08345000	-5.68694200
C	-1	3.65226400	-3.16502300	1.73279200
C	-1	5.08632800	-3.57220000	1.71775200
C	-1	7.78299500	-4.04390100	1.62746400
C	-1	-2.75945600	3.37217200	-0.54842600
C	-1	-3.24196100	4.68677400	-1.08022700
C	-1	-3.92902000	7.11048900	-2.17807200

C	-1	-3.84224800	-1.74393300	-1.14696200
C	-1	-4.79697700	-2.58123400	-1.93947700
C	-1	-6.39799400	-4.29978100	-3.36405700
C	-1	0.67563000	2.84172900	-2.88353300
C	-1	0.38549600	4.08230500	-3.67102900
C	-1	-0.22122200	6.43619100	-4.94261400
C	-1	4.57356100	0.94910100	2.24804200
C	-1	6.05662700	0.79711900	2.35702600
C	-1	8.78222600	0.45976400	2.36172200
C	-1	-0.73172200	-2.22708000	4.67836500
C	-1	-1.50010400	-1.91970000	5.92424900
C	-1	-3.07137200	-1.26357100	8.08057000
H	-1	1.45590500	-0.00051500	-2.53058500
H	-1	1.86330600	2.34164700	2.66744100
H	-1	0.61313600	-3.31657300	2.08682400
C	-1	14.11622500	-2.28788800	-2.14705300
O	-1	14.96348500	-1.58591700	-1.62288800
H	-1	15.37637000	-3.56125500	-2.73158600
H	-1	-7.64863200	-8.77290400	-8.94338000
H	-1	-6.34130000	-12.85168300	-5.96292200
H	-1	-10.53017300	-9.80235100	-5.72371600
H	-1	15.64166400	0.00903300	0.23086900
H	-1	-2.87149300	14.11433900	-3.44714900
C	-1	-1.51092100	11.41104000	-7.44624800
O	-1	-2.64623000	11.83495900	-7.57053700
O	-1	-0.42336500	12.07872800	-7.87840100
H	-1	-0.73145000	12.93045500	-8.24231700
H	-1	-5.50805400	12.66022300	-6.59828900
H	-1	-10.26614400	2.92076000	12.54968000
H	-1	-8.42481700	-0.49075600	12.86902300
H	-1	14.92976500	-3.73241100	2.56005700
H	-1	0.10742100	-0.91089100	6.93814200
H	-1	-1.31725400	-0.28432300	8.89097900
H	-1	-3.31378400	-2.85596100	5.23751700
H	-1	-3.19850900	1.10886200	9.42984000
H	-1	-4.79140200	1.66855000	11.27991800
H	-1	-6.34934300	-2.32110400	10.94364800
H	-1	5.61615600	-2.41793400	3.45529700
H	-1	7.37575500	-5.28831500	-0.09824800
H	-1	4.91412500	-4.83085900	-0.02116900
H	-1	11.78109300	-4.40560700	3.62303700
H	-1	11.83398700	-4.21846600	-0.66372400
H	-1	9.33224400	-4.07752400	-0.60959400
H	-1	5.73692100	-2.99325800	-1.61240500
H	-1	12.02267100	-3.69454200	-3.30905900
H	-1	12.91928100	-0.20885200	-0.96975900
H	-1	10.44997400	0.22189100	-0.82247400
H	-1	8.66832700	0.87932700	-2.20629700
H	-1	6.20148100	1.25029900	-2.02120600
H	-1	2.02283200	5.23963400	-2.88833400
H	-1	0.97159100	10.22020200	-7.04543400
H	-1	-3.23842500	9.65284500	-6.44395400
H	-1	-2.69969200	7.48860200	-5.28712500
H	-1	-1.88303000	5.37476900	-5.83432300
H	-1	-1.32377400	3.23382100	-4.66343500
H	-1	-3.52865400	5.60485300	0.84583100
H	-1	-4.16729300	7.81109900	-0.14167800
H	-1	-3.09483100	4.10206500	-3.14578000
H	-1	-5.70375900	9.44924300	-5.56119000
H	-1	-3.78703900	11.77056500	-2.49637800

H	-1	-3.29038400	9.62693100	-1.30285300
H	-1	-3.54081900	2.12925400	5.69628400
H	-1	-5.73347700	-1.20322700	4.11744800
H	-1	-7.33259300	-0.94953300	6.01682200
H	-1	-8.02193100	3.33030900	10.04427300
H	-1	-9.31702100	-0.76790100	10.08947500
H	-1	-7.82322000	-1.17160500	8.12989000
H	-1	0.61520600	-4.63232500	-4.16008600
H	-1	-0.65503200	-6.35916200	-5.45598900
H	-1	-2.52222900	-7.76315200	-5.17158500
H	-1	-4.05125300	-9.39685300	-6.29797000
H	-1	-5.53173800	-6.15820600	-8.69284700
H	-1	-2.74763800	-2.01387700	-4.62440300
H	-1	-0.43926200	-5.99724900	-2.31303300
H	-1	-4.76097400	-7.28535300	-0.41077400
H	-1	-3.36742400	-5.59378400	0.79388800
H	-1	-6.01664900	-7.41762500	-2.41387900
H	-1	-7.38173200	-9.12985600	-3.64073000
H	-1	-3.74217000	-11.25967700	-4.43860200
H	-1	-4.86929600	-1.27333200	-3.64799200
H	-1	-6.33859900	-2.82345700	-4.94908100
H	-1	-4.97124500	-4.10562800	-0.43117900
H	-1	-9.53256600	-7.50228100	-3.45088200
H	-1	-7.63227600	-6.64417300	-7.20673700
H	-1	-6.29338200	-4.88887800	-6.03094200
H	-1	6.44089400	1.67145900	0.42930000
H	-1	12.80063700	1.74024600	0.86383300
H	-1	12.72679200	-1.94279400	3.07317100
H	-1	10.27014600	-1.60332500	3.39155900
H	-1	8.53181600	-0.41863800	4.32785500
H	-1	6.05038400	-0.11765800	4.30693200
H	-1	2.33346500	8.07227300	-1.67576300
H	-1	2.77294300	5.87163600	-0.56261000
H	-1	-1.11505300	6.15767800	1.22082900
H	-1	0.94992400	8.92709900	-3.39209900
H	-1	0.21182200	11.01780200	-4.56447400
H	-1	-1.71603100	12.21595300	-0.92176400
N	-1	-2.12495600	-7.17169900	-2.53154200
N	-1	-3.53141200	-9.53052000	-3.33597500
N	-1	-2.96000500	-3.87904900	-5.48592400
N	-1	-4.04798000	-5.66309700	-7.35268800
N	-1	-6.03845200	-4.64529200	-2.11217900
N	-1	-8.11804600	-6.00633400	-3.40755300
N	-1	10.96270400	1.19035800	1.60899900
N	-1	8.20832200	1.04904500	1.29348100
N	-1	-0.72271200	10.41340300	-0.84620700
N	-1	-0.59010000	7.73953200	-0.00014300
N	-1	-5.18882100	1.55301600	6.80010400
N	-1	-7.21175000	2.12696100	8.58221300
N	-1	-3.61433900	-2.00213100	7.09221200
N	-1	-4.82861200	-1.85220700	9.63605200
N	-1	7.30083200	-3.28024600	2.62727500
N	-1	9.93361300	-4.28987900	2.71952000
N	-1	7.68268500	-2.33769800	-1.83747400
N	-1	10.38927600	-2.59182400	-2.70526700
N	-1	0.44451900	8.48260800	-6.06805800
N	-1	0.86974700	6.39920600	-4.15243600
N	-1	-3.65516100	6.08318600	-3.00700300
N	-1	-4.92076700	8.37086800	-3.99154000
C	0	0.84560600	2.29734900	5.49847500

Atom		x	y	z
O	0	1.81235900	2.83966500	5.12386100
O	0	-0.12105300	1.75270700	5.86775500

Sum of electronic and thermal Free Energies = -13236.789681 (Hartree/Particle).

Table S11: DFT-optimized geometry of **TS₁** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.38811600	-2.19317400	-0.55059900
Ce	0	-0.98494500	1.82759600	1.88254200
Ce	-1	-1.74588000	-1.64740800	1.54226900
Ce	-1	2.17599600	1.54515200	-0.10810700
Ce	-1	-1.23735000	0.43544600	-1.39986800
Ce	0	1.66453200	-0.69413000	2.89087700
O	-1	-4.59325800	13.13475900	-4.54011400
C	-1	-4.10762200	10.81707700	-2.89928200
C	-1	-3.84756500	9.62482200	-2.23277700
O	-1	-6.08920600	-9.98290300	-7.70469500
C	-1	-4.02811000	-8.35562000	-6.59223500
C	-1	-3.16699400	-7.45043800	-5.98595000
O	-1	14.12610400	-4.06174600	0.40938800
C	-1	11.28902600	-4.25120000	0.27080600
C	-1	9.90265000	-4.19573700	0.30500700
O	-1	14.81990500	0.39292300	0.59288700
C	-1	12.26686700	0.98481700	1.43402500
O	-1	-6.83384900	1.19878700	12.73991500
C	-1	-4.77710100	0.68193500	10.82926600
C	-1	-3.89341300	0.36630100	9.80465800
O	-1	-9.23885700	-8.66433300	-7.25216400
C	-1	-7.76829200	-6.45074300	-6.14986300
C	-1	-7.03755300	-5.46686400	-5.49496300
C	-1	-2.21730900	9.31068200	-6.33394900
C	-1	-1.91525000	8.10984800	-5.70674100
O	-1	-2.29218400	13.61240700	-2.84024300
C	-1	-1.11833700	11.51015100	-1.49201000
C	-1	12.20250300	-0.86226500	-1.45214400
C	-1	10.83633800	-0.61788000	-1.38948700
O	-1	-7.68669900	-11.21640600	-5.05076000
C	-1	-6.30808700	-9.23150100	-3.54069800
C	-1	-5.55014200	-8.29427800	-2.85146100
O	-1	-10.00546600	0.66300500	12.17520800
C	-1	-8.73911600	0.03799500	9.65020700
C	-1	-7.91100500	-0.17923100	8.55589200
O	-1	14.41176500	-3.42789900	-2.80091900
C	-1	11.70493800	-2.81359800	-2.75796900
O	-1	-5.73770500	-12.28263100	-5.44848700
C	-1	-4.27493400	-10.42407300	-3.99239100
O	-1	-9.78169600	2.85470700	11.70375100
C	-1	-8.01119200	2.32630400	9.62861600
O	-1	-1.27792200	13.07816700	-4.78694400
C	-1	-0.02761500	10.84281800	-3.52331100
C	-1	0.39749500	9.69699200	-2.86389200
O	-1	14.99899500	-1.39007700	1.96478800
C	-1	12.22670900	-1.06538000	2.68042200

C	-1	10.86414900	-0.86310300	2.86837500
C	-1	0.13671400	9.63406600	-6.67085300
O	-1	-10.17248100	-9.03587100	-5.23612700
C	-1	-8.82086400	-6.94005000	-4.04922400
O	-1	-7.62978300	-0.89326300	12.45937600
C	-1	-5.66020200	-1.54222700	10.63045700
O	-1	14.02209900	-4.07774100	2.66560700
C	-1	11.26478600	-4.34393400	2.66895500
O	-1	-5.50451400	11.81026800	-6.11788900
C	-1	-5.16781300	9.52067600	-4.61858200
O	-1	-6.84459100	-8.21807200	-8.89570000
C	-1	-4.86779400	-6.54502400	-7.92457300
O	-1	0.14884900	-4.29475700	-0.49694100
C	-1	-1.39399900	-6.26792500	-1.87241000
O	-1	-2.82990200	1.38419700	3.39158600
C	-1	-4.36749500	1.42565400	5.75821900
O	-1	0.10844600	4.08372000	1.80059300
C	-1	1.83865400	6.40104400	-0.41160800
C	-1	1.58806500	7.61742600	-1.03350700
O	-1	3.57258900	-1.68591100	-1.52412900
C	-1	6.36820500	-2.12032800	-1.74411700
O	-1	-3.47750200	-0.73875600	3.00240400
C	-1	-5.58697500	-0.43845800	4.87230400
C	-1	-6.46632900	-0.30206300	5.93948300
O	-1	2.02486300	3.81152300	0.64931900
C	-1	-0.33686500	6.56968000	0.58633500
O	-1	3.91285800	0.53672300	-1.40294200
C	-1	6.62388700	0.25333000	-1.96432500
C	-1	7.99296600	0.04417400	-2.06052700
O	-1	-1.55324000	-3.97103100	0.94311300
C	-1	-3.03190600	-6.03559600	-0.13712500
C	-1	-3.80463900	-6.96995000	-0.81139000
O	-1	-0.87043400	-1.03390200	-3.31574000
C	-1	-2.26654600	-2.97064400	-4.79958100
O	-1	3.23052300	-2.50150800	2.73091400
C	-1	5.98674000	-3.05748000	2.66034700
O	-1	-2.59588900	2.42771400	-1.37842500
C	-1	-3.32520300	4.91208900	-2.46167000
O	-1	-2.50690100	3.30454700	0.69456200
C	-1	-3.55947800	5.74824000	-0.22848700
C	-1	-3.90782200	6.97534800	-0.78131000
O	-1	0.74740000	-2.52253900	-2.82607800
C	-1	-0.38348500	-4.43319700	-4.53313500
C	-1	-1.09417200	-5.39083800	-5.24545400
O	-1	2.95542000	-3.47588000	0.71737500
C	-1	5.58883500	-4.40369900	0.71276000
C	-1	6.95472900	-4.64707800	0.66765500
O	-1	-3.59127800	-2.11043000	0.04181600
C	-1	-5.26314800	-3.80162900	-1.43075400
O	-1	1.72337300	2.79492700	-2.16992800
C	-1	1.15379900	5.24659600	-3.53792600
O	-1	4.12907600	1.64959100	1.28583600
C	-1	6.65958200	0.20285800	3.46860400
C	-1	8.03937800	0.03091900	3.47311100
O	-1	-1.38384500	-2.70870400	3.70670300
C	-1	-2.84737400	-2.29622400	6.04234300
O	-1	-3.31998600	-0.74431500	-1.72821800
C	-1	-5.19857400	-2.21699000	-3.22747200
C	-1	-6.00808500	-3.08551400	-3.95051600
O	-1	0.51508500	-1.94707400	4.65414800

C	-1	-0.93653100	-1.19266600	6.97529400
C	-1	-1.73251000	-0.84425500	8.06022500
O	-1	3.85512000	0.35582100	3.10969400
C	-1	6.88612500	1.20921800	1.30430800
O	-1	-0.18625800	1.91377400	-2.97954400
C	-1	-0.72077600	4.12383700	-4.52426100
C	-1	-1.03061700	5.31300800	-5.16756500
O	-1	2.12109400	-0.51914100	0.79662100
O	-1	0.00913200	1.76767600	-0.04511600
O	-1	-0.45779900	-0.16353100	2.65085000
O	-1	-0.68930300	-1.51524200	-0.43412800
O	-1	0.57888200	-2.41834200	1.72047700
O	-1	1.17854100	-0.04236600	-1.60117400
O	-1	1.41289300	1.58859200	2.25458000
O	-1	-2.08747300	0.39462200	0.68576800
C	-1	-4.93413000	12.02614800	-4.91871200
C	-1	-4.76180100	10.77492200	-4.13410100
C	-1	-4.25385600	8.41625600	-2.81995200
C	-1	-5.97954800	-8.82071900	-8.05354400
C	-1	-4.92448400	-7.89875300	-7.56161900
C	-1	-3.22346800	-6.10346300	-6.38084200
C	-1	13.47526400	-4.15645800	1.43475900
C	-1	11.99745800	-4.29636200	1.47328900
C	-1	9.26160800	-4.19733000	1.55432700
C	-1	14.35087300	-0.45232600	1.53304200
C	-1	12.94731900	-0.14621900	1.91400800
C	-1	10.25822200	0.26317800	2.29125200
C	-1	-6.73649500	0.08963600	12.24144800
C	-1	-5.68957600	-0.28615900	11.25646300
C	-1	-3.95985400	-0.90847400	9.22149900
C	-1	-9.37183300	-8.35828700	-6.07827500
C	-1	-8.66970600	-7.22701700	-5.41619900
C	-1	-7.22393400	-5.28629500	-4.11621400
C	-1	-1.17680600	10.10319900	-6.82396500
C	-1	-0.56805100	7.72951100	-5.59555500
C	-1	-1.45326600	12.87593700	-3.59852100
C	-1	-0.82880100	11.76217400	-2.84095000
C	-1	0.00768000	9.50840700	-1.52804800
C	-1	12.65911200	-1.98959500	-2.13951500
C	-1	9.95896500	-1.50736400	-2.03022600
C	-1	-6.47850500	-11.29206500	-4.91478700
C	-1	-5.66655800	-10.32179100	-4.13473900
C	-1	-4.16005700	-8.48285100	-2.76868500
C	-1	-9.57963000	1.55041000	11.45043300
C	-1	-8.79062700	1.31729300	10.21433300
C	-1	-7.15342300	0.89017500	8.04971100
C	-1	-0.99923000	-4.56875600	-0.03137300
C	-1	-1.80181900	-5.65290200	-0.68159000
C	-1	-3.32532900	-7.50410600	-2.01714300
C	-1	-3.54172400	0.35546600	3.63027400
C	-1	-4.51739000	0.45125200	4.76033100
C	-1	-6.23266500	0.70328800	6.89096600
C	-1	1.00610000	4.49070800	1.00823200
C	-1	0.84892800	5.84606600	0.40438800
C	-1	0.35210500	8.24682100	-0.81868500
C	-1	4.31299200	-0.65878800	-1.56431000
C	-1	5.78200800	-0.84760600	-1.78075500
C	-1	8.48872700	-1.26616400	-1.97493900
C	-1	-0.32138800	-2.16914100	-3.42455600
C	-1	-0.98296800	-3.19523800	-4.28344000

C	-1	-2.39103100	-5.08345000	-5.68694200
C	-1	3.65226400	-3.16502300	1.73279200
C	-1	5.08632800	-3.57220000	1.71775200
C	-1	7.78299500	-4.04390100	1.62746400
C	-1	-2.75945600	3.37217200	-0.54842600
C	-1	-3.24196100	4.68677400	-1.08022700
C	-1	-3.92902000	7.11048900	-2.17807200
C	-1	-3.84224800	-1.74393300	-1.14696200
C	-1	-4.79697700	-2.58123400	-1.93947700
C	-1	-6.39799400	-4.29978100	-3.36405700
C	-1	0.67563000	2.84172900	-2.88353300
C	-1	0.38549600	4.08230500	-3.67102900
C	-1	-0.22122200	6.43619100	-4.94261400
C	-1	4.57356100	0.94910100	2.24804200
C	-1	6.05662700	0.79711900	2.35702600
C	-1	8.78222600	0.45976400	2.36172200
C	-1	-0.73172200	-2.22708000	4.67836500
C	-1	-1.50010400	-1.91970000	5.92424900
C	-1	-3.07137200	-1.26357100	8.08057000
H	-1	1.45590500	-0.00051500	-2.53058500
H	-1	1.86330600	2.34164700	2.66744100
H	-1	0.61313600	-3.31657300	2.08682400
C	-1	14.11622500	-2.28788800	-2.14705300
O	-1	14.96348500	-1.58591700	-1.62288800
H	-1	15.37637000	-3.56125500	-2.73158600
H	-1	-7.64863200	-8.77290400	-8.94338000
H	-1	-6.34130000	-12.85168300	-5.96292200
H	-1	-10.53017300	-9.80235100	-5.72371600
H	-1	15.64166400	0.00903300	0.23086900
H	-1	-2.87149300	14.11433900	-3.44714900
C	-1	-1.51092100	11.41104000	-7.44624800
O	-1	-2.64623000	11.83495900	-7.57053700
O	-1	-0.42336500	12.07872800	-7.87840100
H	-1	-0.73145000	12.93045500	-8.24231700
H	-1	-5.50805400	12.66022300	-6.59828900
H	-1	-10.26614400	2.92076000	12.54968000
H	-1	-8.42481700	-0.49075600	12.86902300
H	-1	14.92976500	-3.73241100	2.56005700
H	-1	0.10742100	-0.91089100	6.93814200
H	-1	-1.31725400	-0.28432300	8.89097900
H	-1	-3.31378400	-2.85596100	5.23751700
H	-1	-3.19850900	1.10886200	9.42984000
H	-1	-4.79140200	1.66855000	11.27991800
H	-1	-6.34934300	-2.32110400	10.94364800
H	-1	5.61615600	-2.41793400	3.45529700
H	-1	7.37575500	-5.28831500	-0.09824800
H	-1	4.91412500	-4.83085900	-0.02116900
H	-1	11.78109300	-4.40560700	3.62303700
H	-1	11.83398700	-4.21846600	-0.66372400
H	-1	9.33224400	-4.07752400	-0.60959400
H	-1	5.73692100	-2.99325800	-1.61240500
H	-1	12.02267100	-3.69454200	-3.30905900
H	-1	12.91928100	-0.20885200	-0.96975900
H	-1	10.44997400	0.22189100	-0.82247400
H	-1	8.66832700	0.87932700	-2.20629700
H	-1	6.20148100	1.25029900	-2.02120600
H	-1	2.02283200	5.23963400	-2.88833400
H	-1	0.97159100	10.22020200	-7.04543400
H	-1	-3.23842500	9.65284500	-6.44395400
H	-1	-2.69969200	7.48860200	-5.28712500

H	-1	-1.88303000	5.37476900	-5.83432300
H	-1	-1.32377400	3.23382100	-4.66343500
H	-1	-3.52865400	5.60485300	0.84583100
H	-1	-4.16729300	7.81109900	-0.14167800
H	-1	-3.09483100	4.10206500	-3.14578000
H	-1	-5.70375900	9.44924300	-5.56119000
H	-1	-3.78703900	11.77056500	-2.49637800
H	-1	-3.29038400	9.62693100	-1.30285300
H	-1	-3.54081900	2.12925400	5.69628400
H	-1	-5.73347700	-1.20322700	4.11744800
H	-1	-7.33259300	-0.94953300	6.01682200
H	-1	-8.02193100	3.33030900	10.04427300
H	-1	-9.31702100	-0.76790100	10.08947500
H	-1	-7.82322000	-1.17160500	8.12989000
H	-1	0.61520600	-4.63232500	-4.16008600
H	-1	-0.65503200	-6.35916200	-5.45598900
H	-1	-2.52222900	-7.76315200	-5.17158500
H	-1	-4.05125300	-9.39685300	-6.29797000
H	-1	-5.53173800	-6.15820600	-8.69284700
H	-1	-2.74763800	-2.01387700	-4.62440300
H	-1	-0.43926200	-5.99724900	-2.31303300
H	-1	-4.76097400	-7.28535300	-0.41077400
H	-1	-3.36742400	-5.59378400	0.79388800
H	-1	-6.01664900	-7.41762500	-2.41387900
H	-1	-7.38173200	-9.12985600	-3.64073000
H	-1	-3.74217000	-11.25967700	-4.43860200
H	-1	-4.86929600	-1.27333200	-3.64799200
H	-1	-6.33859900	-2.82345700	-4.94908100
H	-1	-4.97124500	-4.10562800	-0.43117900
H	-1	-9.53256600	-7.50228100	-3.45088200
H	-1	-7.63227600	-6.64417300	-7.20673700
H	-1	-6.29338200	-4.88887800	-6.03094200
H	-1	6.44089400	1.67145900	0.42930000
H	-1	12.80063700	1.74024600	0.86383300
H	-1	12.72679200	-1.94279400	3.07317100
H	-1	10.27014600	-1.60332500	3.39155900
H	-1	8.53181600	-0.41863800	4.32785500
H	-1	6.05038400	-0.11765800	4.30693200
H	-1	2.33346500	8.07227300	-1.67576300
H	-1	2.77294300	5.87163600	-0.56261000
H	-1	-1.11505300	6.15767800	1.22082900
H	-1	0.94992400	8.92709900	-3.39209900
H	-1	0.21182200	11.01780200	-4.56447400
H	-1	-1.71603100	12.21595300	-0.92176400
N	-1	-2.12495600	-7.17169900	-2.53154200
N	-1	-3.53141200	-9.53052000	-3.33597500
N	-1	-2.96000500	-3.87904900	-5.48592400
N	-1	-4.04798000	-5.66309700	-7.35268800
N	-1	-6.03845200	-4.64529200	-2.11217900
N	-1	-8.11804600	-6.00633400	-3.40755300
N	-1	10.96270400	1.19035800	1.60899900
N	-1	8.20832200	1.04904500	1.29348100
N	-1	-0.72271200	10.41340300	-0.84620700
N	-1	-0.59010000	7.73953200	-0.00014300
N	-1	-5.18882100	1.55301600	6.80010400
N	-1	-7.21175000	2.12696100	8.58221300
N	-1	-3.61433900	-2.00213100	7.09221200
N	-1	-4.82861200	-1.85220700	9.63605200
N	-1	7.30083200	-3.28024600	2.62727500
N	-1	9.93361300	-4.28987900	2.71952000

Atom		x	y	z
N	-1	7.68268500	-2.33769800	-1.83747400
N	-1	10.38927600	-2.59182400	-2.70526700
N	-1	0.44451900	8.48260800	-6.06805800
N	-1	0.86974700	6.39920600	-4.15243600
N	-1	-3.65516100	6.08318600	-3.00700300
N	-1	-4.92076700	8.37086800	-3.99154000
C	0	0.82780809	2.42242457	5.87800527
O	0	1.79456109	2.96474057	5.50339127
O	0	-0.13885091	1.87778257	6.24728527

Sum of electronic and thermal Free Energies = -13236.780863 (Hartree/Particle).

Table S12: DFT-optimized geometry of **f-[Ce^{IV}(COOH)-Ce^{III}]**$^-$ (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.39611600	-2.17645300	-0.57208700
Ce	0	-0.98505500	1.83575900	1.96058600
Ce	-1	-1.73928000	-1.65604300	1.52505700
Ce	-1	2.17182200	1.56100800	-0.10268600
Ce	-1	-1.23796000	0.44967500	-1.40192200
Ce	0	1.67699900	-0.66507600	2.98704800
O	-1	-4.63556000	13.16048700	-4.44957900
C	-1	-4.14214700	10.83256000	-2.82565700
C	-1	-3.87811700	9.63635500	-2.16784900
O	-1	-6.05702900	-9.93835900	-7.78145600
C	-1	-4.00104400	-8.31250600	-6.65751000
C	-1	-3.14277100	-7.40895300	-6.04479600
O	-1	14.14027000	-4.01061900	0.37257700
C	-1	11.30379800	-4.20826800	0.23301300
C	-1	9.91725500	-4.15755200	0.26780400
O	-1	14.81964800	0.44482900	0.58826900
C	-1	12.26483900	1.02232400	1.43402400
O	-1	-6.83466000	1.09236600	12.74377600
C	-1	-4.77655300	0.59605200	10.82915000
C	-1	-3.89201000	0.29072200	9.80216000
O	-1	-9.21086700	-8.63333000	-7.31894700
C	-1	-7.74731400	-6.42302900	-6.20083000
C	-1	-7.01966400	-5.44155700	-5.53891500
C	-1	-2.24750800	9.35724200	-6.27141200
C	-1	-1.94145500	8.15288000	-5.65296700
O	-1	-2.33577400	13.63326500	-2.74660400
C	-1	-1.15490000	11.52511000	-1.41380700
C	-1	12.20600500	-0.80398800	-1.46545000
C	-1	10.83906300	-0.56449600	-1.40083600
O	-1	-7.65008800	-11.19624400	-5.13631300
C	-1	-6.27767900	-9.21787400	-3.61209000
C	-1	-5.52266700	-8.28321900	-2.91618100
O	-1	-10.00461300	0.55040500	12.17563400
C	-1	-8.73664700	-0.05217400	9.64599600
C	-1	-7.90801100	-0.25877500	8.55002100
O	-1	14.42335900	-3.35259600	-2.83309100
C	-1	11.71456100	-2.74740800	-2.78531800
O	-1	-5.69771100	-12.25323000	-5.54202500
C	-1	-4.24074100	-10.40053900	-4.07269400

O	-1	-9.78802800	2.74618000	11.72004600
C	-1	-8.01615200	2.23858000	9.64089300
O	-1	-1.32009700	13.11644200	-4.69726600
C	-1	-0.06234300	10.87606100	-3.45004100
C	-1	0.36658600	9.72687100	-2.79900300
O	-1	15.00474000	-1.34747800	1.94718400
C	-1	12.23153100	-1.03697300	2.66553200
C	-1	10.86835100	-0.84048600	2.85513200
C	-1	0.10540100	9.69069500	-6.60628500
O	-1	-10.14295900	-9.02250000	-5.30552900
C	-1	-8.79795700	-6.93096300	-4.10364900
O	-1	-7.62384900	-1.00016700	12.44818700
C	-1	-5.65246800	-1.62946300	10.61434400
O	-1	14.03667800	-4.04330700	2.62863500
C	-1	11.28024400	-4.31846100	2.63042900
O	-1	-5.54276700	11.84451800	-6.03678900
C	-1	-5.19840200	9.54522400	-4.55416600
O	-1	-6.81832400	-8.16740300	-8.95953200
C	-1	-4.84680800	-6.49503200	-7.97657200
O	-1	0.16370700	-4.28240600	-0.53350800
C	-1	-1.37296200	-6.25054200	-1.92303400
O	-1	-2.83279600	1.35835200	3.39657900
C	-1	-4.37017300	1.37783500	5.76357200
O	-1	0.09649000	4.07902600	1.82470700
C	-1	1.81881900	6.41792600	-0.37087400
C	-1	1.56418700	7.63796400	-0.98390400
O	-1	3.57879700	-1.65509000	-1.54222200
C	-1	6.37577000	-2.07882300	-1.76573900
O	-1	-3.47361500	-0.76364000	2.99201100
C	-1	-5.58374200	-0.48375300	4.86433400
C	-1	-6.46336300	-0.35795100	5.93259300
O	-1	2.01361500	3.82140300	0.67122500
C	-1	-0.35707600	6.57226500	0.62856300
O	-1	3.91186600	0.56769600	-1.40497700
C	-1	6.62371600	0.29718600	-1.96876900
C	-1	7.99345200	0.09317600	-2.06667100
O	-1	-1.53919300	-3.97464300	0.90907700
C	-1	-3.01133700	-6.03611300	-0.18588700
C	-1	-3.78114200	-6.96805700	-0.86680200
O	-1	-0.86660300	-1.00452900	-3.32845100
C	-1	-2.25666700	-2.93497800	-4.82610700
O	-1	3.24017100	-2.50283900	2.70722900
C	-1	5.99805200	-3.04910900	2.63186900
O	-1	-2.60296400	2.43734400	-1.36586700
C	-1	-3.34050900	4.92712500	-2.43097000
O	-1	-2.51651500	3.29953700	0.71337100
C	-1	-3.57713700	5.74630200	-0.19175200
C	-1	-3.92954800	6.97624800	-0.73561800
O	-1	0.75613400	-2.49142500	-2.84982000
C	-1	-0.36883000	-4.39330700	-4.57052800
C	-1	-1.07652100	-5.34806000	-5.28967300
O	-1	2.96779300	-3.46325000	0.68633400
C	-1	5.60420300	-4.38245900	0.67462800
C	-1	6.97087200	-4.62107200	0.62757400
O	-1	-3.58340200	-2.11418200	0.02157500
C	-1	-5.25001900	-3.80007800	-1.46298300
O	-1	1.71495300	2.82429400	-2.15527300
C	-1	1.13721200	5.28395400	-3.50538500
O	-1	4.12491800	1.66177200	1.29177000
C	-1	6.66044600	0.20745000	3.46364700

C	-1	8.04079200	0.03996000	3.46671900
O	-1	-1.37344000	-2.73185700	3.68173200
C	-1	-2.83794400	-2.34105300	6.02050100
O	-1	-3.31683300	-0.73439500	-1.73854600
C	-1	-5.19087100	-2.20225600	-3.24817500
C	-1	-5.99767700	-3.06813700	-3.97738600
O	-1	0.52295300	-1.97114900	4.63443700
C	-1	-0.93053900	-1.23809300	6.96116600
C	-1	-1.72747100	-0.90014000	8.04870200
O	-1	3.85580300	0.35370500	3.10588600
C	-1	6.88337700	1.23020200	1.30667200
O	-1	-0.19194600	1.94284200	-2.97099800
C	-1	-0.73386900	4.16229800	-4.49957600
C	-1	-1.04767000	5.35509000	-5.13420000
O	-1	2.12410100	-0.50965400	0.78711900
O	-1	0.00448800	1.77612000	-0.03776500
O	-1	-0.45606200	-0.17602800	2.64434800
O	-1	-0.68345700	-1.50614900	-0.45043000
O	-1	0.58783000	-2.42064000	1.69742000
O	-1	1.17940700	-0.01880200	-1.60702100
O	-1	1.40889100	1.58503600	2.26045000
O	-1	-2.08762600	0.39106300	0.68343800
C	-1	-4.97289400	12.05355000	-4.83615700
C	-1	-4.79638300	10.79723500	-4.06066000
C	-1	-4.28058000	8.43076600	-2.76371300
C	-1	-5.95119700	-8.77332800	-8.12188500
C	-1	-4.89905000	-7.85153400	-7.62343400
C	-1	-3.20367700	-6.05934100	-6.42990500
C	-1	13.48990300	-4.11487400	1.39732300
C	-1	12.01256600	-4.25984700	1.43504000
C	-1	9.27642200	-4.17028100	1.51716700
C	-1	14.35351100	-0.40873000	1.52233600
C	-1	12.94903300	-0.10994800	1.90570200
C	-1	10.25868300	0.28797700	2.28627200
C	-1	-6.73379000	-0.01282100	12.23727000
C	-1	-5.68581500	-0.37806800	11.24944300
C	-1	-3.95441000	-0.98000000	9.20978400
C	-1	-9.34464700	-8.33623400	-6.14285200
C	-1	-8.64608800	-7.20752200	-5.47269000
C	-1	-7.20640900	-5.27159300	-4.15886700
C	-1	-1.20965900	10.15666200	-6.75581200
C	-1	-0.59301100	7.77611900	-5.54472500
C	-1	-1.49459400	12.90503600	-3.51031500
C	-1	-0.86639900	11.78784300	-2.76092400
C	-1	-0.02240200	9.52734300	-1.46450900
C	-1	12.66615700	-1.92481800	-2.16103800
C	-1	9.96447700	-1.45215400	-2.04788700
C	-1	-6.44163300	-11.26896600	-5.00105800
C	-1	-5.63271300	-10.30174300	-4.21410800
C	-1	-4.13196500	-8.46787600	-2.83496500
C	-1	-9.58177300	1.44441600	11.45725200
C	-1	-8.79221700	1.22282700	10.21938700
C	-1	-7.15398300	0.81672500	8.05150300
C	-1	-0.98341100	-4.56349100	-0.06978200
C	-1	-1.78258300	-5.64549400	-0.72773200
C	-1	-3.30029600	-7.49190100	-2.07646100
C	-1	-3.54127300	0.32578200	3.62780600
C	-1	-4.51706900	0.41021200	4.75866500
C	-1	-6.23280900	0.64122900	6.89130800
C	-1	0.99269200	4.49465700	1.03519400

C	-1	0.83102900	5.85384000	0.44121400
C	-1	0.32622700	8.26177200	-0.76435600
C	-1	4.31585600	-0.62530000	-1.57506100
C	-1	5.78544200	-0.80777800	-1.79307000
C	-1	8.49347400	-1.21613300	-1.99065100
C	-1	-0.31389800	-2.13715700	-3.44557400
C	-1	-0.97228500	-3.15914300	-4.31178300
C	-1	-2.37444100	-5.04169000	-5.72874400
C	-1	3.66378000	-3.15743100	1.70382900
C	-1	5.09916000	-3.55991100	1.68569500
C	-1	7.79733200	-4.02218400	1.59161600
C	-1	-2.76947800	3.37519200	-0.52901600
C	-1	-3.25633100	4.69207000	-1.05120500
C	-1	-3.95140800	7.12144100	-2.13136000
C	-1	-3.83575500	-1.73989500	-1.16447600
C	-1	-4.78789000	-2.57452100	-1.96291000
C	-1	-6.38355200	-4.28788200	-3.39969200
C	-1	0.66694900	2.87286900	-2.86837600
C	-1	0.37266800	4.11817200	-3.64681900
C	-1	-0.24188500	6.47923200	-4.90122400
C	-1	4.57173100	0.95587500	2.24882700
C	-1	6.05538900	0.80783500	2.35652000
C	-1	8.78206700	0.47925800	2.35836600
C	-1	-0.72275600	-2.25511000	4.65680200
C	-1	-1.49192400	-1.95930300	5.90495000
C	-1	-3.06496400	-1.32393400	8.06619000
H	-1	1.45649500	0.03068700	-2.53614800
H	-1	1.85724300	2.33639200	2.67858800
H	-1	0.62533300	-3.32149600	2.05714200
C	-1	14.12422700	-2.21832000	-2.17093700
O	-1	14.96929100	-1.51742100	-1.64181200
H	-1	15.38840300	-3.48332000	-2.76485700
H	-1	-7.62056900	-8.72448000	-9.01112300
H	-1	-6.29953900	-12.82049400	-6.06049000
H	-1	-10.49824100	-9.78658100	-5.79861300
H	-1	15.64259000	0.06624100	0.22336600
H	-1	-2.91680600	14.13770000	-3.34977700
C	-1	-1.54811300	11.46788900	-7.36855300
O	-1	-2.68481000	11.88901100	-7.48961000
O	-1	-0.46279800	12.14221700	-7.79600300
H	-1	-0.77370100	12.99555500	-8.15369300
H	-1	-5.54914100	12.69791700	-6.51101400
H	-1	-10.27255200	2.80452900	12.56649800
H	-1	-8.42011900	-0.60322100	12.86085000
H	-1	14.94320200	-3.69427800	2.52546700
H	-1	0.11248600	-0.95267100	6.92591400
H	-1	-1.31390100	-0.34490000	8.88343700
H	-1	-3.30266400	-2.89645200	5.21170100
H	-1	-3.19957800	1.03823200	9.43264100
H	-1	-4.79398200	1.57932300	11.28694400
H	-1	-6.33902900	-2.41282200	10.92197400
H	-1	5.62552300	-2.41654800	3.43148400
H	-1	7.39385300	-5.25537100	-0.14301500
H	-1	4.93076400	-4.80647500	-0.06228600
H	-1	11.79690100	-4.38537300	3.58397000
H	-1	11.84850100	-4.16699300	-0.70132900
H	-1	9.34632300	-4.03456400	-0.64583800
H	-1	5.74734200	-2.95472800	-1.64027100
H	-1	12.03506200	-3.62329900	-3.34282300
H	-1	12.92073600	-0.15176700	-0.97844000

H	-1	10.45006800	0.26988500	-0.82769900
H	-1	8.66607700	0.93155000	-2.20647500
H	-1	6.19807100	1.29316500	-2.01836300
H	-1	2.00636600	5.27510300	-2.85597900
H	-1	0.93831200	10.28223700	-6.97672100
H	-1	-3.26974600	9.69687900	-6.37879500
H	-1	-2.72381100	7.52606700	-5.23775900
H	-1	-1.90038500	5.41891600	-5.80037800
H	-1	-1.33400000	3.27136400	-4.64511600
H	-1	-3.54567700	5.59523200	0.88149300
H	-1	-4.19162700	7.80649400	-0.08990800
H	-1	-3.10762100	4.12283300	-3.12096500
H	-1	-5.73426500	9.47888600	-5.49719300
H	-1	-3.82459200	11.78413700	-2.41589600
H	-1	-3.32079700	9.63353100	-1.23800900
H	-1	-3.54579200	2.08454400	5.70662600
H	-1	-5.72788400	-1.24350100	4.10397400
H	-1	-7.32751000	-1.00877200	6.00535500
H	-1	-8.03008200	3.23950500	10.06381900
H	-1	-9.31186500	-0.86310400	10.07948900
H	-1	-7.81707600	-1.24774500	8.11682400
H	-1	0.63056100	-4.59189300	-4.19906800
H	-1	-0.63427700	-6.31340300	-5.50728100
H	-1	-2.49686400	-7.72546800	-5.23280700
H	-1	-4.02076200	-9.35591300	-6.37079800
H	-1	-5.51212600	-6.10481200	-8.74193200
H	-1	-2.74083100	-1.98107300	-4.64393200
H	-1	-0.41917800	-5.97358300	-2.36181500
H	-1	-4.73638500	-7.28945600	-0.46835200
H	-1	-3.34813600	-5.60215200	0.74835000
H	-1	-5.99194600	-7.41127800	-2.47219300
H	-1	-7.35166500	-9.11899200	-3.71123700
H	-1	-3.70534100	-11.23115300	-4.52502400
H	-1	-4.86472400	-1.25451200	-3.66188900
H	-1	-6.32919900	-2.79992400	-4.97398000
H	-1	-4.95697100	-4.11036700	-0.46567800
H	-1	-9.50773500	-7.49982300	-3.50930100
H	-1	-7.61083900	-6.60835200	-7.25909600
H	-1	-6.27745700	-4.85729100	-6.07079100
H	-1	6.43650900	1.69732600	0.43509800
H	-1	12.79606500	1.78359500	0.86925100
H	-1	12.73451800	-1.91558400	3.05184100
H	-1	10.27683600	-1.58640300	3.37301800
H	-1	8.53482300	-0.41418100	4.31811400
H	-1	6.05242300	-0.12110900	4.29971300
H	-1	2.30800400	8.09987100	-1.62294700
H	-1	2.75479600	5.89266000	-0.52583600
H	-1	-1.13382200	6.15315200	1.26015900
H	-1	0.92142400	8.96262300	-3.33285300
H	-1	0.17635800	11.05936300	-4.48994100
H	-1	-1.75478700	12.22481700	-0.83837700
N	-1	-2.10109000	-7.15188200	-2.58860100
N	-1	-3.50001700	-9.50936000	-3.40992000
N	-1	-2.94728600	-3.84063000	-5.51892200
N	-1	-4.02976800	-5.61461900	-7.39842200
N	-1	-6.02269200	-4.64129100	-2.15040100
N	-1	-8.09806700	-5.99964700	-3.45532200
N	-1	10.96004400	1.22236000	1.61066100
N	-1	8.20608500	1.07440200	1.29450400
N	-1	-0.75561600	10.42499900	-0.77602500

N	-1	-0.61419800	7.74551000	0.05061600
N	-1	-5.19174100	1.49497600	6.80646500
N	-1	-7.21623600	2.04942200	8.59296500
N	-1	-3.60569000	-2.05706900	7.07257900
N	-1	-4.82003600	-1.92952700	9.61760400
N	-1	7.31285400	-3.26736500	2.59700300
N	-1	9.94891000	-4.26909400	2.68156600
N	-1	7.69093300	-2.29124500	-1.86084800
N	-1	10.39819400	-2.53029200	-2.73083000
N	-1	0.41703500	8.53590300	-6.01189500
N	-1	0.84932500	6.44006000	-4.11148400
N	-1	-3.67435200	6.10106700	-2.96775400
N	-1	-4.94752800	8.39170800	-3.93550900
C	0	0.98280700	0.99433500	4.96145400
O	0	1.32255100	1.04456300	6.12990500
O	0	-0.03135400	1.91355300	4.57035200
H	0	-0.32035000	2.41961700	5.36068300

Sum of electronic and thermal Free Energies = -13237.217312 (Hartree/Particle).

Table S13: DFT-optimized geometry of **f-[Ce^{IV}(COOH)-Ce^{IV}(CO$_2$$^-$)]$^-$** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.39041100	-2.20607700	-0.59971400
Ce	0	-1.02586900	1.85942500	1.83282800
Ce	-1	-1.73795400	-1.66133600	1.50174800
Ce	-1	2.15945300	1.53968500	-0.18921800
Ce	-1	-1.25283900	0.40152800	-1.45829100
Ce	0	1.68476500	-0.67027300	2.87356600
O	-1	-4.69115900	13.05784900	-4.68197600
C	-1	-4.18612900	10.75553700	-3.02543600
C	-1	-3.91681900	9.56987900	-2.35088600
O	-1	-6.07315800	-10.09127900	-7.66301900
C	-1	-4.01650100	-8.44427300	-6.57156900
C	-1	-3.15789800	-7.52977200	-5.97579500
O	-1	14.14228500	-3.99772800	0.32207400
C	-1	11.30574700	-4.20371400	0.19663800
C	-1	9.91923900	-4.15555200	0.23612400
O	-1	14.81238100	0.46193800	0.46855200
C	-1	12.25958600	1.04634800	1.31563700
O	-1	-6.79575500	1.24307000	12.69814900
C	-1	-4.74401100	0.72276600	10.78306200
C	-1	-3.86279000	0.40408700	9.75727200
O	-1	-9.22812300	-8.78646800	-7.20763800
C	-1	-7.76524200	-6.55647900	-6.12841100
C	-1	-7.03724600	-5.56362100	-5.48409000
C	-1	-2.30160200	9.23310600	-6.45621000
C	-1	-1.99040400	8.03879700	-5.82106200
O	-1	-2.38582600	13.56109900	-2.99531200
C	-1	-1.19497700	11.47570600	-1.63584700
C	-1	12.19358700	-0.82319700	-1.55599500
C	-1	10.82636800	-0.58579200	-1.48958600
O	-1	-7.65302500	-11.31303300	-4.99314400
C	-1	-6.27917600	-9.30908400	-3.50403800

C	-1	-5.52357900	-8.36246900	-2.82513600
O	-1	-9.96666100	0.68567100	12.15063800
C	-1	-8.70720900	0.04817800	9.62530800
C	-1	-7.88238700	-0.17293700	8.52928800
O	-1	14.41137100	-3.38703900	-2.89414900
C	-1	11.70141300	-2.78719900	-2.84475900
O	-1	-5.69985000	-12.37163900	-5.39071000
C	-1	-4.24137000	-10.49398700	-3.95494600
O	-1	-9.75684200	2.87486900	11.66147200
C	-1	-7.99194300	2.34018900	9.58317300
O	-1	-1.37659600	13.01744400	-4.94202100
C	-1	-0.10890200	10.79873200	-3.66644700
C	-1	0.32517200	9.66034700	-3.00001900
O	-1	15.00684300	-1.30945700	1.85333400
C	-1	12.23575900	-0.99439200	2.57787200
C	-1	10.87288600	-0.79811100	2.76988100
C	-1	0.04921900	9.56672500	-6.80527900
O	-1	-10.15146600	-9.14757900	-5.18498200
C	-1	-8.80653900	-7.03535100	-4.01976300
O	-1	-7.58133700	-0.85538600	12.43694000
C	-1	-5.61570100	-1.50764300	10.60495300
O	-1	14.04757000	-3.99694100	2.57875800
C	-1	11.29179700	-4.27813500	2.59550700
O	-1	-5.60156100	11.71631300	-6.24578100
C	-1	-5.24619400	9.44019000	-4.73036400
O	-1	-6.84306300	-8.33980700	-8.86439800
C	-1	-4.87153000	-6.64858200	-7.91428000
O	-1	0.16294800	-4.31394000	-0.52485000
C	-1	-1.37465700	-6.30600800	-1.87878200
O	-1	-2.83100200	1.37825300	3.33234800
C	-1	-4.35917300	1.42969000	5.70481700
O	-1	0.08594400	4.08161700	1.70852000
C	-1	1.79437800	6.39126300	-0.52849400
C	-1	1.53458600	7.60144100	-1.15866300
O	-1	3.56810100	-1.69443600	-1.58610500
C	-1	6.36513500	-2.11527200	-1.81427500
O	-1	-3.46857300	-0.75095800	2.96202900
C	-1	-5.57201100	-0.44780400	4.83825300
C	-1	-6.44774100	-0.30800400	5.90796800
O	-1	1.99913400	3.81103300	0.55147800
C	-1	-0.37794600	6.55570000	0.47708100
O	-1	3.89665400	0.53088300	-1.48337200
C	-1	6.60689200	0.25798200	-2.05372800
C	-1	7.97669500	0.05556300	-2.15396300
O	-1	-1.53500600	-3.98843100	0.91966900
C	-1	-3.00672500	-6.06927900	-0.13859600
C	-1	-3.77706300	-7.01299100	-0.80248800
O	-1	-0.88569900	-1.08046700	-3.36434200
C	-1	-2.27720800	-3.03614300	-4.82753000
O	-1	3.24798200	-2.47936000	2.67682800
C	-1	6.00678100	-3.02059300	2.59878100
O	-1	-2.62220200	2.38648900	-1.44654300
C	-1	-3.36955000	4.85844500	-2.54578700
O	-1	-2.52960000	3.27983400	0.61923600
C	-1	-3.59929900	5.71045300	-0.31813500
C	-1	-3.95662200	6.93135500	-0.87891100
O	-1	0.74226500	-2.55645300	-2.86995500
C	-1	-0.38508200	-4.48631100	-4.55763800
C	-1	-1.09340400	-5.45326400	-5.25965900
O	-1	2.96990400	-3.47045200	0.67158300

C	-1	5.60832900	-4.38389900	0.66322900
C	-1	6.97534200	-4.62016400	0.61436400
O	-1	-3.58688200	-2.14596200	0.01254100
C	-1	-5.25544500	-3.85752900	-1.44011300
O	-1	1.69171200	2.77115600	-2.25862200
C	-1	1.10312400	5.20909000	-3.64302000
O	-1	4.11774000	1.66558900	1.19588300
C	-1	6.66501800	0.24948600	3.37923600
C	-1	8.04574300	0.08511500	3.37937600
O	-1	-1.36126000	-2.70400200	3.67278700
C	-1	-2.81751200	-2.28154700	6.01120600
O	-1	-3.33031500	-0.79203500	-1.76901800
C	-1	-5.20689100	-2.28642500	-3.24917900
C	-1	-6.01456700	-3.16488500	-3.96220100
O	-1	0.53710400	-1.92495400	4.60656100
C	-1	-0.90896200	-1.16044100	6.92778700
C	-1	-1.70241000	-0.80804400	8.01328400
O	-1	3.85867600	0.38417500	3.03037000
C	-1	6.87721000	1.24039400	1.20637200
O	-1	-0.21634800	1.87340000	-3.05358700
C	-1	-0.76927000	4.06857100	-4.61298500
C	-1	-1.08825200	5.25105300	-5.26410600
O	-1	2.11990600	-0.51755400	0.73158200
O	-1	-0.00809400	1.75094800	-0.11898800
O	-1	-0.45374200	-0.16193100	2.59376100
O	-1	-0.69018800	-1.53863300	-0.47989600
O	-1	0.59154200	-2.41812300	1.67634900
O	-1	1.16476700	-0.06461100	-1.66588300
O	-1	1.40569400	1.59732300	2.17627900
O	-1	-2.09422800	0.37219400	0.63103900
C	-1	-5.02748500	11.94451700	-5.05065500
C	-1	-4.84509600	10.70032000	-4.25718900
C	-1	-4.31886500	8.35463500	-2.92709700
C	-1	-5.97130000	-8.93123200	-8.02121600
C	-1	-4.91931300	-7.99977000	-7.54072600
C	-1	-3.22337100	-6.18620200	-6.38076700
C	-1	13.49616000	-4.08810200	1.35081300
C	-1	12.01931500	-4.23576400	1.39650300
C	-1	9.28331500	-4.15103400	1.48805000
C	-1	14.35183100	-0.37860300	1.41708400
C	-1	12.94818400	-0.07723600	1.80147000
C	-1	10.25844200	0.32037700	2.18664000
C	-1	-6.69435200	0.13066600	12.20780500
C	-1	-5.64941200	-0.24697700	11.22142500
C	-1	-3.92461500	-0.87547800	9.18418300
C	-1	-9.35798800	-8.47213300	-6.03559200
C	-1	-8.65938400	-7.33199300	-5.38510900
C	-1	-7.21899100	-5.37347500	-4.10601000
C	-1	-1.26746900	10.02749600	-6.95657100
C	-1	-0.64069600	7.66667900	-5.71251500
C	-1	-1.54598100	12.82340600	-3.75137000
C	-1	-0.91233100	11.71892400	-2.98786100
C	-1	-0.05815200	9.47991600	-1.66117400
C	-1	12.65356700	-1.95327200	-2.23657700
C	-1	9.95128200	-1.48495000	-2.11986600
C	-1	-6.44389000	-11.38105300	-4.86157400
C	-1	-5.63410400	-10.40039500	-4.09234100
C	-1	-4.13215500	-8.54281500	-2.74664500
C	-1	-9.54865900	1.56978500	11.41733100
C	-1	-8.76343600	1.33147600	10.17981500

C	-1	-7.13275400	0.89666100	8.01180600
C	-1	-0.98171100	-4.59060300	-0.05247000
C	-1	-1.78098600	-5.68408000	-0.69104300
C	-1	-3.29975100	-7.55378100	-2.00607500
C	-1	-3.53622400	0.34768700	3.58175000
C	-1	-4.50779000	0.44684100	4.71505400
C	-1	-6.21571800	0.70589300	6.85074500
C	-1	0.97811300	4.48738900	0.90937000
C	-1	0.81104700	5.83718700	0.29580500
C	-1	0.29607900	8.22571900	-0.94358300
C	-1	4.30268600	-0.66362300	-1.63721400
C	-1	5.77182100	-0.84608600	-1.85825500
C	-1	8.47998100	-1.25135500	-2.06037300
C	-1	-0.33088600	-2.21349200	-3.46671600
C	-1	-0.99032400	-3.24975700	-4.31497400
C	-1	-2.39371800	-5.15635800	-5.69814400
C	-1	3.66915800	-3.14792800	1.68165300
C	-1	5.10536700	-3.54745900	1.66388100
C	-1	7.80419400	-4.00511500	1.56609800
C	-1	-2.78758000	3.33636200	-0.62313700
C	-1	-3.27945500	4.64421300	-1.16300900
C	-1	-3.98425600	7.05563400	-2.27656800
C	-1	-3.84470900	-1.78999300	-1.17796300
C	-1	-4.79805400	-2.63855700	-1.96009500
C	-1	-6.39541400	-4.37671500	-3.36484900
C	-1	0.64082600	2.80675400	-2.96824200
C	-1	0.34068300	4.03963600	-3.76402500
C	-1	-0.28411900	6.38032900	-5.05111100
C	-1	4.56988600	0.97505800	2.16160600
C	-1	6.05428500	0.83192600	2.26565800
C	-1	8.78168900	0.50944600	2.26168100
C	-1	-0.70786100	-2.21130400	4.63806400
C	-1	-1.47282300	-1.89858800	5.88467300
C	-1	-3.03885800	-1.23448800	8.04236000
H	-1	1.43811500	-0.02839400	-2.59672900
H	-1	1.85396700	2.35583200	2.58138700
H	-1	0.63249400	-3.31342000	2.04933000
C	-1	14.11225000	-2.24366300	-2.24783100
O	-1	14.95777800	-1.53307100	-1.73255800
H	-1	15.37696900	-3.51459500	-2.82776900
H	-1	-7.64423600	-8.89936600	-8.90451000
H	-1	-6.30240600	-12.94791400	-5.89827600
H	-1	-10.50693400	-9.91972500	-5.66520300
H	-1	15.63475000	0.07976200	0.10610500
H	-1	-2.97035100	14.05518200	-3.60365700
C	-1	-1.61128800	11.32867100	-7.58748200
O	-1	-2.74940200	11.74542200	-7.71033900
O	-1	-0.52918300	11.99893800	-8.02921800
H	-1	-0.84341600	12.84614800	-8.39838200
H	-1	-5.61172300	12.56251700	-6.73266500
H	-1	-10.23819200	2.94478300	12.50885800
H	-1	-8.37689000	-0.45408300	12.84676100
H	-1	14.95289000	-3.64748700	2.46682500
H	-1	0.13326800	-0.87327000	6.88417500
H	-1	-1.28684800	-0.23948300	8.83800300
H	-1	-3.28412200	-2.84999200	5.21262200
H	-1	-3.17350400	1.14752300	9.37391300
H	-1	-4.76188700	1.71272400	11.22619100
H	-1	-6.29927600	-2.28783600	10.92694300
H	-1	5.63593900	-2.37698300	3.39032300

H	-1	7.39675300	-5.26496500	-0.14832800
H	-1	4.93298500	-4.82036400	-0.06461900
H	-1	11.81232000	-4.32965300	3.54789900
H	-1	11.84670500	-4.17519700	-0.74035200
H	-1	9.34446900	-4.04748900	-0.67699900
H	-1	5.73919200	-2.99059300	-1.67327300
H	-1	12.02172400	-3.67060900	-3.39038200
H	-1	12.90873000	-0.16219500	-1.08159200
H	-1	10.43771900	0.25619400	-0.92744200
H	-1	8.64686400	0.89324100	-2.30891300
H	-1	6.17879600	1.25216500	-2.11651100
H	-1	1.97482300	5.21186300	-2.99697900
H	-1	0.87933300	10.15450900	-7.18777900
H	-1	-3.32502000	9.56883900	-6.56462800
H	-1	-2.76970900	7.41652700	-5.39346800
H	-1	-1.94370200	5.30303400	-5.92780200
H	-1	-1.36793900	3.17423600	-4.74284600
H	-1	-3.56330900	5.57550200	0.75711500
H	-1	-4.21806400	7.77057300	-0.24464200
H	-1	-3.13752900	4.04445200	-3.22460900
H	-1	-5.78558000	9.35858700	-5.67017900
H	-1	-3.86914000	11.71382900	-2.63117900
H	-1	-3.35587100	9.58217700	-1.42330800
H	-1	-3.53662800	2.13729100	5.63408400
H	-1	-5.71739200	-1.21914200	4.08989400
H	-1	-7.31011700	-0.95957600	5.99383800
H	-1	-8.00649500	3.34728700	9.99116000
H	-1	-9.27888800	-0.75745600	10.07312000
H	-1	-7.79089800	-1.16806400	8.11054900
H	-1	0.61619900	-4.67711400	-4.18719000
H	-1	-0.64982000	-6.42076800	-5.46457000
H	-1	-2.50811200	-7.83269300	-5.16171900
H	-1	-4.03273100	-9.48332300	-6.26923600
H	-1	-5.54071300	-6.27131200	-8.68275500
H	-1	-2.76282400	-2.08069600	-4.65771300
H	-1	-0.42322400	-6.03352500	-2.32539800
H	-1	-4.73001200	-7.33051500	-0.39552900
H	-1	-3.34086200	-5.62215600	0.79037600
H	-1	-5.99310100	-7.48503400	-2.39237200
H	-1	-7.35376200	-9.21407000	-3.60042300
H	-1	-3.70585400	-11.33007900	-4.39692800
H	-1	-4.88451300	-1.34424700	-3.67827600
H	-1	-6.35058300	-2.91232300	-4.96137700
H	-1	-4.95780400	-4.15223600	-0.43944800
H	-1	-9.51269900	-7.59683800	-3.41420100
H	-1	-7.63247600	-6.75728700	-7.18432100
H	-1	-6.29844900	-4.98572400	-6.02754600
H	-1	6.42588500	1.69345700	0.32968700
H	-1	12.78687400	1.80027100	0.73747600
H	-1	12.74224400	-1.86601900	2.97527300
H	-1	10.28509200	-1.53751600	3.30116800
H	-1	8.54412100	-0.35516300	4.23550600
H	-1	6.06101000	-0.06789200	4.22249900
H	-1	2.27485400	8.05539500	-1.80745300
H	-1	2.73093400	5.86581300	-0.67927900
H	-1	-1.15126900	6.14435100	1.11791600
H	-1	0.87965800	8.88943900	-3.52457900
H	-1	0.12532300	10.96700700	-4.70989900
H	-1	-1.79420300	12.18260200	-1.06857100
N	-1	-2.10332800	-7.21879800	-2.52794800

Atom		x	y	z
N	-1	-3.50009100	-9.59137100	-3.30847000
N	-1	-2.96846600	-3.95356800	-5.50402400
N	-1	-4.05424200	-5.75782600	-7.35255600
N	-1	-6.02888100	-4.71062400	-2.11185000
N	-1	-8.10624200	-6.09290900	-3.38817100
N	-1	10.95503900	1.24611300	1.49440100
N	-1	8.20021000	1.08735600	1.19132700
N	-1	-0.79071100	10.38613200	-0.98328900
N	-1	-0.63998400	7.71960900	-0.11730100
N	-1	-5.17693000	1.56057800	6.74907000
N	-1	-7.19569300	2.13716900	8.53504500
N	-1	-3.58179100	-1.98357700	7.06194000
N	-1	-4.78648500	-1.82072000	9.60953600
N	-1	7.32193000	-3.23643500	2.56200400
N	-1	9.96056300	-4.23095500	2.65113900
N	-1	7.68039700	-2.32618100	-1.91137600
N	-1	10.38477900	-2.57220600	-2.78833900
N	-1	0.36579100	8.42163300	-6.19494600
N	-1	0.81025000	6.35537300	-4.26517400
N	-1	-3.70814900	6.02349500	-3.09872000
N	-1	-4.99028900	8.29660200	-4.09554700
C	0	-0.49001000	2.65117800	4.05597500
C	0	1.75106800	0.46610100	5.00913500
O	0	0.64101200	0.78531800	5.60851600
O	0	2.89665500	0.75584700	5.55416700
O	0	-1.44357400	3.02658600	4.85795200
O	0	0.75071000	2.70005600	4.44534100
H	0	2.92485800	1.20661400	6.40128700

Sum of electronic and thermal Free Energies = -13425.800511 (Hartree/Particle).

Table S14: DFT-optimized geometry of **TS₂** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.39041100	-2.20607700	-0.59971400
Ce	0	-1.02586900	1.85942500	1.83282800
Ce	-1	-1.73795400	-1.66133600	1.50174800
Ce	-1	2.15945300	1.53968500	-0.18921800
Ce	-1	-1.25283900	0.40152800	-1.45829100
Ce	0	1.68476500	-0.67027300	2.87356600
O	-1	-4.69115900	13.05784900	-4.68197600
C	-1	-4.18612900	10.75553700	-3.02543600
C	-1	-3.91681900	9.56987900	-2.35088600
O	-1	-6.07315800	-10.09127900	-7.66301900
C	-1	-4.01650100	-8.44427300	-6.57156900
C	-1	-3.15789800	-7.52977200	-5.97579500
O	-1	14.14228500	-3.99772800	0.32207400
C	-1	11.30574700	-4.20371400	0.19663800
C	-1	9.91923900	-4.15555200	0.23612400
O	-1	14.81238100	0.46193800	0.46855200
C	-1	12.25958600	1.04634800	1.31563700
O	-1	-6.79575500	1.24307000	12.69814900
C	-1	-4.74401100	0.72276600	10.78306200
C	-1	-3.86279000	0.40408700	9.75727200

O	-1	-9.22812300	-8.78646800	-7.20763800
C	-1	-7.76524200	-6.55647900	-6.12841100
C	-1	-7.03724600	-5.56362100	-5.48409000
C	-1	-2.30160200	9.23310600	-6.45621000
C	-1	-1.99040400	8.03879700	-5.82106200
O	-1	-2.38582600	13.56109900	-2.99531200
C	-1	-1.19497700	11.47570600	-1.63584700
C	-1	12.19358700	-0.82319700	-1.55599500
C	-1	10.82636800	-0.58579200	-1.48958600
O	-1	-7.65302500	-11.31303300	-4.99314400
C	-1	-6.27917600	-9.30908400	-3.50403800
C	-1	-5.52357900	-8.36246900	-2.82513600
O	-1	-9.96666100	0.68567100	12.15063800
C	-1	-8.70720900	0.04817800	9.62530800
C	-1	-7.88238700	-0.17293700	8.52928800
O	-1	14.41137100	-3.38703900	-2.89414900
C	-1	11.70141300	-2.78719900	-2.84475900
O	-1	-5.69985000	-12.37163900	-5.39071000
C	-1	-4.24137000	-10.49398700	-3.95494600
O	-1	-9.75684200	2.87486900	11.66147200
C	-1	-7.99194300	2.34018900	9.58317300
O	-1	-1.37659600	13.01744400	-4.94202100
C	-1	-0.10890200	10.79873200	-3.66644700
C	-1	0.32517200	9.66034700	-3.00001900
O	-1	15.00684300	-1.30945700	1.85333400
C	-1	12.23575900	-0.99439200	2.57787200
C	-1	10.87288600	-0.79811100	2.76988100
C	-1	0.04921900	9.56672500	-6.80527900
O	-1	-10.15146600	-9.14757900	-5.18498200
C	-1	-8.80653900	-7.03535100	-4.01976300
O	-1	-7.58133700	-0.85538600	12.43694000
C	-1	-5.61570100	-1.50764300	10.60495300
O	-1	14.04757000	-3.99694100	2.57875800
C	-1	11.29179700	-4.27813500	2.59550700
O	-1	-5.60156100	11.71631300	-6.24578100
C	-1	-5.24619400	9.44019000	-4.73036400
O	-1	-6.84306300	-8.33980700	-8.86439800
C	-1	-4.87153000	-6.64858200	-7.91428000
O	-1	0.16294800	-4.31394000	-0.52485000
C	-1	-1.37465700	-6.30600800	-1.87878200
O	-1	-2.83100200	1.37825300	3.33234800
C	-1	-4.35917300	1.42969000	5.70481700
O	-1	0.08594400	4.08161700	1.70852000
C	-1	1.79437800	6.39126300	-0.52849400
C	-1	1.53458600	7.60144100	-1.15866300
O	-1	3.56810100	-1.69443600	-1.58610500
C	-1	6.36513500	-2.11527200	-1.81427500
O	-1	-3.46857300	-0.75095800	2.96202900
C	-1	-5.57201100	-0.44780400	4.83825300
C	-1	-6.44774100	-0.30800400	5.90796800
O	-1	1.99913400	3.81103300	0.55147800
C	-1	-0.37794600	6.55570000	0.47708100
O	-1	3.89665400	0.53088300	-1.48337200
C	-1	6.60689200	0.25798200	-2.05372800
C	-1	7.97669500	0.05556300	-2.15396300
O	-1	-1.53500600	-3.98843100	0.91966900
C	-1	-3.00672500	-6.06927900	-0.13859600
C	-1	-3.77706300	-7.01299100	-0.80248800
O	-1	-0.88569900	-1.08046700	-3.36434200
C	-1	-2.27720800	-3.03614300	-4.82753000

O	-1	3.24798200	-2.47936000	2.67682800
C	-1	6.00678100	-3.02059300	2.59878100
O	-1	-2.62220200	2.38648900	-1.44654300
C	-1	-3.36955000	4.85844500	-2.54578700
O	-1	-2.52960000	3.27983400	0.61923600
C	-1	-3.59929900	5.71045300	-0.31813500
C	-1	-3.95662200	6.93135500	-0.87891100
O	-1	0.74226500	-2.55645300	-2.86995500
C	-1	-0.38508200	-4.48631100	-4.55763800
C	-1	-1.09340400	-5.45326400	-5.25965900
O	-1	2.96990400	-3.47045200	0.67158300
C	-1	5.60832900	-4.38389900	0.66322900
C	-1	6.97534200	-4.62016400	0.61436400
O	-1	-3.58688200	-2.14596200	0.01254100
C	-1	-5.25544500	-3.85752900	-1.44011300
O	-1	1.69171200	2.77115600	-2.25862200
C	-1	1.10312400	5.20909000	-3.64302000
O	-1	4.11774000	1.66558900	1.19588300
C	-1	6.66501800	0.24948600	3.37923600
C	-1	8.04574300	0.08511500	3.37937600
O	-1	-1.36126000	-2.70400200	3.67278700
C	-1	-2.81751200	-2.28154700	6.01120600
O	-1	-3.33031500	-0.79203500	-1.76901800
C	-1	-5.20689100	-2.28642500	-3.24917900
C	-1	-6.01456700	-3.16488500	-3.96220100
O	-1	0.53710400	-1.92495400	4.60656100
C	-1	-0.90896200	-1.16044100	6.92778700
C	-1	-1.70241000	-0.80804400	8.01328400
O	-1	3.85867600	0.38417500	3.03037000
C	-1	6.87721000	1.24039400	1.20637200
O	-1	-0.21634800	1.87340000	-3.05358700
C	-1	-0.76927000	4.06857100	-4.61298500
C	-1	-1.08825200	5.25105300	-5.26410600
O	-1	2.11990600	-0.51755400	0.73158200
O	-1	-0.00809400	1.75094800	-0.11898800
O	-1	-0.45374200	-0.16193100	2.59376100
O	-1	-0.69018800	-1.53863300	-0.47989600
O	-1	0.59154200	-2.41812300	1.67634900
O	-1	1.16476700	-0.06461100	-1.66588300
O	-1	1.40569400	1.59732300	2.17627900
O	-1	-2.09422800	0.37219400	0.63103900
C	-1	-5.02748500	11.94451700	-5.05065500
C	-1	-4.84509600	10.70032000	-4.25718900
C	-1	-4.31886500	8.35463500	-2.92709700
C	-1	-5.97130000	-8.93123200	-8.02121600
C	-1	-4.91931300	-7.99977000	-7.54072600
C	-1	-3.22337100	-6.18620200	-6.38076700
C	-1	13.49616000	-4.08810200	1.35081300
C	-1	12.01931500	-4.23576400	1.39650300
C	-1	9.28331500	-4.15103400	1.48805000
C	-1	14.35183100	-0.37860300	1.41708400
C	-1	12.94818400	-0.07723600	1.80147000
C	-1	10.25844200	0.32037700	2.18664000
C	-1	-6.69435200	0.13066600	12.20780500
C	-1	-5.64941200	-0.24697700	11.22142500
C	-1	-3.92461500	-0.87547800	9.18418300
C	-1	-9.35798800	-8.47213300	-6.03559200
C	-1	-8.65938400	-7.33199300	-5.38510900
C	-1	-7.21899100	-5.37347500	-4.10601000
C	-1	-1.26746900	10.02749600	-6.95657100

C	-1	-0.64069600	7.66667900	-5.71251500
C	-1	-1.54598100	12.82340600	-3.75137000
C	-1	-0.91233100	11.71892400	-2.98786100
C	-1	-0.05815200	9.47991600	-1.66117400
C	-1	12.65356700	-1.95327200	-2.23657700
C	-1	9.95128200	-1.48495000	-2.11986600
C	-1	-6.44389000	-11.38105300	-4.86157400
C	-1	-5.63410400	-10.40039500	-4.09234100
C	-1	-4.13215500	-8.54281500	-2.74664500
C	-1	-9.54865900	1.56978500	11.41733100
C	-1	-8.76343600	1.33147600	10.17981500
C	-1	-7.13275400	0.89666100	8.01180600
C	-1	-0.98171100	-4.59060300	-0.05247000
C	-1	-1.78098600	-5.68408000	-0.69104300
C	-1	-3.29975100	-7.55378100	-2.00607500
C	-1	-3.53622400	0.34768700	3.58175000
C	-1	-4.50779000	0.44684100	4.71505400
C	-1	-6.21571800	0.70589300	6.85074500
C	-1	0.97811300	4.48738900	0.90937000
C	-1	0.81104700	5.83718700	0.29580500
C	-1	0.29607900	8.22571900	-0.94358300
C	-1	4.30268600	-0.66362300	-1.63721400
C	-1	5.77182100	-0.84608600	-1.85825500
C	-1	8.47998100	-1.25135500	-2.06037300
C	-1	-0.33088600	-2.21349200	-3.46671600
C	-1	-0.99032400	-3.24975700	-4.31497400
C	-1	-2.39371800	-5.15635800	-5.69814400
C	-1	3.66915800	-3.14792800	1.68165300
C	-1	5.10536700	-3.54745900	1.66388100
C	-1	7.80419400	-4.00511500	1.56609800
C	-1	-2.78758000	3.33636200	-0.62313700
C	-1	-3.27945500	4.64421300	-1.16300900
C	-1	-3.98425600	7.05563400	-2.27656800
C	-1	-3.84470900	-1.78999300	-1.17796300
C	-1	-4.79805400	-2.63855700	-1.96009500
C	-1	-6.39541400	-4.37671500	-3.36484900
C	-1	0.64082600	2.80675400	-2.96824200
C	-1	0.34068300	4.03963600	-3.76402500
C	-1	-0.28411900	6.38032900	-5.05111100
C	-1	4.56988600	0.97505800	2.16160600
C	-1	6.05428500	0.83192600	2.26565800
C	-1	8.78168900	0.50944600	2.26168100
C	-1	-0.70786100	-2.21130400	4.63806400
C	-1	-1.47282300	-1.89858800	5.88467300
C	-1	-3.03885800	-1.23448800	8.04236000
H	-1	1.43811500	-0.02839400	-2.59672900
H	-1	1.85396700	2.35583200	2.58138700
H	-1	0.63249400	-3.31342000	2.04933000
C	-1	14.11225000	-2.24366300	-2.24783100
O	-1	14.95777800	-1.53307100	-1.73255800
H	-1	15.37696900	-3.51459500	-2.82776900
H	-1	-7.64423600	-8.89936600	-8.90451000
H	-1	-6.30240600	-12.94791400	-5.89827600
H	-1	-10.50693400	-9.91972500	-5.66520300
H	-1	15.63475000	0.07976200	0.10610500
H	-1	-2.97035100	14.05518200	-3.60365700
C	-1	-1.61128800	11.32867100	-7.58748200
O	-1	-2.74940200	11.74542200	-7.71033900
O	-1	-0.52918300	11.99893800	-8.02921800
H	-1	-0.84341600	12.84614800	-8.39838200

H	-1	-5.61172300	12.56251700	-6.73266500
H	-1	-10.23819200	2.94478300	12.50885800
H	-1	-8.37689000	-0.45408300	12.84676100
H	-1	14.95289000	-3.64748700	2.46682500
H	-1	0.13326800	-0.87327000	6.88417500
H	-1	-1.28684800	-0.23948300	8.83800300
H	-1	-3.28412200	-2.84999200	5.21262200
H	-1	-3.17350400	1.14752300	9.37391300
H	-1	-4.76188700	1.71272400	11.22619100
H	-1	-6.29927600	-2.28783600	10.92694300
H	-1	5.63593900	-2.37698300	3.39032300
H	-1	7.39675300	-5.26496500	-0.14832800
H	-1	4.93298500	-4.82036400	-0.06461900
H	-1	11.81232000	-4.32965300	3.54789900
H	-1	11.84670500	-4.17519700	-0.74035200
H	-1	9.34446900	-4.04748900	-0.67699900
H	-1	5.73919200	-2.99059300	-1.67327300
H	-1	12.02172400	-3.67060900	-3.39038200
H	-1	12.90873000	-0.16219500	-1.08159200
H	-1	10.43771900	0.25619400	-0.92744200
H	-1	8.64686400	0.89324100	-2.30891300
H	-1	6.17879600	1.25216500	-2.11651100
H	-1	1.97482300	5.21186300	-2.99697900
H	-1	0.87933300	10.15450900	-7.18777900
H	-1	-3.32502000	9.56883900	-6.56462800
H	-1	-2.76970900	7.41652700	-5.39346800
H	-1	-1.94370200	5.30303400	-5.92780200
H	-1	-1.36793900	3.17423600	-4.74284600
H	-1	-3.56330900	5.57550200	0.75711500
H	-1	-4.21806400	7.77057300	-0.24464200
H	-1	-3.13752900	4.04445200	-3.22460900
H	-1	-5.78558000	9.35858700	-5.67017900
H	-1	-3.86914000	11.71382900	-2.63117900
H	-1	-3.35587100	9.58217700	-1.42330800
H	-1	-3.53662800	2.13729100	5.63408400
H	-1	-5.71739200	-1.21914200	4.08989400
H	-1	-7.31011700	-0.95957600	5.99383800
H	-1	-8.00649500	3.34728700	9.99116000
H	-1	-9.27888800	-0.75745600	10.07312000
H	-1	-7.79089800	-1.16806400	8.11054900
H	-1	0.61619900	-4.67711400	-4.18719000
H	-1	-0.64982000	-6.42076800	-5.46457000
H	-1	-2.50811200	-7.83269300	-5.16171900
H	-1	-4.03273100	-9.48332300	-6.26923600
H	-1	-5.54071300	-6.27131200	-8.68275500
H	-1	-2.76282400	-2.08069600	-4.65771300
H	-1	-0.42322400	-6.03352500	-2.32539800
H	-1	-4.73001200	-7.33051500	-0.39552900
H	-1	-3.34086200	-5.62215600	0.79037600
H	-1	-5.99310100	-7.48503400	-2.39237200
H	-1	-7.35376200	-9.21407000	-3.60042300
H	-1	-3.70585400	-11.33007900	-4.39692800
H	-1	-4.88451300	-1.34424700	-3.67827600
H	-1	-6.35058300	-2.91232300	-4.96137700
H	-1	-4.95780400	-4.15223600	-0.43944800
H	-1	-9.51269900	-7.59683800	-3.41420100
H	-1	-7.63247600	-6.75728700	-7.18432100
H	-1	-6.29844900	-4.98572400	-6.02754600
H	-1	6.42588500	1.69345700	0.32968700
H	-1	12.78687400	1.80027100	0.73747600

Atom		x	y	z
H	-1	12.74224400	-1.86601900	2.97527300
H	-1	10.28509200	-1.53751600	3.30116800
H	-1	8.54412100	-0.35516300	4.23550600
H	-1	6.06101000	-0.06789200	4.22249900
H	-1	2.27485400	8.05539500	-1.80745300
H	-1	2.73093400	5.86581300	-0.67927900
H	-1	-1.15126900	6.14435100	1.11791600
H	-1	0.87965800	8.88943900	-3.52457900
H	-1	0.12532300	10.96700700	-4.70989900
H	-1	-1.79420300	12.18260200	-1.06857100
N	-1	-2.10332800	-7.21879800	-2.52794800
N	-1	-3.50009100	-9.59137100	-3.30847000
N	-1	-2.96846600	-3.95356800	-5.50402400
N	-1	-4.05424200	-5.75782600	-7.35255600
N	-1	-6.02888100	-4.71062400	-2.11185000
N	-1	-8.10624200	-6.09290900	-3.38817100
N	-1	10.95503900	1.24611300	1.49440100
N	-1	8.20021000	1.08735600	1.19132700
N	-1	-0.79071100	10.38613200	-0.98328900
N	-1	-0.63998400	7.71960900	-0.11730100
N	-1	-5.17693000	1.56057800	6.74907000
N	-1	-7.19569300	2.13716900	8.53504500
N	-1	-3.58179100	-1.98357700	7.06194000
N	-1	-4.78648500	-1.82072000	9.60953600
N	-1	7.32193000	-3.23643500	2.56200400
N	-1	9.96056300	-4.23095500	2.65113900
N	-1	7.68039700	-2.32618100	-1.91137600
N	-1	10.38477900	-2.57220600	-2.78833900
N	-1	0.36579100	8.42163300	-6.19494600
N	-1	0.81025000	6.35537300	-4.26517400
N	-1	-3.70814900	6.02349500	-3.09872000
N	-1	-4.99028900	8.29660200	-4.09554700
C	0	-0.42358121	2.74932918	4.33157168
C	0	1.75106800	0.46610100	5.00913500
O	0	0.64101200	0.78531800	5.60851600
O	0	2.89665500	0.75584700	5.55416700
O	0	-1.37714521	3.12473718	5.13354868
O	0	0.81713879	2.79820718	4.72093768
H	0	2.92485800	1.20661400	6.40128700

Sum of electronic and thermal Free Energies = -13425.793162 (Hartree/Particle).

Table S15: DFT-optimized geometry of **f-[Ce^IV(COOH)-Ce^IV(COOH)]** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.39219100	-2.20821200	-0.59911600
Ce	0	-1.02654200	1.85990200	1.82661100
Ce	-1	-1.73705500	-1.66164500	1.50056000
Ce	-1	2.15954300	1.53847900	-0.19396600
Ce	-1	-1.25187900	0.39700600	-1.46240100
Ce	0	1.68482300	-0.66710800	2.87196200
O	-1	-4.69447400	13.04706900	-4.70602200
C	-1	-4.18900000	10.74744100	-3.04589400
C	-1	-3.91940500	9.56290200	-2.36949300

O	-1	-6.06588800	-10.10705200	-7.65297400
C	-1	-4.01025800	-8.45756200	-6.56334300
C	-1	-3.15222200	-7.54181600	-5.96866600
O	-1	14.14452400	-3.99316200	0.32930600
C	-1	11.30811100	-4.20051900	0.20329600
C	-1	9.92157100	-4.15287700	0.24227900
O	-1	14.81271300	0.46699700	0.46934200
C	-1	12.25941100	1.05160400	1.31476200
O	-1	-6.79955400	1.25733800	12.69104500
C	-1	-4.74699700	0.73503600	10.77737300
C	-1	-3.86532400	0.41519600	9.75233400
O	-1	-9.22153900	-8.80288100	-7.20052000
C	-1	-7.75992400	-6.57067500	-6.12416500
C	-1	-7.03254300	-5.57655400	-5.48109900
C	-1	-2.30276900	9.22068400	-6.47380800
C	-1	-1.99127100	8.02745300	-5.83678400
O	-1	-2.38987700	13.55379700	-3.01939300
C	-1	-1.19858200	11.47093100	-1.65645000
C	-1	12.19508700	-0.82224800	-1.55409900
C	-1	10.82774800	-0.58531500	-1.48846900
O	-1	-7.64607600	-11.32548300	-4.98177200
C	-1	-6.27352700	-9.31874300	-3.49522900
C	-1	-5.51853700	-8.37080200	-2.81750400
O	-1	-9.97005600	0.69779900	12.14338000
C	-1	-8.70955200	0.05706800	9.61939500
C	-1	-7.88429700	-0.16533600	8.52396300
O	-1	14.41435600	-3.38715600	-2.88774000
C	-1	11.70413300	-2.78837500	-2.84008600
O	-1	-5.69233600	-12.38386600	-5.37715200
C	-1	-4.23508700	-10.50346700	-3.94373600
O	-1	-9.76099800	2.88635300	11.65101600
C	-1	-7.99522900	2.34931200	9.57406500
O	-1	-1.37981400	13.00766200	-4.96497600
C	-1	-0.11159200	10.79138300	-3.68570200
C	-1	0.32275000	9.65417400	-3.01744200
O	-1	15.00748300	-1.30224900	1.85682500
C	-1	12.23604200	-0.98726200	2.58003200
C	-1	10.87302800	-0.79126400	2.77132300
C	-1	0.04802000	9.55476400	-6.82264400
O	-1	-10.14536100	-9.16136200	-5.17761600
C	-1	-8.80167800	-7.04683800	-4.01512900
O	-1	-7.58417900	-0.84183200	12.43272100
C	-1	-5.61770100	-1.49599900	10.60232000
O	-1	14.04910600	-3.98904900	2.58595700
C	-1	11.29344500	-4.27136900	2.60226900
O	-1	-5.60382900	11.70282400	-6.26810800
C	-1	-5.24798500	9.42911100	-4.74918800
O	-1	-6.83615000	-8.35769500	-8.85720300
C	-1	-4.86561800	-6.66423200	-7.90899500
O	-1	0.16558400	-4.31647400	-0.52149000
C	-1	-1.37076800	-6.31120000	-1.87292800
O	-1	-2.83194100	1.38021300	3.32628500
C	-1	-4.36087200	1.43454900	5.69820000
O	-1	0.08438200	4.08237100	1.69933600
C	-1	1.79255000	6.38939300	-0.54058800
C	-1	1.53244900	7.59852200	-1.17264200
O	-1	3.56997500	-1.69713300	-1.58559100
C	-1	6.36725500	-2.11714000	-1.81226400
O	-1	-3.46850900	-0.74981400	2.95894400
C	-1	-5.57265700	-0.44474100	4.83406000

C	-1	-6.44877800	-0.30371200	5.90329300
O	-1	1.99804500	3.81086200	0.54329300
C	-1	-0.38015600	6.55442100	0.46406500
O	-1	3.89756700	0.52847400	-1.48607400
C	-1	6.60809600	0.25585500	-2.05518000
C	-1	7.97801500	0.05385900	-2.15468700
O	-1	-1.53295500	-3.98952000	0.92201400
C	-1	-3.00347700	-6.07255800	-0.13360400
C	-1	-3.77321400	-7.01758100	-0.79632800
O	-1	-0.88352800	-1.08767500	-3.36612600
C	-1	-2.27376500	-3.04611200	-4.82682800
O	-1	3.24885600	-2.47583400	2.67840800
C	-1	6.00790400	-3.01603000	2.60202500
O	-1	-2.62207400	2.38141100	-1.45403800
C	-1	-3.37011000	4.85141200	-2.55719900
O	-1	-2.53048800	3.27787300	0.61043500
C	-1	-3.60090800	5.70664500	-0.33089100
C	-1	-3.95856500	6.92656000	-0.89359800
O	-1	0.74489800	-2.56224300	-2.86903200
C	-1	-0.38111800	-4.49508500	-4.55418700
C	-1	-1.08881700	-5.46337900	-5.25498500
O	-1	2.97181500	-3.47003100	0.67455700
C	-1	5.61062400	-4.38238700	0.66838400
C	-1	6.97775000	-4.61815300	0.62029700
O	-1	-3.58531700	-2.14926300	0.01150200
C	-1	-5.25271400	-3.86369000	-1.43911700
O	-1	1.69193200	2.76666800	-2.26534900
C	-1	1.10275900	5.20228900	-3.65356300
O	-1	4.11734600	1.66726600	1.19155400
C	-1	6.66453400	0.25548300	3.37780800
C	-1	8.04532700	0.09168900	3.37862200
O	-1	-1.36060200	-2.70091600	3.67326800
C	-1	-2.81775900	-2.27558200	6.01060100
O	-1	-3.32876000	-0.79788600	-1.77199300
C	-1	-5.20425100	-2.29526500	-3.25050800
C	-1	-6.01133900	-3.17512400	-3.96247100
O	-1	0.53714500	-1.91968400	4.60646900
C	-1	-0.90996200	-1.15231400	6.92610300
C	-1	-1.70389500	-0.79863100	8.01082700
O	-1	3.85824500	0.38848000	3.02786900
C	-1	6.87698900	1.24323900	1.20353500
O	-1	-0.21550500	1.86693100	-3.05956800
C	-1	-0.76885700	4.05954300	-4.62240900
C	-1	-1.08812900	5.24092000	-5.27539200
O	-1	2.12056700	-0.51740100	0.72988800
O	-1	-0.00811500	1.74894100	-0.12472500
O	-1	-0.45380900	-0.16007700	2.59073500
O	-1	-0.68872300	-1.54145900	-0.48093900
O	-1	0.59270100	-2.41719800	1.67701200
O	-1	1.16598600	-0.06843200	-1.66854600
O	-1	1.40502300	1.59932900	2.17120900
O	-1	-2.09390600	0.37043500	0.62670800
C	-1	-5.03022000	11.93304900	-5.07314500
C	-1	-4.84756000	10.69011300	-4.27776900
C	-1	-4.32076500	8.34663300	-2.94401700
C	-1	-5.96440300	-8.94749800	-8.01287000
C	-1	-4.91295400	-8.01488100	-7.53344200
C	-1	-3.21812900	-6.19887800	-6.37566100
C	-1	13.49811600	-4.08227100	1.35797800
C	-1	12.02131800	-4.23048100	1.40342900

C	-1	9.28525500	-4.14675800	1.49399900
C	-1	14.35221900	-0.37232000	1.41898400
C	-1	12.94832700	-0.07096700	1.80248400
C	-1	10.25830000	0.32609700	2.18622400
C	-1	-6.69753400	0.14424700	12.20239200
C	-1	-5.65213000	-0.23443000	11.21690100
C	-1	-3.92643600	-0.86524700	9.18113400
C	-1	-9.35190000	-8.48685400	-6.02898500
C	-1	-8.65397400	-7.34545300	-5.37998600
C	-1	-7.21479700	-5.38442900	-4.10336000
C	-1	-1.26881200	10.01475900	-6.97503100
C	-1	-0.64144200	7.65606200	-5.72726200
C	-1	-1.54948800	12.81532800	-3.77409000
C	-1	-0.91561600	11.71225100	-3.00873800
C	-1	-0.06091600	9.47557900	-1.67844900
C	-1	12.65575000	-1.95314500	-2.23285300
C	-1	9.95323400	-1.48577700	-2.11768000
C	-1	-6.43695400	-11.39280200	-4.84972500
C	-1	-5.62781700	-10.41066000	-4.08170300
C	-1	-4.12706300	-8.55045000	-2.73831200
C	-1	-9.55219500	1.58099300	11.40888600
C	-1	-8.76648800	1.34116800	10.17197100
C	-1	-7.13494900	0.90380300	8.00511900
C	-1	-0.97910700	-4.59291000	-0.04905300
C	-1	-1.77772600	-5.68767100	-0.68624400
C	-1	-3.29530200	-7.55996500	-1.99895800
C	-1	-3.53681100	0.34972600	3.57700500
C	-1	-4.50877100	0.45016300	4.70985800
C	-1	-6.21747200	0.71168600	6.84462900
C	-1	0.97663100	4.48732400	0.89985800
C	-1	0.80919300	5.83613600	0.28423000
C	-1	0.29361400	8.22260200	-0.95887800
C	-1	4.30414500	-0.66609100	-1.63800900
C	-1	5.77342500	-0.84826900	-1.85832100
C	-1	8.48181700	-1.25270800	-2.05899200
C	-1	-0.32820900	-2.22062100	-3.46663800
C	-1	-0.98695100	-3.25842400	-4.31355500
C	-1	-2.38911900	-5.16767100	-5.69431700
C	-1	3.67062000	-3.14570900	1.68436200
C	-1	5.10700100	-3.54466600	1.66763200
C	-1	7.80604900	-4.00134000	1.57137000
C	-1	-2.78810400	3.33244100	-0.63210100
C	-1	-3.28035700	4.63928000	-1.17407500
C	-1	-3.98581700	7.04874400	-2.29144800
C	-1	-3.84292200	-1.79517600	-1.17961100
C	-1	-4.79566900	-2.64530400	-1.96077400
C	-1	-6.39186600	-4.38622100	-3.36343000
C	-1	0.64125300	2.80076900	-2.97534800
C	-1	0.34084300	4.03233800	-3.77306100
C	-1	-0.28453400	6.37084800	-5.06383000
C	-1	4.56947900	0.97836400	2.15844600
C	-1	6.05390500	0.83600700	2.26317300
C	-1	8.78144400	0.51466100	2.26052400
C	-1	-0.70771000	-2.20650600	4.63801200
C	-1	-1.47319100	-1.89225100	5.88391600
C	-1	-3.04017400	-1.22558900	8.04012400
H	-1	1.43960900	-0.03348900	-2.59936000
H	-1	1.85285300	2.35862800	2.57532400
H	-1	0.63391100	-3.31192100	2.05134100
C	-1	14.11455700	-2.24294300	-2.24322000

O	-1	14.95962800	-1.53123000	-1.72874400
H	-1	15.37998700	-3.51420900	-2.82086900
H	-1	-7.63707600	-8.91764800	-8.89672900
H	-1	-6.29449400	-12.96114900	-5.88404600
H	-1	-10.50035700	-9.93437100	-5.65679500
H	-1	15.63535500	0.08462500	0.10772200
H	-1	-2.97441800	14.04672800	-3.62865600
C	-1	-1.61297800	11.31484800	-7.60798900
O	-1	-2.75122700	11.73094100	-7.73182100
O	-1	-0.53101400	11.98490800	-8.05038800
H	-1	-0.84548600	12.83143500	-8.42091200
H	-1	-5.61419200	12.54829700	-6.75625600
H	-1	-10.24264100	2.95733000	12.49814800
H	-1	-8.38002700	-0.44025100	12.84169600
H	-1	14.95431500	-3.63938400	2.47378400
H	-1	0.13216100	-0.86477400	6.88238700
H	-1	-1.28882700	-0.22866800	8.83482600
H	-1	-3.28388300	-2.84541200	5.21272200
H	-1	-3.17622800	1.15834800	9.36808100
H	-1	-4.76542400	1.72564700	11.21902000
H	-1	-6.30105100	-2.27599700	10.92526000
H	-1	5.63654700	-2.37139600	3.39249100
H	-1	7.39966800	-5.26391500	-0.14130200
H	-1	4.93568800	-4.82021900	-0.05902100
H	-1	11.81369300	-4.32124900	3.55489900
H	-1	11.84934900	-4.17317200	-0.73356800
H	-1	9.34704000	-4.04641500	-0.67118300
H	-1	5.74163300	-2.99251200	-1.67015200
H	-1	12.02498300	-3.67246300	-3.38429200
H	-1	12.90980600	-0.16024100	-1.08046000
H	-1	10.43857200	0.25734600	-0.92770300
H	-1	8.64788200	0.89158400	-2.31067800
H	-1	6.17960500	1.24976400	-2.11957800
H	-1	1.97425600	5.20639000	-3.00725600
H	-1	0.87800900	10.14232300	-7.20576200
H	-1	-3.32629300	9.55582800	-6.58304500
H	-1	-2.77045000	7.40549700	-5.40850500
H	-1	-1.94339500	5.29155400	-5.93943000
H	-1	-1.36711300	3.16476600	-4.75112200
H	-1	-3.56519700	5.57331200	0.74456900
H	-1	-4.22055500	7.76661300	-0.26066200
H	-1	-3.13753900	4.03650500	-3.23473500
H	-1	-5.78704400	9.34588200	-5.68904800
H	-1	-3.87253300	11.70645200	-2.65296800
H	-1	-3.35875100	9.57681800	-1.44176100
H	-1	-3.53860000	2.14238800	5.62666800
H	-1	-5.71748300	-1.21725400	4.08680600
H	-1	-7.31090900	-0.95551500	5.98986600
H	-1	-8.01032900	3.35701100	9.98054600
H	-1	-9.28103400	-0.74813600	10.06823000
H	-1	-7.79226200	-1.16104800	8.10673700
H	-1	0.62012700	-4.68491800	-4.18314400
H	-1	-0.64476700	-6.43100300	-5.45831500
H	-1	-2.50256300	-7.84325000	-5.15393700
H	-1	-4.02614900	-9.49616700	-6.25946600
H	-1	-5.53471900	-6.28838700	-8.67824000
H	-1	-2.75983200	-2.09061500	-4.65858700
H	-1	-0.41930900	-6.03898600	-2.31965400
H	-1	-4.72615700	-7.33489500	-0.38919200
H	-1	-3.33808900	-5.62419000	0.79459600

H	-1	-5.98855900	-7.49291800	-2.38619500
H	-1	-7.34812300	-9.22432200	-3.59208900
H	-1	-3.69908500	-11.33999300	-4.38430500
H	-1	-4.88213300	-1.35359300	-3.68090900
H	-1	-6.34714900	-2.92419200	-4.96212600
H	-1	-4.95526100	-4.15678100	-0.43792100
H	-1	-9.50779300	-7.60771600	-3.40895000
H	-1	-7.62674600	-6.77300100	-7.17973300
H	-1	-6.29381800	-4.99915900	-6.02518600
H	-1	6.42574900	1.69480500	0.32603500
H	-1	12.78656500	1.80488400	0.73564100
H	-1	12.74276700	-1.85808400	2.97888900
H	-1	10.28537700	-1.53012100	3.30353000
H	-1	8.54362300	-0.34710400	4.23556300
H	-1	6.06039600	-0.06088900	4.22135600
H	-1	2.27273000	8.05181600	-1.82187800
H	-1	2.72937200	5.86411000	-0.69029900
H	-1	-1.15350600	6.14370500	1.10527200
H	-1	0.87772100	8.88271600	-3.54067900
H	-1	0.12288900	10.95820000	-4.72933100
H	-1	-1.79827800	12.17842100	-1.09041600
N	-1	-2.09885600	-7.22526000	-2.52095900
N	-1	-3.49438600	-9.59957800	-3.29837600
N	-1	-2.96443000	-3.96483300	-5.50216900
N	-1	-4.04887700	-5.77229800	-7.34834600
N	-1	-6.02558500	-4.71810800	-2.10982100
N	-1	-8.10197100	-6.10316300	-3.38472500
N	-1	10.95472500	1.25109000	1.49282300
N	-1	8.20005800	1.09073100	1.18912900
N	-1	-0.79406400	10.38249900	-1.00214300
N	-1	-0.64249500	7.71733300	-0.13213300
N	-1	-5.17900900	1.56665300	6.74200300
N	-1	-7.19856900	2.14506200	8.52648900
N	-1	-3.58248900	-1.97636600	7.06065200
N	-1	-4.78804400	-1.81021300	9.60762800
N	-1	7.32315400	-3.23137800	2.56597800
N	-1	9.96217500	-4.22466200	2.65741700
N	-1	7.68263500	-2.32764500	-1.90864200
N	-1	10.38739200	-2.57384800	-2.78439600
N	-1	0.36488100	8.41071500	-6.21050600
N	-1	0.80960100	6.34752100	-4.27751700
N	-1	-3.70902300	6.01549500	-3.11197300
N	-1	-4.99180100	8.28657800	-4.11258700
C	0	-0.49170600	2.65519300	4.04874100
C	0	1.74998700	0.47247600	5.00585500
O	0	0.63961100	0.79212200	5.60441500
O	0	2.89528300	0.76351300	5.55081000
O	0	-1.44567600	3.03139800	4.84986200
O	0	0.74887200	2.70517000	4.43842000
H	0	2.92303400	1.21555400	6.39726600
H	0	-1.23535900	3.34716000	5.73171300

Sum of electronic and thermal Free Energies = -13426.189189 (Hartree/Particle).

Table S16: DFT-optimized geometry of **f-[Ce^III(HOOC-COOH)-Ce^IV]⁻** (doublet), computed at the UB3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM. The spin density plot is also shown below. (Isovalue = 0.0004)
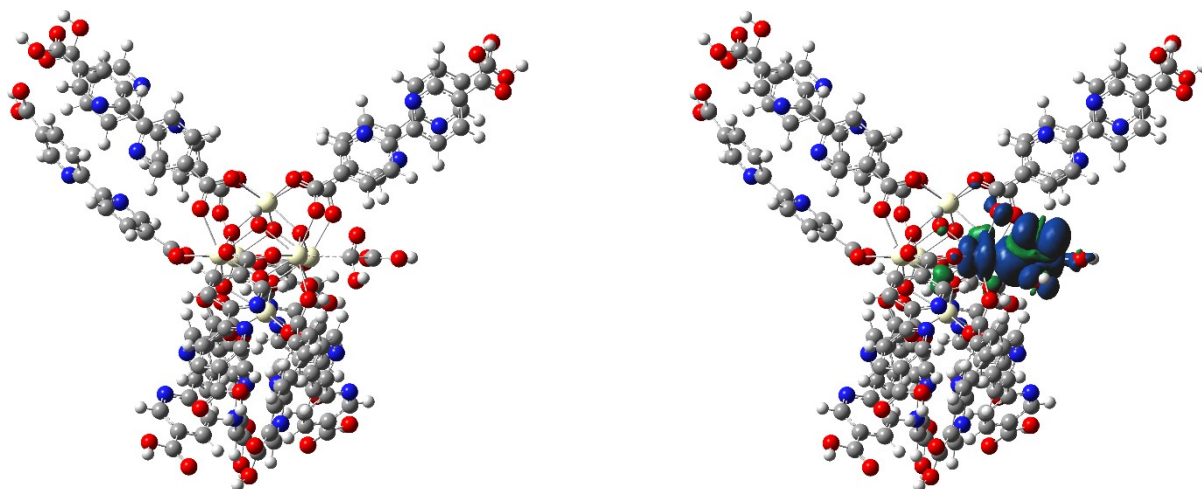
Spin Density Distribution

Atom		x	y	z
Ce	-1	1.35400100	-2.20129400	-0.63861300
Ce	0	-1.01786500	1.87109900	1.82590300
Ce	-1	-1.75271300	-1.64468200	1.49165900
Ce	-1	2.14777100	1.53894600	-0.22485300
Ce	-1	-1.28188200	0.42348000	-1.46698900
Ce	0	1.68743300	-0.67664600	2.83605000
O	-1	-4.67669400	13.10769700	-4.62650400
C	-1	-4.17020200	10.79807100	-2.98062600
C	-1	-3.90170300	9.60908100	-2.31164100
O	-1	-6.21558500	-10.02507200	-7.65726100
C	-1	-4.14017200	-8.39265200	-6.57948800
C	-1	-3.27122900	-7.48462600	-5.98882200
O	-1	14.10312600*	-4.06721000	0.16649100
C	-1	11.26447900	-4.25688100	0.06538900
C	-1	9.87866400	-4.20102300	0.11716400
O	-1	14.79967900	0.38819700	0.31902100
C	-1	12.25774300	0.98465800	1.19002700
O	-1	-6.69578500	1.25761800	12.73972600
C	-1	-4.66386300	0.73099500	10.80533000
C	-1	-3.79347300	0.41015700	9.77100200
O	-1	-9.35901500	-8.70376600	-7.17073400
C	-1	-7.87415700	-6.48499900	-6.09841400
C	-1	-7.13494600	-5.49801500	-5.45784900
C	-1	-2.32442400	9.27441400	-6.43186000
C	-1	-2.01443300	8.07664400	-5.80266600
O	-1	-2.35387300	13.59336200	-2.95878500
C	-1	-1.16297400	11.49760000	-1.61540400
C	-1	12.15603500	-0.87665100	-1.68590900
C	-1	10.79081300	-0.63173500	-1.60687500
O	-1	-7.77889500	-11.24518600	-4.97691100
C	-1	-6.38075300	-9.25306900	-3.49455400
C	-1	-5.61390200	-8.31257700	-2.81977400
O	-1	-9.87446300	0.71957300	12.21855900

C	-1	-8.64079600	0.08188700	9.68058200
C	-1	-7.82686600	-0.14087900	8.57678200
O	-1	14.34748800	-3.44928000	-3.05032300
C	-1	11.64150000	-2.83433100	-2.97555900
O	-1	-5.83529200	-12.31368300	-5.39442500
C	-1	-4.35370500	-10.44819300	-3.96648900
O	-1	-9.65656300	2.90888100	11.73343300
C	-1	-7.91298000	2.36994100	9.63831000
O	-1	-1.36481600	13.04934300	-4.91572000
C	-1	-0.09856500	10.82006000	-3.65725700
C	-1	0.33488600	9.67743700	-2.99771100
O	-1	14.99624100	-1.38803200	1.69729900
C	-1	12.23343300	-1.05934900	2.44695600
C	-1	10.87342500	-0.85592300	2.65143600
C	-1	0.02509900	9.59574300	-6.80064100
O	-1	-10.26663900	-9.06518700	-5.14103000
C	-1	-8.89964100	-6.96374800	-3.98200300
O	-1	-7.49547400	-0.83566200	12.47980200
C	-1	-5.54967300	-1.49397700	10.62890500
O	-1	14.02818000	-4.07204100	2.42391300
C	-1	11.27111300	-4.33776200	2.46408000
O	-1	-5.60832200	11.77557600	-6.18584900
C	-1	-5.25257300	9.49336600	-4.67970500
O	-1	-6.98606700	-8.26602500	-8.84714800
C	-1	-4.99676100	-6.58852200	-7.90983600
O	-1	0.11534400	-4.30241100	-0.55862700
C	-1	-1.44529400	-6.28209300	-1.90434700
O	-1	-2.81249100	1.39601000	3.33990500
C	-1	-4.31951400	1.44958200	5.72581600
O	-1	0.10536100	4.08732700	1.69779600
C	-1	1.80717200	6.39340900	-0.54792700
C	-1	1.54871800	7.60674400	-1.17255200
O	-1	3.52582900	-1.69923400	-1.64269400
C	-1	6.31833400	-2.13518600	-1.89651400
O	-1	-3.46530600	-0.72856000	2.96949500
C	-1	-5.55048700	-0.41868500	4.86490200
C	-1	-6.41601300	-0.27687500	5.94262700
O	-1	2.00678700	3.80913300	0.52329700
C	-1	-0.35529900	6.56733000	0.47710000
O	-1	3.86784400	0.52391200	-1.53689000
C	-1	6.57139700	0.23731400	-2.13172500
C	-1	7.93910400	0.02746100	-2.24451200
O	-1	-1.56802900	-3.97128700	0.90159600
C	-1	-3.06069800	-6.04092400	-0.14928600
C	-1	-3.84214200	-6.97847200	-0.80891900
O	-1	-0.93982900	-1.05535700	-3.38014700
C	-1	-2.35513000	-2.99917200	-4.83630200
O	-1	3.23861600	-2.49396100	2.62076700
C	-1	5.99352200	-3.05050100	2.51707600
O	-1	-2.63984700	2.41607900	-1.43791700
C	-1	-3.38280400	4.89519000	-2.52394400
O	-1	-2.52411100	3.30325400	0.62935300
C	-1	-3.58821900	5.74240300	-0.29209000
C	-1	-3.94353000	6.96682100	-0.84644000
O	-1	0.68403100	-2.54182600	-2.90401000
C	-1	-0.46894200	-4.46069900	-4.58690000
C	-1	-1.18883800	-5.42173200	-5.28526700
O	-1	2.93739200	-3.47800200	0.61539300
C	-1	5.57043700	-4.40626100	0.58145100
C	-1	6.93561200	-4.65008400	0.51996600

O	-1	-3.61732100	-2.11483000	0.01743500
C	-1	-5.30818800	-3.81301000	-1.42510400
O	-1	1.66889700	2.77866700	-2.28677200
C	-1	1.08200200	5.22364000	-3.65942300
O	-1	4.11879200	1.65004800	1.14335000
C	-1	6.67704400	0.21368100	3.30047700
C	-1	8.05676600	0.04154000	3.28806700
O	-1	-1.36292500	-2.69536600	3.65651200
C	-1	-2.79623400	-2.27109600	6.00873600
O	-1	-3.36871300	-0.75751700	-1.76267500
C	-1	-5.26659500	-2.23727900	-3.23031500
C	-1	-6.08543700	-3.10923200	-3.93857400
O	-1	0.54791600	-1.92956600	4.57568000
C	-1	-0.87342400	-1.16325500	6.91153900
C	-1	-1.65533200	-0.80935700	8.00489400
O	-1	3.86856100	0.36511600	2.97660200
C	-1	6.87580000	1.20929800	1.12849600
O	-1	-0.25109500	1.89383800	-3.06737000
C	-1	-0.80523100	4.09632900	-4.61597700
C	-1	-1.12321200	5.28235800	-5.26110800
O	-1	2.10466000	-0.52054000	0.69074800
O	-1	-0.01784900	1.76221500	-0.13504900
O	-1	-0.45053400	-0.15551200	2.57637500
O	-1	-0.72166200	-1.52247800	-0.49876300
O	-1	0.57390600	-2.41504400	1.64379400
O	-1	1.13114000	-0.05569300	-1.69702600
O	-1	1.41509200	1.59437800	2.14731000
O	-1	-2.10509700	0.39318700	0.62955400
C	-1	-5.02252300	11.99728500	-4.99519800
C	-1	-4.84023100	10.74992300	-4.20669600
C	-1	-4.31564300	8.39769600	-2.88755400
C	-1	-6.11031200	-8.86464400	-8.01323100
C	-1	-5.04890800	-7.94043200	-7.53949600
C	-1	-3.33264900	-6.13960900	-6.38960600
C	-1	13.46553300	-4.15674900	1.20061200
C	-1	11.98833300	-4.29621800	1.25885900
C	-1	9.25376200	-4.19633800	1.37462700
C	-1	14.34270700	-0.45232000	1.26930400
C	-1	12.94420600	-0.14410500	1.66679200
C	-1	10.26023100	0.26759200	2.07660200
C	-1	-6.60496900	0.14600200	12.24553600
C	-1	-5.57085800	-0.23482700	11.24902100
C	-1	-3.86754600	-0.86747200	9.19505400
C	-1	-9.47683400	-8.39190200	-5.99675700
C	-1	-8.76612700	-7.25749000	-5.34937700
C	-1	-7.30354000	-5.31060600	-4.07772300
C	-1	-1.29023700	10.06433000	-6.93914500
C	-1	-0.66595200	7.69664000	-5.70695800
C	-1	-1.52486300	12.85301700	-3.72415200
C	-1	-0.89080700	11.74290800	-2.96918900
C	-1	-0.03771500	9.49551800	-1.65604400
C	-1	12.60364200	-2.00743800	-2.37352300
C	-1	9.90517400	-1.52423100	-2.23186000
C	-1	-6.56905800	-11.32037000	-4.85613400
C	-1	-5.74703700	-10.34638700	-4.09141100
C	-1	-4.22288600	-8.50096700	-2.75397400
C	-1	-9.45790700	1.60331600	11.48398400
C	-1	-8.68491000	1.36396500	10.23899400
C	-1	-7.07575800	0.92588900	8.05560900
C	-1	-1.02668100	-4.57391200	-0.07696700

C	-1	-1.83768400	-5.66112700	-0.71143000
C	-1	-3.37845200	-7.51865700	-2.01808900
C	-1	-3.52131700	0.36875500	3.59272400
C	-1	-4.48234600	0.47028700	4.73476700
C	-1	-6.17001600	0.73312700	6.88604300
C	-1	0.99277800	4.49024800	0.89194000
C	-1	0.82798000	5.84263200	0.28347900
C	-1	0.31569000	8.23739500	-0.94494700
C	-1	4.26575400	-0.67243700	-1.69748500
C	-1	5.73184200	-0.86256400	-1.93189100
C	-1	8.43579400	-1.28252000	-2.15883900
C	-1	-0.39234700	-2.19120400	-3.49041600
C	-1	-1.06503500	-3.22142400	-4.33562800
C	-1	-2.49124300	-5.11631700	-5.71153300
C	-1	3.64727600	-3.16217500	1.62015000
C	-1	5.08099300	-3.56973400	1.58871300
C	-1	7.77623000	-4.04230700	1.46603600
C	-1	-2.79263600	3.36462000	-0.61055400
C	-1	-3.28181800	4.67668600	-1.14258800
C	-1	-3.98269900	7.09506300	-2.24346400
C	-1	-3.88354600	-1.75417100	-1.16980500
C	-1	-4.84848400	-2.59522000	-1.94581300
C	-1	-6.46788400	-4.32052200	-3.34114900
C	-1	0.61205700	2.82211500	-2.98704900
C	-1	0.31193200	4.05883200	-3.77686500
C	-1	-0.31087400	6.40650500	-5.05215200
C	-1	4.57546500	0.95435200	2.10321700
C	-1	6.05988600	0.80258300	2.19386200
C	-1	8.78528300	0.46476600	2.16509900
C	-1	-0.69832400	-2.20898800	4.61733500
C	-1	-1.45056200	-1.89536900	5.87143900
C	-1	-2.99386400	-1.22834900	8.04454900
H	-1	1.39652700	-0.01847900	-2.63013300
H	-1	1.87117500	2.34924400	2.55049900
H	-1	0.61306100	-3.31157100	2.01400400
C	-1	14.06050600	-2.30600500	-2.39834700
O	-1	14.91451700	-1.60159100	-1.88861000
H	-1	15.31289300	-3.58245000	-2.99275600
H	-1	-7.79071000	-8.82095400	-8.88172800
H	-1	-6.44551800	-12.88517100	-5.89822700
H	-1	-10.63065700	-9.83400700	-5.62018000
H	-1	15.61666900	0.00238700	-0.05164600
H	-1	-2.94089900	14.09238400	-3.56065500
C	-1	-1.63220600	11.36913500	-7.56353100
O	-1	-2.76897800	11.79262000	-7.67528400
O	-1	-0.55023900	12.03450200	-8.01294600
H	-1	-0.86289800	12.88447100	-8.37707000
H	-1	-5.61796400	12.62314700	-6.67035900
H	-1	-10.13007200	2.97919400	12.58519300
H	-1	-8.28512700	-0.43100500	12.89765800
H	-1	14.93444600	-3.72738500	2.30497900
H	-1	0.16999000	-0.88183800	6.85955600
H	-1	-1.22935800	-0.24539500	8.82745400
H	-1	-3.27302500	-2.83472600	5.21275800
H	-1	-3.10337800	1.15074400	9.38360300
H	-1	-4.67226100	1.71982700	11.25124700
H	-1	-6.23480200	-2.27118500	10.95478900
H	-1	5.63327000	-2.40697400	3.31356000
H	-1	7.34667700	-5.29516600	-0.24811600
H	-1	4.88628900	-4.83693200	-0.14161000

H	-1	11.79965600	-4.39480500	3.41172900
H	-1	11.79736500	-4.22885600	-0.87623000
H	-1	9.29654100	-4.08723700	-0.79059000
H	-1	5.68871100	-3.00735000	-1.75237000
H	-1	11.95202300	-3.71803900	-3.52633300
H	-1	12.87903000	-0.22098100	-1.21603000
H	-1	10.41186800	0.21089000	-1.03909300
H	-1	8.61261500	0.86177200	-2.40309200
H	-1	6.14839500	1.23405900	-2.18808900
H	-1	1.95932600	5.21974600	-3.02104800
H	-1	0.85514200	10.17988600	-7.18883400
H	-1	-3.34683700	9.61619700	-6.53039900
H	-1	-2.79347000	7.45760900	-5.36992000
H	-1	-1.98413400	5.34096300	-5.91713300
H	-1	-1.41006100	3.20573600	-4.74297500
H	-1	-3.54357900	5.60432100	0.78243800
H	-1	-4.19466000	7.80576500	-0.20765800
H	-1	-3.16134200	4.08175800	-3.20695200
H	-1	-5.80062000	9.41736300	-5.61496800
H	-1	-3.84436000	11.75348600	-2.58660100
H	-1	-3.33259300	9.61569300	-1.38898900
H	-1	-3.49363300	2.15273200	5.64976500
H	-1	-5.70677400	-1.18715000	4.11578400
H	-1	-7.28127400	-0.92381300	6.03431300
H	-1	-7.91826600	3.37598900	10.04910300
H	-1	-9.21307700	-0.72173400	10.13123300
H	-1	-7.74467300	-1.13536100	8.15459500
H	-1	0.53445000	-4.65814500	-4.22576100
H	-1	-0.75254200	-6.39115600	-5.49664900
H	-1	-2.61606300	-7.79341700	-5.18129000
H	-1	-4.15962800	-9.43241400	-6.27980700
H	-1	-5.67050300	-6.20539700	-8.67140000
H	-1	-2.83383100	-2.04147300	-4.65967600
H	-1	-0.49628200	-6.01375400	-2.35856000
H	-1	-4.79327100	-7.29173400	-0.39446800
H	-1	-3.38415400	-5.59446200	0.78377500
H	-1	-6.07464900	-7.43369600	-2.38056200
H	-1	-7.45558800	-9.15174500	-3.58125500
H	-1	-3.82681500	-11.28607800	-4.41538800
H	-1	-4.94266600	-1.29576500	-3.65969900
H	-1	-6.42875600	-2.85205900	-4.93408400
H	-1	-5.00346700	-4.11211600	-0.42788000
H	-1	-9.60363500	-7.52289900	-3.37177500
H	-1	-7.75178000	-6.68367100	-7.15598200
H	-1	-6.39768100	-4.92280700	-6.00621500
H	-1	6.41938500	1.66728200	0.25701900
H	-1	12.78420200	1.73717300	0.60928300
H	-1	12.73844300	-1.93489400	2.83756400
H	-1	10.28613500	-1.59345300	3.18587700
H	-1	8.56012400	-0.40386900	4.13861100
H	-1	6.07865800	-0.10258900	4.14815400
H	-1	2.28583100	8.05829000	-1.82659300
H	-1	2.73938600	5.86310800	-0.70832700
H	-1	-1.12529400	6.15859600	1.12359000
H	-1	0.88039000	8.90485200	-3.52917600
H	-1	0.12746300	10.98985800	-4.70227000
H	-1	-1.75320400	12.20630900	-1.04100400
N	-1	-2.18476900	-7.18899300	-2.54953800
N	-1	-3.60170300	-9.55152900	-3.32412600
N	-1	-3.05746100	-3.91084400	-5.50916000

Atom		x	y	z
N	-1	-4.16956300	-5.70391500	-7.35292100
N	-1	-6.09228700	-4.65990400	-2.09231200
N	-1	-8.18852400	-6.02698800	-3.35405800
N	-1	10.95596100	1.19127500	1.38076000
N	-1	8.19773200	1.04885600	1.10143800
N	-1	-0.75917500	10.40399200	-0.96933600
N	-1	-0.61594800	7.73431200	-0.11184300
N	-1	-5.12734300	1.58222500	6.77754800
N	-1	-7.12709900	2.16530000	8.58269900
N	-1	-3.54958700	-1.97169400	7.06692700
N	-1	-4.73098800	-1.80900300	9.62541900
N	-1	7.30705700	-3.27364300	2.46818700
N	-1	9.94070600	-4.28324000	2.53151300
N	-1	7.63148200	-2.35323000	-2.00571200
N	-1	10.32664800	-2.61208400	-2.90701700
N	-1	0.34052500	8.44722800	-6.19617600
N	-1	0.79017600	6.37324700	-4.27591400
N	-1	-3.71964000	6.06363100	-3.07076500
N	-1	-4.99758900	8.34662900	-4.05022000
C	0	1.78552400	0.53593300	5.12990900
O	0	1.55405700	-0.38755900	6.01702100
C	0	0.94494300	1.77802400	5.59522600
O	0	3.15256400	0.92172700	5.29502700
O	0	0.11105400	2.33564100	4.88969000
O	0	1.21830200	2.17911700	6.83639400
H	0	3.69157400	0.50223700	5.96963500
H	0	0.60784700	2.90683400	7.07576900

Sum of electronic and thermal Free Energies = -13426.370458 (Hartree/Particle).

Table S17: DFT-optimized geometry of **f-[Ce^{IV}(OC-COOH)-Ce^{IV}]** (doublet), computed at the UB3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.37431600	-2.23334500	-0.56066800
Ce	0	-1.01006700	1.89292800	1.84106700
Ce	-1	-1.75256700	-1.63866600	1.52945900
Ce	-1	2.17629800	1.50948700	-0.18755800
Ce	-1	-1.24401700	0.38899000	-1.45074000
Ce	0	1.66285900	-0.68755400	2.88149400
O	-1	-4.56284900	13.04172700	-4.81083900
C	-1	-4.08131200	10.75221000	-3.12975200
C	-1	-3.82380800	9.57121200	-2.44253500
O	-1	-6.14846900	-10.12360900	-7.55522600
C	-1	-4.07885400	-8.48397300	-6.47725700
C	-1	-3.21302700	-7.57112100	-5.88945900
O	-1	14.10789000	-4.12990000	0.40169900
C	-1	11.26982100	-4.31165500	0.27346300
C	-1	9.88373900	-4.25062100	0.31003900
O	-1	14.81789900	0.32483400	0.50331000
C	-1	12.26908300	0.94090200	1.33987900
O	-1	-6.80242200	1.42660800	12.68660100
C	-1	-4.75230000	0.86811000	10.78055600
C	-1	-3.87229800	0.53093400	9.75964400
O	-1	-9.29229300	-8.78584100	-7.11882200

C	-1	-7.81115700	-6.55806300	-6.06012400
C	-1	-7.07530600	-5.56518700	-5.42481800
C	-1	-2.20493500	9.17751800	-6.54134900
C	-1	-1.90555800	7.98708600	-5.89337100
O	-1	-2.25585500	13.54163100	-3.12545200
C	-1	-1.08608400	11.45977500	-1.74246900
C	-1	12.19096900	-0.95755300	-1.51241700
C	-1	10.82583600	-0.70718900	-1.45083800
O	-1	-7.74367300	-11.30344700	-4.87563600
C	-1	-6.35427500	-9.29665000	-3.40490300
C	-1	-5.59129800	-8.34990300	-2.73449400
O	-1	-9.97731600	0.89212000	12.13935800
C	-1	-8.71950400	0.21726200	9.62293600
C	-1	-7.89490500	-0.02257800	8.53069200
O	-1	14.38776000	-3.55492800	-2.82018300
C	-1	11.68323900	-2.93026500	-2.78169700
O	-1	-5.79946200	-12.38362700	-5.25885900
C	-1	-4.32649000	-10.50442900	-3.84001400
O	-1	-9.74697400	3.07417000	11.62799100
C	-1	-7.98354600	2.50219000	9.55839300
O	-1	-1.24836100	12.96883100	-5.06469000
C	-1	-0.00281100	10.75211000	-3.76408500
C	-1	0.41989000	9.61681600	-3.08518900
O	-1	14.99411200	-1.43383100	1.90663600
C	-1	12.22479200	-1.08638800	2.62306400
C	-1	10.86342900	-0.87588400	2.81066800
C	-1	0.14936800	9.48635600	-6.88975500
O	-1	-10.22218100	-9.11771000	-5.09415700
C	-1	-8.86019600	-7.00573300	-3.94846000
O	-1	-7.60644900	-0.66728500	12.44569600
C	-1	-5.64375600	-1.35609000	10.62395900
O	-1	14.00947100	-4.10493900	2.65808700
C	-1	11.25125200	-4.36115100	2.67294400
O	-1	-5.48272700	11.69234300	-6.36229700
C	-1	-5.15037800	9.42889900	-4.82285600
O	-1	-6.90058200	-8.37779300	-8.77595400
C	-1	-4.91545700	-6.69463800	-7.83991200
O	-1	0.12765100	-4.32910200	-0.46623300
C	-1	-1.42557800	-6.32116600	-1.80219900
O	-1	-2.82119700	1.42933300	3.32682900
C	-1	-4.35274900	1.51902300	5.69596400
O	-1	0.12265400	4.08942900	1.68027600
C	-1	1.85551100	6.36036900	-0.57750800
C	-1	1.60767100	7.56625900	-1.22058300
O	-1	3.55804200	-1.75145100	-1.54853600
C	-1	6.35154300	-2.19976100	-1.76748400
O	-1	-3.47733000	-0.69779700	2.97738000
C	-1	-5.58102700	-0.35634300	4.84671400
C	-1	-6.45722100	-0.19762600	5.91340400
O	-1	2.03521800	3.78970600	0.52938500
C	-1	-0.31689600	6.55472000	0.42253700
O	-1	3.90645700	0.47175700	-1.46820500
C	-1	6.61506900	0.16862200	-2.03099500
C	-1	7.98315600	-0.04713300	-2.12675300
O	-1	-1.56963200	-3.97343400	0.97187200
C	-1	-3.05830800	-6.05179700	-0.06738900
C	-1	-3.83602600	-6.99535400	-0.72284600
O	-1	-0.88710900	-1.11586800	-3.34075200
C	-1	-2.29377500	-3.07396700	-4.78610000
O	-1	3.22364100	-2.48941300	2.72145500

C	-1	5.97778400	-3.05616500	2.65404900
O	-1	-2.59545900	2.38620300	-1.46186000
C	-1	-3.31869100	4.85328500	-2.58785200
O	-1	-2.49821600	3.29998000	0.59476800
C	-1	-3.54442200	5.73030200	-0.36951400
C	-1	-3.88980500	6.94850900	-0.94348000
O	-1	0.72665900	-2.60122500	-2.82833000
C	-1	-0.41523900	-4.53822500	-4.49796600
C	-1	-1.13108800	-5.50597300	-5.19120200
O	-1	2.94015000	-3.49859300	0.72632100
C	-1	5.57024900	-4.43576300	0.73198000
C	-1	6.93515700	-4.68480400	0.68793400
O	-1	-3.60333100	-2.12205900	0.04222700
C	-1	-5.28486400	-3.83348300	-1.39557100
O	-1	1.72305600	2.72363200	-2.27036400
C	-1	1.15876000	5.15233400	-3.68086500
O	-1	4.13335700	1.63207400	1.19957700
C	-1	6.66417400	0.21575400	3.40185900
C	-1	8.04335900	0.03898300	3.40609700
O	-1	-1.38886100	-2.66224500	3.71190800
C	-1	-2.84509600	-2.20256300	6.04331500
O	-1	-3.33165000	-0.78899100	-1.75274300
C	-1	-5.21917700	-2.28166000	-3.22066700
C	-1	-6.03356100	-3.16014300	-3.92598900
O	-1	0.51485000	-1.89073700	4.64075500
C	-1	-0.92803500	-1.08925300	6.95159500
C	-1	-1.72006000	-0.71853500	8.03201800
O	-1	3.85972700	0.37205200	3.04675200
C	-1	6.88886100	1.18220400	1.21925700
O	-1	-0.19168200	1.83491600	-3.05933600
C	-1	-0.72223500	4.01873700	-4.64226400
C	-1	-1.02947800	5.19724700	-5.30610700
O	-1	2.11661500	-0.53746200	0.75432200
O	-1	0.01061800	1.74094800	-0.12326200
O	-1	-0.45676800	-0.13975900	2.60821000
O	-1	-0.70048100	-1.54590500	-0.45140000
O	-1	0.56990600	-2.41502300	1.71648800
O	-1	1.16962400	-0.10099300	-1.64930000
O	-1	1.41934800	1.59845200	2.17597100
O	-1	-2.08906100	0.38882100	0.63731700
C	-1	-4.90858600	11.92771400	-5.16859300
C	-1	-4.73872200	10.69019500	-4.36201500
C	-1	-4.23583800	8.35374400	-3.00687300
C	-1	-6.03557300	-8.96828800	-7.92519900
C	-1	-4.97602700	-8.04140800	-7.45251700
C	-1	-3.26572400	-6.23127400	-6.30838900
C	-1	13.45928400	-4.20382300	1.43019100
C	-1	11.98109400	-4.33771800	1.47483400
C	-1	9.24582200	-4.22744600	1.56074300
C	-1	14.34823300	-0.50168200	1.45966400
C	-1	12.94672900	-0.18374800	1.83847900
C	-1	10.26004900	0.24199700	2.21484600
C	-1	-6.71023900	0.30833000	12.20794000
C	-1	-5.66712100	-0.08886800	11.22732800
C	-1	-3.94470700	-0.75387800	9.19968300
C	-1	-9.42125100	-8.45825600	-5.95031100
C	-1	-8.71347300	-7.31778100	-5.31041400
C	-1	-7.25759800	-5.35918200	-4.04909200
C	-1	-1.16286300	9.95736200	-7.04808200
C	-1	-0.55943700	7.60398800	-5.77864200

C	-1	-1.42144700	12.78864000	-3.87239600
C	-1	-0.79903300	11.68645500	-3.09642800
C	-1	0.03275200	9.45368600	-1.74522200
C	-1	12.64186700	-2.09869300	-2.18049900
C	-1	9.94372300	-1.60490500	-2.07332800
C	-1	-6.53541700	-11.38097300	-4.74126900
C	-1	-5.71809500	-10.39974100	-3.98078900
C	-1	-4.20168700	-8.54193500	-2.65172600
C	-1	-9.55015800	1.76481300	11.39769400
C	-1	-8.76507800	1.50667500	10.16407100
C	-1	-7.13481400	1.03483000	8.00350400
C	-1	-1.02019900	-4.59058000	0.00699500
C	-1	-1.82824100	-5.68336600	-0.62164900
C	-1	-3.36162500	-7.55282500	-1.91995500
C	-1	-3.53609600	0.40777900	3.58560000
C	-1	-4.50858900	0.52737400	4.71613700
C	-1	-6.21762400	0.82383300	6.84607000
C	-1	1.01974500	4.47887600	0.87849100
C	-1	0.86586800	5.82370600	0.25075000
C	-1	0.37448700	8.20383800	-1.01411100
C	-1	4.30197100	-0.72787000	-1.60900000
C	-1	5.76976200	-0.92581200	-1.82559100
C	-1	8.47449000	-1.35748600	-2.01880700
C	-1	-0.34236100	-2.25483200	-3.43046600
C	-1	-1.00971300	-3.29383600	-4.26913000
C	-1	-2.42795100	-5.20193300	-5.63498800
C	-1	3.64075100	-3.17188100	1.73423100
C	-1	5.07319700	-3.58454200	1.72307400
C	-1	7.76794900	-4.06743100	1.63471000
C	-1	-2.75362900	3.34597200	-0.64858800
C	-1	-3.23280900	4.65255400	-1.20278100
C	-1	-3.91401800	7.05858000	-2.34239200
C	-1	-3.85598900	-1.77611800	-1.15231800
C	-1	-4.81565200	-2.62411300	-1.92730800
C	-1	-6.42629500	-4.36226100	-3.31682500
C	-1	0.67372400	2.76135600	-2.98213700
C	-1	0.38601300	3.98859700	-3.79112100
C	-1	-0.21555400	6.32138800	-5.10337900
C	-1	4.57767100	0.94757400	2.17320500
C	-1	6.06054600	0.79210600	2.28125900
C	-1	8.78493700	0.44510400	2.28536400
C	-1	-0.73264700	-2.16545400	4.67326400
C	-1	-1.49680700	-1.83303500	5.91517400
C	-1	-3.06034300	-1.13261900	8.06316900
H	-1	1.44482300	-0.07685700	-2.57999900
H	-1	1.87369800	2.35690700	2.57388500
H	-1	0.60183900	-3.30628200	2.09838700
C	-1	14.09789000	-2.40229100	-2.18621900
O	-1	14.94893700	-1.69404300	-1.67683600
H	-1	15.35205900	-3.69047000	-2.75081000
H	-1	-7.70669700	-8.93051000	-8.81168200
H	-1	-6.40635200	-12.95967600	-5.76149900
H	-1	-10.58380100	-9.89155000	-5.56700000
H	-1	15.63738600	-0.06844700	0.14625900
H	-1	-2.83490200	14.03463600	-3.73987900
C	-1	-1.49390500	11.25498600	-7.69298500
O	-1	-2.62801500	11.68066400	-7.82211600
O	-1	-0.40508000	11.91089400	-8.13973300
H	-1	-0.71105800	12.75703500	-8.51816500
H	-1	-5.48446200	12.53352700	-6.85790500

H	-1	-10.22906900	3.15716500	12.47377300
H	-1	-8.39902800	-0.25463000	12.84997000
H	-1	14.91808700	-3.76481600	2.54412700
H	-1	0.11681000	-0.81193200	6.90683600
H	-1	-1.30075100	-0.14524200	8.85154600
H	-1	-3.31549500	-2.77501200	5.24983100
H	-1	-3.17571200	1.26414000	9.36983100
H	-1	-4.76198300	1.86271700	11.21341300
H	-1	-6.33486300	-2.12673600	10.95279300
H	-1	5.61145300	-2.40110000	3.43826100
H	-1	7.35199600	-5.34121700	-0.06733000
H	-1	4.89219900	-4.87363600	0.00750200
H	-1	11.76972100	-4.40750100	3.62672100
H	-1	11.81255600	-4.29768900	-0.66283000
H	-1	9.31147100	-4.14683500	-0.60514900
H	-1	5.71750900	-3.06791300	-1.61854500
H	-1	11.99647500	-3.82211100	-3.31761700
H	-1	12.91125700	-0.29814000	-1.04361800
H	-1	10.44386500	0.14402300	-0.89809100
H	-1	8.66109900	0.78283800	-2.28917400
H	-1	6.19605100	1.16591300	-2.10477900
H	-1	2.02938400	5.15394700	-3.03337300
H	-1	0.98537300	10.06266700	-7.27685600
H	-1	-3.22510700	9.52130200	-6.65500600
H	-1	-2.69114000	7.37630200	-5.46073400
H	-1	-1.88333200	5.25005800	-5.97179000
H	-1	-1.32872400	3.12852800	-4.76392900
H	-1	-3.51141900	5.60615400	0.70713200
H	-1	-4.14471800	7.79655300	-0.31836200
H	-1	-3.09289800	4.03026700	-3.25783400
H	-1	-5.68892900	9.34244100	-5.76271500
H	-1	-3.75635000	11.71163700	-2.74485400
H	-1	-3.26429800	9.58805300	-1.51416000
H	-1	-3.52374700	2.21842900	5.61936200
H	-1	-5.73212100	-1.13403600	4.10610200
H	-1	-7.32557300	-0.84049300	6.00449300
H	-1	-7.98969600	3.51354000	9.95594000
H	-1	-9.29915500	-0.57852800	10.07804200
H	-1	-7.81169700	-1.02276200	8.12240500
H	-1	0.58367100	-4.73418600	-4.12382900
H	-1	-0.69590300	-6.47949300	-5.38534500
H	-1	-2.56733800	-7.87144400	-5.07117200
H	-1	-4.10494300	-9.51965500	-6.16424600
H	-1	-5.57994800	-6.31932700	-8.61340200
H	-1	-2.77104000	-2.11248700	-4.62699600
H	-1	-0.47099500	-6.06188000	-2.24994700
H	-1	-4.79246600	-7.30007300	-0.31428900
H	-1	-3.38993200	-5.59211000	0.85633600
H	-1	-6.05360700	-7.46385600	-2.31162400
H	-1	-7.42780200	-9.19297900	-3.50413200
H	-1	-3.79780200	-11.34982600	-4.27241400
H	-1	-4.88761800	-1.34690500	-3.65890200
H	-1	-6.36564300	-2.91491000	-4.92830100
H	-1	-4.99153800	-4.12049800	-0.39140100
H	-1	-9.57238300	-7.55455800	-3.33836400
H	-1	-7.67846900	-6.77095900	-7.11367300
H	-1	-6.33043700	-4.99960400	-5.97292400
H	-1	6.44308100	1.63022200	0.33716000
H	-1	12.80409400	1.68403600	0.75488600
H	-1	12.72274700	-1.95838000	3.03031900

Atom		x	y	z
H	-1	10.26812200	-1.60444200	3.34853300
H	-1	8.53634000	-0.39688800	4.26759100
H	-1	6.05594200	-0.08744700	4.24730200
H	-1	2.35306600	8.00680600	-1.87273500
H	-1	2.78754100	5.82498800	-0.72123300
H	-1	-1.09494800	6.15698600	1.06623700
H	-1	0.96826900	8.83557100	-3.60080000
H	-1	0.23463900	10.90747900	-4.80880800
H	-1	-1.67984900	12.17785500	-1.18356200
N	-1	-2.16137400	-7.23402600	-2.44317700
N	-1	-3.57817300	-9.60188200	-3.20160100
N	-1	-2.99215700	-3.99208000	-5.45429100
N	-1	-4.09110100	-5.80550900	-7.28599100
N	-1	-6.06484900	-4.68648500	-2.05981100
N	-1	-8.15247600	-6.06315000	-3.32541000
N	-1	10.96609600	1.15422800	1.51430300
N	-1	8.21045200	1.01712700	1.20809400
N	-1	-0.69272700	10.37341100	-1.07800000
N	-1	-0.56745800	7.71473200	-0.18428000
N	-1	-5.17101100	1.66804500	6.73738600
N	-1	-7.18743400	2.28119400	8.51380300
N	-1	-3.60838900	-1.88689000	7.08958800
N	-1	-4.81575800	-1.68688400	9.63326900
N	-1	7.29099200	-3.28419300	2.62178900
N	-1	9.92040900	-4.30142800	2.72577100
N	-1	7.66501000	-2.42348100	-1.86011700
N	-1	10.36850600	-2.70286800	-2.72978900
N	-1	0.45460500	8.34483200	-6.26708700
N	-1	0.87725100	6.29471500	-4.31532400
N	-1	-3.64586900	6.01555700	-3.15336700
N	-1	-4.90583300	8.28968000	-4.17582600
C	0	1.82749300	2.61544600	5.23344500
O	0	2.55977500	3.53703900	5.26533900
C	0	0.34484800	2.42639200	5.34330200
O	0	-0.36946500	2.58078000	4.36641000
O	0	-0.01268200	1.91359700	6.51062900
H	0	-0.95630100	1.65016100	6.47718100

Sum of electronic and thermal Free Energies = -13350.372871 (Hartree/Particle).

Table S18: DFT-optimized geometry of **f-[Ce^{III}(OC-COOH)-Ce^{IV}]$^-$** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z

Atom		x	y	z
Ce	-1	1.39364900	-2.19697000	-0.59351200
Ce	0	-0.98858500	1.84683700	1.88401500
Ce	-1	-1.73900100	-1.65381400	1.50196600
Ce	-1	2.16662100	1.54664800	-0.17100900
Ce	-1	-1.24412400	0.41643600	-1.45129300
Ce	0	1.69302100	-0.65728600	2.94047500
O	-1	-4.65814900	13.08597900	-4.64875500
C	-1	-4.16009000	10.77851600	-2.99727900
C	-1	-3.89394500	9.59067700	-2.32531400
O	-1	-6.06338400	-10.05313200	-7.69597100
C	-1	-4.00717800	-8.41180600	-6.59515500

C	-1	-3.14880000	-7.50005700	-5.99485500
O	-1	14.14092900	-4.00791700	0.35377100
C	-1	11.30443000	-4.20982400	0.22102100
C	-1	9.91789600	-4.15994300	0.25733500
O	-1	14.81652000	0.45044800	0.51396100
C	-1	12.26248000	1.03592000	1.35655000
O	-1	-6.81968100	1.22685500	12.69414100
C	-1	-4.76405900	0.70904800	10.78253900
C	-1	-3.88081200	0.39199300	9.75798800
O	-1	-9.21771200	-8.74540500	-7.24456200
C	-1	-7.75448700	-6.52028300	-6.15579800
C	-1	-7.02672900	-5.53013800	-5.50705000
C	-1	-2.26938300	9.26292100	-6.42767900
C	-1	-1.96126800	8.06648300	-5.79504000
O	-1	-2.35618700	13.58161200	-2.95524400
C	-1	-1.17131900	11.49097000	-1.59861800
C	-1	12.20088000	-0.82573600	-1.52030100
C	-1	10.83381800	-0.58671100	-1.45650300
O	-1	-7.65121500	-11.28004500	-5.03319600
C	-1	-6.27829500	-9.28195600	-3.53538200
C	-1	-5.52307900	-8.33818400	-2.85211300
O	-1	-9.99000000	0.67512300	12.13756700
C	-1	-8.72536500	0.04282800	9.61352100
C	-1	-7.89822200	-0.17639800	8.51887200
O	-1	14.41848500	-3.38885600	-2.86013100
C	-1	11.70920600	-2.78558300	-2.81556500
O	-1	-5.69848600	-12.34014100	-5.42898400
C	-1	-4.24097500	-10.46831600	-3.98465400
O	-1	-9.77614400	2.86536200	11.65485300
C	-1	-8.00699600	2.33400000	9.57931700
O	-1	-1.34303000	13.04191300	-4.90101500
C	-1	-0.08129200	10.81807900	-3.62845900
C	-1	0.34969800	9.67731800	-2.96409400
O	-1	15.00535500	-1.32495300	1.89438400
C	-1	12.23296700	-1.00820500	2.61317500
C	-1	10.86989900	-0.81065000	2.80247000
C	-1	0.08269900	9.59438700	-6.77024100
O	-1	-10.14635000	-9.11078800	-5.22509900
C	-1	-8.80143700	-7.00350500	-4.05094500
O	-1	-7.60738800	-0.86984700	12.42536100
C	-1	-5.63824500	-1.51971800	10.59629500
O	-1	14.04083300	-4.01313000	2.61021700
C	-1	11.28466100	-4.29073700	2.61963800
O	-1	-5.56657600	11.74989300	-6.21836300
C	-1	-5.21780900	9.46919900	-4.70829400
O	-1	-6.82812400	-8.29739200	-8.89441700
C	-1	-4.85664700	-6.61135200	-7.93501400
O	-1	0.16324800	-4.30341000	-0.52729900
C	-1	-1.37373300	-6.28976800	-1.89029700
O	-1	-2.83242700	1.38223300	3.33821000
C	-1	-4.36618300	1.42924500	5.70716500
O	-1	0.09192600	4.08614900	1.72868600
C	-1	1.80871800	6.39960500	-0.49796900
C	-1	1.55201600	7.61183100	-1.12546500
O	-1	3.57435500	-1.68552400	-1.57332000
C	-1	6.37137100	-2.10942400	-1.79597000
O	-1	-3.47190400	-0.74512300	2.96059000
C	-1	-5.57941100	-0.44429000	4.83261600
C	-1	-6.45750600	-0.30624100	5.90061900
O	-1	2.00751400	3.81618600	0.57547300

C	-1	-0.36578100	6.56417400	0.50287300
O	-1	3.90558000	0.53907400	-1.46375800
C	-1	6.61681000	0.26415100	-2.02839800
C	-1	7.98658200	0.06020000	-2.12591900
O	-1	-1.53771800	-3.97958500	0.91405100
C	-1	-3.00963500	-6.05561200	-0.15336600
C	-1	-3.77962500	-6.99650300	-0.82165300
O	-1	-0.87438300	-1.06086300	-3.36048400
C	-1	-2.26496100	-3.01072500	-4.83229000
O	-1	3.24304100	-2.48159200	2.68669000
C	-1	6.00130600	-3.02624600	2.61374300
O	-1	-2.61090800	2.40316100	-1.43741200
C	-1	-3.35238900	4.87907300	-2.53171200
O	-1	-2.52206200	3.29077300	0.63100100
C	-1	-3.58633400	5.72533400	-0.30230600
C	-1	-3.94071700	6.94822400	-0.86061200
O	-1	0.75046100	-2.54032900	-2.86623300
C	-1	-0.37538700	-4.46411200	-4.56183400
C	-1	-1.08329900	-5.42822200	-5.26816500
O	-1	2.96844600	-3.46687100	0.67810300
C	-1	5.60568400	-4.38376700	0.67355000
C	-1	6.97249900	-4.62170000	0.62730000
O	-1	-3.58500700	-2.13195900	0.00704900
C	-1	-5.25234300	-3.83737700	-1.45422000
O	-1	1.70543200	2.78434600	-2.23816700
C	-1	1.12334500	5.22680100	-3.61733300
O	-1	4.12176200	1.66621100	1.21908900
C	-1	6.66196700	0.24083300	3.40464600
C	-1	8.04247100	0.07464300	3.40762800
O	-1	-1.36885400	-2.70286300	3.67105500
C	-1	-2.83012400	-2.28483800	6.00713800
O	-1	-3.32241600	-0.77354100	-1.77020800
C	-1	-5.19741400	-2.26143400	-3.25889000
C	-1	-6.00453800	-3.13689100	-3.97621800
O	-1	0.52829600	-1.92885500	4.61146100
C	-1	-0.92229800	-1.16873900	6.93130500
C	-1	-1.71787000	-0.81824500	8.01586400
O	-1	3.85664400	0.38016600	3.04946500
C	-1	6.88063900	1.23735400	1.23499400
O	-1	-0.20190200	1.89126600	-3.04011100
C	-1	-0.74822400	4.09138700	-4.59485000
C	-1	-1.06410200	5.27605100	-5.24351400
O	-1	2.12218100	-0.51302900	0.74410100
O	-1	-0.00080900	1.76057500	-0.10536700
O	-1	-0.45543300	-0.15907100	2.60110500
O	-1	-0.68635300	-1.52711300	-0.47683600
O	-1	0.58907600	-2.41414000	1.68005700
O	-1	1.17335700	-0.05232300	-1.65439200
O	-1	1.40729900	1.59885900	2.19283500
O	-1	-2.09053200	0.38254000	0.63594000
C	-1	-4.99505300	11.97409600	-5.02125700
C	-1	-4.81618900	10.72751100	-4.23074400
C	-1	-4.29620800	8.37753300	-2.90578100
C	-1	-5.95915100	-8.89225200	-8.05077200
C	-1	-4.90709200	-7.96348400	-7.56524800
C	-1	-3.21154500	-6.15530700	-6.39633000
C	-1	13.49223400	-4.10023100	1.38071900
C	-1	12.01509100	-4.24607000	1.42249000
C	-1	9.27899500	-4.15798500	1.50775000
C	-1	14.35260700	-0.39205600	1.45910700

C	-1	12.94844400	-0.08988400	1.84096700
C	-1	10.25831500	0.31022500	2.22080800
C	-1	-6.71856700	0.11565400	12.20101900
C	-1	-5.67177300	-0.26068700	11.21610800
C	-1	-3.94294800	-0.88592900	9.18127900
C	-1	-9.34996100	-8.43408300	-6.07197900
C	-1	-8.65141600	-7.29663300	-5.41673800
C	-1	-7.21151100	-5.34349400	-4.12889500
C	-1	-1.23301900	10.05730200	-6.92341500
C	-1	-0.61231100	7.69229400	-5.68429000
C	-1	-1.51550900	12.84486800	-3.71130200
C	-1	-0.88513100	11.73748400	-2.94929000
C	-1	-0.03705500	9.49375900	-1.62666100
C	-1	12.66099900	-1.95456500	-2.20285400
C	-1	9.95906000	-1.48300000	-2.09130700
C	-1	-6.44248700	-11.35001400	-4.89893200
C	-1	-5.63325300	-10.37251600	-4.12511000
C	-1	-4.13208400	-8.52057600	-2.77079900
C	-1	-9.56909100	1.56067200	11.40766300
C	-1	-8.78123200	1.32468900	10.17137800
C	-1	-7.14595500	0.89361200	8.00608500
C	-1	-0.98289600	-4.57984500	-0.05839900
C	-1	-1.78207800	-5.67053000	-0.70184300
C	-1	-3.30015200	-7.53465300	-2.02556400
C	-1	-3.53959300	0.35192400	3.58313100
C	-1	-4.51372800	0.44928200	4.71438300
C	-1	-6.22640300	0.70478700	6.84669700
C	-1	0.98653000	4.49291300	0.93276800
C	-1	0.82269700	5.84459000	0.32247700
C	-1	0.31381900	8.23715400	-0.91163900
C	-1	4.31041100	-0.65554500	-1.61987800
C	-1	5.77982800	-0.83934200	-1.83791500
C	-1	8.48792900	-1.24762900	-2.03468300
C	-1	-0.32081200	-2.19433600	-3.46461500
C	-1	-0.97958400	-3.22742500	-4.31725300
C	-1	-2.38217400	-5.12841400	-5.70893700
C	-1	3.66571200	-3.14801200	1.69070800
C	-1	5.10143400	-3.54938400	1.67527100
C	-1	7.79988400	-4.01032900	1.58267300
C	-1	-2.77700300	3.35101200	-0.61182500
C	-1	-3.26587400	4.66097000	-1.14931000
C	-1	-3.96485500	7.07633200	-2.25798900
C	-1	-3.83952700	-1.77242000	-1.18309400
C	-1	-4.79211500	-2.61760200	-1.96979700
C	-1	-6.38839800	-4.34983500	-3.38306900
C	-1	0.65628900	2.82325400	-2.95018800
C	-1	0.35966200	4.05868600	-3.74333100
C	-1	-0.25899900	6.40368500	-5.02553600
C	-1	4.57069800	0.97246600	2.18400600
C	-1	6.05465600	0.82709700	2.29120400
C	-1	8.78163600	0.50103500	2.29284600
C	-1	-0.71711400	-2.21364900	4.63922000
C	-1	-1.48463700	-1.90330900	5.88485000
C	-1	-3.05494200	-1.24300500	8.04059800
H	-1	1.44897200	-0.01394000	-2.58448300
H	-1	1.85559700	2.35567300	2.60106800
H	-1	0.62796500	-3.31049900	2.05070100
C	-1	14.11932300	-2.24684600	-2.21142300
O	-1	14.96455000	-1.53876900	-1.69220800
H	-1	15.38375400	-3.51786300	-2.79179800

H	-1	-7.62993200	-8.85578500	-8.93795700
H	-1	-6.30058600	-12.91424200	-5.93954800
H	-1	-10.50168300	-9.88115900	-5.70826100
H	-1	15.63924900	0.06817400	0.15243800
H	-1	-2.93861100	14.07811300	-3.56363500
C	-1	-1.57362600	11.36063700	-7.55160600
O	-1	-2.71089700	11.77921900	-7.67604000
O	-1	-0.48959300	12.03067400	-7.98894100
H	-1	-0.80183300	12.87929600	-8.35654800
H	-1	-5.57446700	12.59742800	-6.70296900
H	-1	-10.25942200	2.93361100	12.50127700
H	-1	-8.40339000	-0.46861000	12.83437500
H	-1	14.94687500	-3.66456600	2.50139000
H	-1	0.12040800	-0.88282500	6.89095600
H	-1	-1.30353100	-0.25247300	8.84311100
H	-1	-3.29557300	-2.85049800	5.20590500
H	-1	-3.18964000	1.13555800	9.37829300
H	-1	-4.78169300	1.69782300	11.22831200
H	-1	-6.32360800	-2.29988100	10.91453400
H	-1	5.62942100	-2.38429900	3.40614500
H	-1	7.39488200	-5.26498300	-0.13613600
H	-1	4.93150600	-4.81736500	-0.05708700
H	-1	11.80284300	-4.34552500	3.57312400
H	-1	11.84765900	-4.17947600	-0.71459800
H	-1	9.34544800	-4.04864400	-0.65685700
H	-1	5.74394700	-2.98429900	-1.65883800
H	-1	12.02965900	-3.66793000	-3.36282200
H	-1	12.91575500	-0.16696600	-1.04240200
H	-1	10.44493400	0.25425800	-0.89300100
H	-1	8.65821600	0.89741100	-2.27699600
H	-1	6.19016800	1.25906400	-2.08949800
H	-1	1.99350300	5.22667300	-2.96921300
H	-1	0.91449300	10.18211300	-7.14916500
H	-1	-3.29209900	9.60029500	-6.53762200
H	-1	-2.74240500	7.44408200	-5.37099500
H	-1	-1.91789800	5.33096100	-5.90910100
H	-1	-1.34775400	3.19819800	-4.72856600
H	-1	-3.55308600	5.58741800	0.77265500
H	-1	-4.20257000	7.78606000	-0.22469000
H	-1	-3.11981800	4.06662100	-3.21218900
H	-1	-5.75505800	9.39085800	-5.64960900
H	-1	-3.84278600	11.73531600	-2.59966500
H	-1	-3.33519400	9.59972000	-1.39637300
H	-1	-3.54254500	2.13595100	5.64031400
H	-1	-5.72401900	-1.21340200	4.08182000
H	-1	-7.32093800	-0.95690600	5.98266300
H	-1	-8.02120100	3.34000500	9.99000400
H	-1	-9.29916600	-0.76326500	10.05777900
H	-1	-7.80703900	-1.17050500	8.09765000
H	-1	0.62475700	-4.65723900	-4.18952300
H	-1	-0.64049700	-6.39575000	-5.47464700
H	-1	-2.50135500	-7.80604200	-5.18006000
H	-1	-4.02549200	-9.45165000	-6.29568600
H	-1	-5.52350100	-6.23111600	-8.70405300
H	-1	-2.74972700	-2.05510300	-4.66103400
H	-1	-0.42088100	-6.01732700	-2.33390300
H	-1	-4.73395700	-7.31387500	-0.41782800
H	-1	-3.34540000	-5.61057300	0.77601900
H	-1	-5.99248100	-7.46130900	-2.41808600
H	-1	-7.35252300	-9.18526600	-3.63406800

Atom		x	y	z
H	-1	-3.70550300	-11.30391000	-4.42763000
H	-1	-4.87277900	-1.31852100	-3.68465500
H	-1	-6.33783900	-2.88117500	-4.97550100
H	-1	-4.95747600	-4.13519100	-0.45365300
H	-1	-9.50977600	-7.56570200	-3.44859400
H	-1	-7.61946700	-6.71839900	-7.21193100
H	-1	-6.28588000	-4.95174200	-6.04717300
H	-1	6.43200100	1.69338800	0.35847100
H	-1	12.79213400	1.79071400	0.78169600
H	-1	12.73735900	-1.88157400	3.00941100
H	-1	10.27987000	-1.55071900	3.33034400
H	-1	8.53822800	-0.36861400	4.26374300
H	-1	6.05553300	-0.07803700	4.24560300
H	-1	2.29442400	8.06656700	-1.77125400
H	-1	2.74494100	5.87333300	-0.64795000
H	-1	-1.14116900	6.15210700	1.14074400
H	-1	0.90442200	8.90710600	-3.48942500
H	-1	0.15564200	10.98887600	-4.67088900
H	-1	-1.77096900	12.19711200	-1.03085300
N	-1	-2.10205000	-7.19983100	-2.54367400
N	-1	-3.50005700	-9.56843500	-3.33396500
N	-1	-2.95580600	-3.92539900	-5.51291900
N	-1	-4.03953400	-5.72320100	-7.36892800
N	-1	-6.02529300	-4.68762600	-2.13011200
N	-1	-8.10141300	-6.06370400	-3.41512800
N	-1	10.95777300	1.23691800	1.53274800
N	-1	8.20347000	1.08261400	1.22268400
N	-1	-0.77004000	10.39909600	-0.94806200
N	-1	-0.62487500	7.73003600	-0.08896700
N	-1	-5.18625600	1.55837600	6.74981900
N	-1	-7.20851600	2.13277600	8.53254100
N	-1	-3.59651600	-1.98871500	7.05685500
N	-1	-4.80706800	-1.83118500	9.60200800
N	-1	7.31625400	-3.24372000	2.57951100
N	-1	9.95336200	-4.24195400	2.67222800
N	-1	7.68658300	-2.32180100	-1.89051200
N	-1	10.39272500	-2.56900900	-2.76169700
N	-1	0.39631300	8.44722700	-6.16227000
N	-1	0.83345900	6.37515400	-4.23706600
N	-1	-3.68814100	6.04606500	-3.08228200
N	-1	-4.96491900	8.32355700	-4.07597900
C	0	1.36020600	0.86337000	5.01857200
O	0	2.19465300	0.75709400	5.90390000
C	0	0.19765200	1.88537600	5.28327100
O	0	-0.39644900	2.48269900	4.39209500
O	0	-0.13585200	2.00076300	6.56844900
H	0	-0.90907100	2.59765200	6.64246600

Sum of electronic and thermal Free Energies = -13350.535940 (Hartree/Particle).

Table S19: DFT-optimized geometry of **f-[Ce^{III}(OC-COOH)-Ce^{III}]$^{2-}$** (doublet), computed at the UB3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.37197400	-2.19095800	-0.61326100

Ce	0	-0.98130000	1.82736500	1.84086000
Ce	-1	-1.74634800	-1.64848400	1.50365500
Ce	-1	2.15663100	1.54910600	-0.18093800
Ce	-1	-1.26469000	0.43212400	-1.44450500
Ce	0	1.68817000	-0.66023000	2.86257900
O	-1	-4.66761000	13.12227100	-4.57131800
C	-1	-4.16496900	10.80716400	-2.93197200
C	-1	-3.89756500	9.61606500	-2.26630800
O	-1	-6.14783500	-10.00127800	-7.70007400
C	-1	-4.08089100	-8.36922600	-6.60559900
C	-1	-3.21661000	-7.46190400	-6.00706500
O	-1	14.12042400	-4.03625200	0.24809200
C	-1	11.28267800	-4.23081600	0.13210000
C	-1	9.89652000	-4.17774300	0.17718300
O	-1	14.80781900	0.41981300	0.42150100
C	-1	12.26046000	1.00812000	1.28214800
O	-1	-6.75080600	1.20052200	12.73819500
C	-1	-4.70829200	0.68526600	10.81191000
C	-1	-3.83216100	0.37010500	9.78068700
O	-1	-9.29613100	-8.68774800	-7.22406500
C	-1	-7.82080900	-6.47043400	-6.13569500
C	-1	-7.08665600	-5.48459100	-5.48760100
C	-1	-2.29916800	9.30047800	-6.37989000
C	-1	-1.99005900	8.10083300	-5.75384300
O	-1	-2.35403800	13.60572700	-2.89015500
C	-1	-1.16589700	11.50694300	-1.54905300
C	-1	12.17657500	-0.84209700	-1.60151100
C	-1	10.81051800	-0.60003600	-1.52832700
O	-1	-7.72216800	-11.23479100	-5.03234000
C	-1	-6.33517600	-9.24589400	-3.53525800
C	-1	-5.57346600	-8.30662500	-2.85299500
O	-1	-9.92583200	0.65860000	12.19909000
C	-1	-8.67834700	0.03315900	9.66482300
C	-1	-7.85851500	-0.18376500	8.56423200
O	-1	14.37963200	-3.40527300	-2.96502400
C	-1	11.67215300	-2.79566500	-2.90134900
O	-1	-5.77450200	-12.29802100	-5.44433100
C	-1	-4.30355700	-10.43538000	-4.00174800
O	-1	-9.70964200	2.85019300	11.72361500
C	-1	-7.95464000	2.32271400	9.63512000
O	-1	-1.35423000	13.07122200	-4.84424600
C	-1	-0.09006300	10.83939100	-3.58820700
C	-1	0.34225000	9.69500300	-2.93097800
O	-1	15.00086200	-1.36143100	1.79379000
C	-1	12.23374200	-1.04083600	2.53094300
C	-1	10.87235300	-0.84074700	2.72943400
C	-1	0.05155100	9.62762700	-6.73569500
O	-1	-10.21316500	-9.05880600	-5.20033900
C	-1	-8.85591300	-6.95937900	-4.02631000
O	-1	-7.54524900	-0.89321100	12.46611100
C	-1	-5.58902200	-1.54064400	10.62237900
O	-1	14.03425200	-4.05006500	2.50507700
C	-1	11.27752400	-4.32107800	2.53046000
O	-1	-5.58895500	11.79453300	-6.14048100
C	-1	-5.23641100	9.50710900	-4.64151100
O	-1	-6.91569500	-8.23902200	-8.88690600
C	-1	-4.93424200	-6.56149900	-7.93314100
O	-1	0.13689300	-4.29467600	-0.54766200
C	-1	-1.41329600	-6.27197700	-1.90887000
O	-1	-2.82103600	1.38296600	3.35846200

C	-1	-4.34001600	1.42438400	5.73702200
O	-1	0.09988100	4.08612700	1.74144800
C	-1	1.80850400	6.40415400	-0.48673500
C	-1	1.55087800	7.61944200	-1.10789500
O	-1	3.54782400	-1.68092300	-1.60453300
C	-1	6.34237400	-2.11067200	-1.84613100
O	-1	-3.46799900	-0.74135100	2.97650400
C	-1	-5.56316800	-0.44278800	4.86268800
C	-1	-6.43431400	-0.30681300	5.93663100
O	-1	2.00765000	3.81607800	0.57536500
C	-1	-0.35936600	6.57002900	0.52817100
O	-1	3.88512100	0.54242500	-1.48834000
C	-1	6.59213700	0.26319800	-2.07080500
C	-1	7.96078100	0.05633700	-2.17759200
O	-1	-1.55434900	-3.97241200	0.90543300
C	-1	-3.03786800	-6.04069500	-0.16095500
C	-1	-3.81425200	-6.97710600	-0.82813400
O	-1	-0.91033400	-1.03856800	-3.36169800
C	-1	-2.31470700	-2.97929900	-4.83247500
O	-1	3.24088900	-2.49287700	2.65430500
C	-1	5.99732000	-3.04387200	2.56217500
O	-1	-2.62653200	2.42206000	-1.41441800
C	-1	-3.36874100	4.90401700	-2.49443900
O	-1	-2.52275900	3.30134500	0.65685500
C	-1	-3.58685800	5.74209700	-0.26034300
C	-1	-3.94171000	6.96801300	-0.81167000
O	-1	0.71393200	-2.52386200	-2.88328400
C	-1	-0.42703400	-4.43827400	-4.57938500
C	-1	-1.14163400	-5.39790400	-5.28508200
O	-1	2.95150500	-3.46961500	0.64362400
C	-1	5.58642900	-4.39282600	0.61918200
C	-1	6.95235000	-4.63386100	0.56355200
O	-1	-3.60270500	-2.11632800	0.01832900
C	-1	-5.28317100	-3.81199300	-1.43924600
O	-1	1.68569400	2.79599900	-2.24035900
C	-1	1.10103500	5.24523200	-3.60635500
O	-1	4.12060400	1.65852000	1.19749700
C	-1	6.67078600	0.21848500	3.36172300
C	-1	8.05087400	0.04896500	3.35551800
O	-1	-1.36536300	-2.70691100	3.66630200
C	-1	-2.81116000	-2.29452900	6.01299200
O	-1	-3.34779600	-0.75159200	-1.75520300
C	-1	-5.23555900	-2.22912900	-3.23805600
C	-1	-6.04922200	-3.09982500	-3.95379000
O	-1	0.53943300	-1.94115800	4.59797100
C	-1	-0.89495800	-1.18665100	6.92969100
C	-1	-1.68296300	-0.83849700	8.02050900
O	-1	3.86367000	0.36595400	3.02444400
C	-1	6.87847700	1.22297000	1.19466600
O	-1	-0.22871900	1.91065700	-3.03397000
C	-1	-0.77928700	4.11816000	-4.57670200
C	-1	-1.09628500	5.30611300	-5.21877100
O	-1	2.11284000	-0.51402800	0.72638300
O	-1	-0.00982600	1.76798500	-0.10105900
O	-1	-0.45239100	-0.16115000	2.60066000
O	-1	-0.70563400	-1.51656400	-0.48111000
O	-1	0.58093100	-2.41509900	1.66437600
O	-1	1.15034500	-0.04164700	-1.66438000
O	-1	1.41204900	1.59388100	2.18774200
O	-1	-2.09827200	0.39208600	0.64777400

C	-1	-5.00950800	12.01266900	-4.94606700
C	-1	-4.82879400	10.76257000	-4.16154600
C	-1	-4.30635100	8.40617600	-2.84900600
C	-1	-6.04297600	-8.83927000	-8.05097900
C	-1	-4.98568700	-7.91494500	-7.56835100
C	-1	-3.27856600	-6.11544400	-6.40289200
C	-1	13.47786100	-4.13102900	1.27866400
C	-1	12.00065500	-4.27347800	1.32900100
C	-1	9.26535900	-4.17914800	1.43152400
C	-1	14.34770600	-0.42526900	1.36620200
C	-1	12.94666600	-0.12122000	1.75791500
C	-1	10.25991300	0.28386700	2.15594600
C	-1	-6.65543800	0.09102100	12.24012400
C	-1	-5.61566400	-0.28397400	11.24729700
C	-1	-3.90096000	-0.90539400	9.19939000
C	-1	-9.42037900	-8.38070400	-6.04948000
C	-1	-8.71504000	-7.24751400	-5.39413800
C	-1	-7.26247000	-5.30290300	-4.10761100
C	-1	-1.26395800	10.09430100	-6.87892200
C	-1	-0.64135700	7.72297100	-5.65289900
C	-1	-1.51983600	12.86993200	-3.65426700
C	-1	-0.88745600	11.75805800	-2.90049600
C	-1	-0.03668100	9.50713500	-1.59190500
C	-1	12.62972700	-1.96934600	-2.29129700
C	-1	9.92968200	-1.49172600	-2.16120200
C	-1	-6.51280800	-11.30819300	-4.90582800
C	-1	-5.69643900	-10.33568200	-4.13321600
C	-1	-4.18244200	-8.49267900	-2.78099700
C	-1	-9.50728900	1.54598800	11.47005900
C	-1	-8.72765500	1.31295600	10.22801300
C	-1	-7.10683200	0.88643400	8.05098200
C	-1	-1.00700200	-4.57019000	-0.07276500
C	-1	-1.81278900	-5.65642000	-0.71550700
C	-1	-3.34353200	-7.51168700	-2.03707900
C	-1	-3.52917600	0.35340900	3.60372900
C	-1	-4.49606800	0.44867600	4.74135500
C	-1	-6.19491800	0.69994200	6.88520100
C	-1	0.99053800	4.49385300	0.94160700
C	-1	0.82622400	5.84830100	0.33762100
C	-1	0.31554700	8.24689800	-0.88397700
C	-1	4.28607800	-0.65254200	-1.65162300
C	-1	5.75367000	-0.83901700	-1.87945900
C	-1	8.45950400	-1.25304100	-2.09456300
C	-1	-0.36017200	-2.17295300	-3.47367300
C	-1	-1.02670400	-3.20110600	-4.32624700
C	-1	-2.44247400	-5.09324900	-5.71663900
C	-1	3.65578200	-3.15640300	1.65313400
C	-1	5.09040300	-3.56116400	1.62725200
C	-1	7.78710200	-4.02823000	1.51616800
C	-1	-2.78522300	3.36706700	-0.58412600
C	-1	-3.27422100	4.68029300	-1.11346100
C	-1	-3.97416600	7.10165300	-2.20836000
C	-1	-3.86369600	-1.75151800	-1.16880500
C	-1	-4.82317400	-2.59131800	-1.95289500
C	-1	-6.43235600	-4.31415700	-3.36301700
C	-1	0.63227200	2.84022000	-2.94572000
C	-1	0.33375400	4.07945900	-3.73218500
C	-1	-0.28711500	6.43094400	-5.00137700
C	-1	4.57380300	0.95992200	2.15690400
C	-1	6.05803700	0.81056600	2.25435400

C	-1	8.78417500	0.47794400	2.23785800
C	-1	-0.70647100	-2.22306200	4.63232000
C	-1	-1.46553100	-1.91576100	5.88387500
C	-1	-3.02088500	-1.26013300	8.05185400
H	-1	1.42030300	-0.00028400	-2.59600000
H	-1	1.86469700	2.34801000	2.59614600
H	-1	0.61993100	-3.31299400	2.03127000
C	-1	14.08725600	-2.26509700	-2.31002600
O	-1	14.93739100	-1.56109500	-1.79328900
H	-1	15.34498800	-3.53686800	-2.90316700
H	-1	-7.71911000	-8.79531000	-8.92766500
H	-1	-6.38113600	-12.86866800	-5.95339800
H	-1	-10.57334500	-9.82642100	-5.68429800
H	-1	15.62736900	0.03698100	0.05340700
H	-1	-2.93900000	14.10600800	-3.49298900
C	-1	-1.60527200	11.40090200	-7.49990200
O	-1	-2.74226900	11.82270300	-7.61566500
O	-1	-0.52233500	12.07003900	-7.94131400
H	-1	-0.83477800	12.92084300	-8.30366900
H	-1	-5.59778000	12.64397700	-6.62171700
H	-1	-10.18751700	2.91628700	12.57327200
H	-1	-8.33773200	-0.49166600	12.88160300
H	-1	14.94044800	-3.70325700	2.39200900
H	-1	0.14817100	-0.90308900	6.88401000
H	-1	-1.26215200	-0.27696800	8.84738000
H	-1	-3.28292000	-2.85592500	5.21245000
H	-1	-3.14154200	1.11348800	9.39963000
H	-1	-4.72077100	1.67232700	11.26164000
H	-1	-6.27430000	-2.32039800	10.94180400
H	-1	5.63189600	-2.40414200	3.35936200
H	-1	7.36844700	-5.27516300	-0.20498700
H	-1	4.90670100	-4.82193500	-0.10895800
H	-1	11.80145000	-4.38084800	3.48050200
H	-1	11.82019100	-4.19810900	-0.80673500
H	-1	9.31870900	-4.06148700	-0.73301000
H	-1	5.71368500	-2.98456700	-1.70853700
H	-1	11.98707600	-3.67663000	-3.45401700
H	-1	12.89598600	-0.18692600	-1.12547500
H	-1	10.42716400	0.23965100	-0.95915300
H	-1	8.63350100	0.89251600	-2.32955100
H	-1	6.16754500	1.25936600	-2.12538200
H	-1	1.97517700	5.24047200	-2.96363400
H	-1	0.88241500	10.21483100	-7.11745900
H	-1	-3.32172100	9.64073900	-6.48218700
H	-1	-2.77007300	7.47865700	-5.32740800
H	-1	-1.95403900	5.36568300	-5.87884600
H	-1	-1.38179900	3.22694600	-4.71019300
H	-1	-3.54730700	5.59989100	0.81384500
H	-1	-4.19759600	7.80397900	-0.17087500
H	-1	-3.14235000	4.09368000	-3.17950800
H	-1	-5.77965100	9.43374800	-5.57978400
H	-1	-3.84289300	11.76163300	-2.53259800
H	-1	-3.33306900	9.62012400	-1.34081200
H	-1	-3.51509200	2.12936400	5.66783700
H	-1	-5.71427700	-1.20860200	4.10980400
H	-1	-7.29880100	-0.95571600	6.02147400
H	-1	-7.96386500	3.32713300	10.04981000
H	-1	-9.25135000	-0.77328600	10.10947100
H	-1	-7.77234900	-1.17643000	8.13857700
H	-1	0.57491700	-4.63526300	-4.21402300

H	-1	-0.70246700	-6.36567800	-5.49807300
H	-1	-2.56489100	-7.77263400	-5.19749000
H	-1	-4.09988000	-9.41018900	-6.31008300
H	-1	-5.60490500	-6.17665000	-8.69655100
H	-1	-2.79608300	-2.02319300	-4.65449600
H	-1	-0.46254200	-6.00009300	-2.35729500
H	-1	-4.76684100	-7.29376200	-0.41965700
H	-1	-3.36680500	-5.59849400	0.77221900
H	-1	-6.03804700	-7.43033100	-2.41265300
H	-1	-7.40975500	-9.14623500	-3.62692000
H	-1	-3.77286200	-11.27051800	-4.45128500
H	-1	-4.91127000	-1.28533800	-3.66213800
H	-1	-6.38806500	-2.83939500	-4.94998700
H	-1	-4.98285500	-4.11443400	-0.44169200
H	-1	-9.56188100	-7.52222700	-3.42178800
H	-1	-7.69279500	-6.66473400	-7.19340800
H	-1	-6.34775400	-4.90586600	-6.03003300
H	-1	6.42554400	1.68351300	0.32272100
H	-1	12.78838600	1.76388400	0.70698000
H	-1	12.73844900	-1.91696100	2.92064100
H	-1	10.28379900	-1.58145700	3.25805500
H	-1	8.55083100	-0.39883300	4.20681400
H	-1	6.06878500	-0.10221700	4.20516300
H	-1	2.29038600	8.07491900	-1.75648300
H	-1	2.74250200	5.87622300	-0.64455700
H	-1	-1.13179900	6.15733100	1.16921200
H	-1	0.89184700	8.92552300	-3.46273100
H	-1	0.14084400	11.01370100	-4.63140800
H	-1	-1.76031200	12.21229600	-0.97483800
N	-1	-2.14784200	-7.17771900	-2.56127800
N	-1	-3.55645200	-9.53984000	-3.35214600
N	-1	-3.01196100	-3.88963600	-5.51238300
N	-1	-4.11149300	-5.67754100	-7.36865700
N	-1	-6.06234300	-4.65772600	-2.11365900
N	-1	-8.14969500	-6.02376200	-3.39117100
N	-1	10.95735900	1.21156300	1.46719500
N	-1	8.20082600	1.06509900	1.17357100
N	-1	-0.76326100	10.41156700	-0.90525800
N	-1	-0.61927700	7.73882100	-0.05750000
N	-1	-5.15331900	1.55140000	6.78522400
N	-1	-7.16313000	2.12367300	8.58264800
N	-1	-3.57033300	-2.00067900	7.06857600
N	-1	-4.76476000	-1.85021100	9.62176300
N	-1	7.31150000	-3.26437200	2.51896300
N	-1	9.94669700	-4.26930000	2.59147200
N	-1	7.65645700	-2.32584000	-1.94963300
N	-1	10.35655900	-2.57613900	-2.83849500
N	-1	0.36612700	8.47734300	-6.13415700
N	-1	0.81011800	6.39669800	-4.21979600
N	-1	-3.70505000	6.07396100	-3.03836300
N	-1	-4.98240400	8.35839200	-4.01524800
C	0	1.82962400	0.46354100	5.18618900
O	0	2.55528700	-0.00546400	6.04926400
C	0	0.86826300	1.62044300	5.64186600
O	0	0.15401900	2.22470300	4.86675300
O	0	0.98006400	1.94738800	6.93137200
H	0	0.35572100	2.69012400	7.05392100

Sum of electronic and thermal Free Energies = -13350.741828 (Hartree/Particle).

Table S20: DFT-optimized geometry of **f-[Ce^{III}(OHC-COOH)-Ce^{III}]$^{2-}$** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.37773700	-2.19896000	-0.61379500
Ce	0	-0.97804800	1.83082000	1.77407300
Ce	-1	-1.74458300	-1.64288300	1.49367800
Ce	-1	2.16335000	1.54314300	-0.20130900
Ce	-1	-1.25596200	0.42057800	-1.46536800
Ce	0	1.69745900	-0.60421300	2.91955500
O	-1	-4.64635800	13.09423600	-4.67165500
C	-1	-4.14815800	10.78831400	-3.01806800
C	-1	-3.88267900	9.60091900	-2.34505600
O	-1	-6.13158400	-10.04614200	-7.67094700
C	-1	-4.06605300	-8.40883700	-6.58166200
C	-1	-3.20253800	-7.49851500	-5.98658800
O	-1	14.12351800	-4.04538200	0.28385800
C	-1	11.28591800	-4.23925100	0.16325000
C	-1	9.89969700	-4.18525900	0.20522900
O	-1	14.81274300	0.41127400	0.43313900
C	-1	12.26394100	1.00571600	1.28525600
O	-1	-6.77029800	1.27280300	12.70159000
C	-1	-4.72415500	0.74554900	10.78241600
C	-1	-3.84610000	0.42406800	9.75478600
O	-1	-9.28019100	-8.72840300	-7.20882700
C	-1	-7.80598200	-6.50559800	-6.13019200
C	-1	-7.07265500	-5.51641100	-5.48627200
C	-1	-2.27614300	9.26101700	-6.45352700
C	-1	-1.96888500	8.06483000	-5.81999900
O	-1	-2.33594500	13.58620600	-2.98861700
C	-1	-1.15153900	11.49456800	-1.63312400
C	-1	12.18496700	-0.86094300	-1.58792600
C	-1	10.81888400	-0.61781400	-1.51888800
O	-1	-7.71189800	-11.26360500	-4.99938000
C	-1	-6.32695600	-9.26683000	-3.51091100
C	-1	-5.56616400	-8.32403400	-2.83250000
O	-1	-9.94449400	0.72932000	12.15918500
C	-1	-8.69220700	0.08878000	9.63106500
C	-1	-7.87026200	-0.13483500	8.53339300
O	-1	14.38951600	-3.43293700	-2.93228800
C	-1	11.68221200	-2.82168100	-2.87757400
O	-1	-5.76392500	-12.33010700	-5.40134200
C	-1	-4.29498200	-10.45993900	-3.96647900
O	-1	-9.72627400	2.91805000	11.67160800
C	-1	-7.96732000	2.37778200	9.58971500
O	-1	-1.33246000	13.04004100	-4.93759300
C	-1	-0.07192100	10.81483600	-3.66624500
C	-1	0.35850600	9.67402400	-3.00160300
O	-1	15.00214500	-1.36217400	1.81599100
C	-1	12.23370100	-1.03604100	2.54570500
C	-1	10.87201200	-0.83416800	2.74029800
C	-1	0.07544900	9.58500000	-6.80645100
O	-1	-10.20148600	-9.08742800	-5.18486600
C	-1	-8.84557800	-6.98196100	-4.02013700
O	-1	-7.56521500	-0.82207400	12.43989500
C	-1	-5.60559000	-1.48099000	10.60385500
O	-1	14.03278700	-4.04622900	2.54070600

C	-1	11.27588100	-4.31577500	2.56207200
O	-1	-5.56518500	11.75797400	-6.23504800
C	-1	-5.21678500	9.47900300	-4.72229700
O	-1	-6.89618600	-8.29034400	-8.86939800
C	-1	-4.91584000	-6.60833400	-7.92125300
O	-1	0.14149600	-4.30167800	-0.53864700
C	-1	-1.40691200	-6.28600000	-1.89163900
O	-1	-2.82152800	1.39965300	3.32892300
C	-1	-4.34528200	1.45541600	5.70413400
O	-1	0.10396800	4.09211300	1.70236200
C	-1	1.81821500	6.39652600	-0.53560100
C	-1	1.56243800	7.60835900	-1.16422800
O	-1	3.55583000	-1.69565000	-1.60357300
C	-1	6.35065200	-2.12811000	-1.83706200
O	-1	-3.46875800	-0.72650700	2.95782800
C	-1	-5.56758100	-0.41614800	4.83803600
C	-1	-6.44082500	-0.27360800	5.90942200
O	-1	2.01395300	3.81448000	0.54169900
C	-1	-0.35161500	6.56924600	0.47395800
O	-1	3.89398100	0.52816500	-1.49943100
C	-1	6.60202800	0.24431500	-2.07481900
C	-1	7.97078400	0.03619100	-2.17765600
O	-1	-1.55251600	-3.97028900	0.90916000
C	-1	-3.03489300	-6.04393700	-0.14836200
C	-1	-3.81038700	-6.98378100	-0.81173500
O	-1	-0.89845900	-1.06123800	-3.37338900
C	-1	-2.30081200	-3.00968800	-4.83586400
O	-1	3.23990900	-2.48305500	2.65921500
C	-1	5.99625000	-3.03588600	2.57580900
O	-1	-2.61688800	2.41130400	-1.44942500
C	-1	-3.35570200	4.88739000	-2.54513600
O	-1	-2.51686300	3.30238600	0.61698500
C	-1	-3.57791600	5.73835400	-0.31632000
C	-1	-3.93105500	6.96126200	-0.87537300
O	-1	0.72411100	-2.54454400	-2.88319900
C	-1	-0.41436800	-4.46809200	-4.57061200
C	-1	-1.12801300	-5.43140600	-5.27224500
O	-1	2.95410300	-3.47115300	0.65357900
C	-1	5.58861900	-4.39574800	0.63974600
C	-1	6.95453100	-4.63775000	0.58825600
O	-1	-3.59817000	-2.11833800	0.00730900
C	-1	-5.27652200	-3.82151800	-1.44392600
O	-1	1.69717800	2.77844700	-2.26878200
C	-1	1.11647400	5.22009700	-3.64995700
O	-1	4.12459100	1.65951000	1.18044100
C	-1	6.66969800	0.23067400	3.35802300
C	-1	8.04971300	0.06046200	3.35557700
O	-1	-1.36847900	-2.68908900	3.66311500
C	-1	-2.81880500	-2.26258500	6.00448000
O	-1	-3.33901600	-0.76390200	-1.77349000
C	-1	-5.22450700	-2.24900500	-3.25166900
C	-1	-6.03715100	-3.12339700	-3.96404800
O	-1	0.53480800	-1.91892400	4.59422900
C	-1	-0.90391500	-1.15039200	6.91868900
C	-1	-1.69394800	-0.79562000	8.00590200
O	-1	3.86334100	0.37755000	3.01423600
C	-1	6.88225100	1.22263300	1.18567500
O	-1	-0.21606400	1.88948900	-3.06117600
C	-1	-0.76243900	4.08838500	-4.61763100
C	-1	-1.07756000	5.27279300	-5.26713000

O	-1	2.11671900	-0.51474000	0.71772000
O	-1	-0.00315700	1.76351100	-0.12706000
O	-1	-0.45211400	-0.14990900	2.58476000
O	-1	-0.69980400	-1.52282800	-0.48970400
O	-1	0.58199100	-2.40967700	1.66348600
O	-1	1.15928000	-0.05559800	-1.67764700
O	-1	1.41401300	1.60183700	2.16556700
O	-1	-2.09378300	0.39292100	0.62541800
C	-1	-4.98804200	11.98266900	-5.04073500
C	-1	-4.80952300	10.73699700	-4.24870500
C	-1	-4.29088200	8.38790800	-2.92164300
C	-1	-6.02544800	-8.88621300	-8.02828700
C	-1	-4.96868300	-7.95964400	-7.54882500
C	-1	-3.26303600	-6.15431400	-6.39024200
C	-1	13.47883200	-4.13394900	1.31365600
C	-1	12.00145700	-4.27540200	1.36182400
C	-1	9.26600700	-4.17917900	1.45828000
C	-1	14.35031200	-0.42816400	1.38173100
C	-1	12.94863300	-0.12120800	1.76886600
C	-1	10.26128100	0.28743500	2.15914400
C	-1	-6.67446900	0.16042200	12.21007400
C	-1	-5.63287700	-0.22074900	11.22151300
C	-1	-3.91435100	-0.85470500	9.18066500
C	-1	-9.40665800	-8.41457900	-6.03627200
C	-1	-8.70208700	-7.27799100	-5.38600600
C	-1	-7.25116400	-5.32673900	-4.10770300
C	-1	-1.23954000	10.05147500	-6.95500500
C	-1	-0.62057400	7.68690700	-5.71416900
C	-1	-1.50056400	12.84564800	-3.74681800
C	-1	-0.87024900	11.73780700	-2.98541700
C	-1	-0.02321700	9.49400800	-1.66224400
C	-1	12.63895800	-1.99234000	-2.27032900
C	-1	9.93889000	-1.51269200	-2.14842500
C	-1	-6.50283200	-11.33685900	-4.87000700
C	-1	-5.68754800	-10.36033000	-4.10132900
C	-1	-4.17537900	-8.51033800	-2.75662800
C	-1	-9.52404800	1.61231800	11.42593200
C	-1	-8.74202400	1.37180500	10.18681800
C	-1	-7.11702200	0.93204800	8.01554300
C	-1	-1.00348900	-4.57392100	-0.06449100
C	-1	-1.80850900	-5.66342900	-0.70262900
C	-1	-3.33749100	-7.52550200	-2.01664700
C	-1	-3.53066400	0.37185500	3.57865000
C	-1	-4.49980200	0.47409700	4.71375700
C	-1	-6.20285000	0.73844800	6.85269400
C	-1	0.99643600	4.49482600	0.90200000
C	-1	0.83400300	5.84587200	0.28993900
C	-1	0.32696500	8.23767800	-0.94640200
C	-1	4.29468100	-0.66790800	-1.65506000
C	-1	5.76263800	-0.85638600	-1.87886000
C	-1	8.46869800	-1.27292700	-2.08612300
C	-1	-0.34862800	-2.19650800	-3.47775500
C	-1	-1.01394100	-3.22920800	-4.32577300
C	-1	-2.42783000	-5.12860500	-5.70816600
C	-1	3.65649600	-3.15250200	1.66270000
C	-1	5.09096700	-3.55808900	1.64203300
C	-1	7.78765600	-4.02707200	1.53907200
C	-1	-2.77679100	3.36112600	-0.62488000
C	-1	-3.26407800	4.67153200	-1.16271200
C	-1	-3.96062800	7.08691700	-2.27286800

C	-1	-3.85658700	-1.76020800	-1.18242000
C	-1	-4.81489300	-2.60402500	-1.96362500
C	-1	-6.42207000	-4.33414200	-3.36710700
C	-1	0.64520200	2.81913200	-2.97651100
C	-1	0.34887800	4.05398800	-3.77066000
C	-1	-0.26827900	6.39846400	-5.05454600
C	-1	4.57551200	0.96620100	2.14474600
C	-1	6.05947300	0.81669700	2.24604800
C	-1	8.78547700	0.48268400	2.23696300
C	-1	-0.71130100	-2.20003200	4.62767500
C	-1	-1.47273300	-1.88520600	5.87591500
C	-1	-3.03213600	-1.21643000	8.03695900
H	-1	1.43113600	-0.01970000	-2.60894200
H	-1	1.86620500	2.35807700	2.57056100
H	-1	0.61981100	-3.30547400	2.03559300
C	-1	14.09637700	-2.28888900	-2.28442100
O	-1	14.94581200	-1.58234600	-1.77000700
H	-1	15.35468000	-3.56463800	-2.86772800
H	-1	-7.69978900	-8.84647200	-8.90859400
H	-1	-6.36981100	-12.90337100	-5.90835700
H	-1	-10.56106500	-9.85763000	-5.66514900
H	-1	15.63284600	0.02594900	0.06889900
H	-1	-2.91944500	14.08330600	-3.59548700
C	-1	-1.57896200	11.35466100	-7.58414300
O	-1	-2.71551600	11.77633600	-7.70461500
O	-1	-0.49481000	12.02074200	-8.02719100
H	-1	-0.80610400	12.86960600	-8.39504200
H	-1	-5.57262400	12.60465200	-6.72115600
H	-1	-10.20582900	2.98923700	12.51990500
H	-1	-8.35833700	-0.41777800	12.85147900
H	-1	14.93937900	-3.70050700	2.42748500
H	-1	0.13944300	-0.86759500	6.87349300
H	-1	-1.27453000	-0.22956600	8.83039300
H	-1	-3.28922400	-2.82833100	5.20621400
H	-1	-3.15435000	1.16492700	9.37087500
H	-1	-4.73705800	1.73517400	11.22646100
H	-1	-6.29189200	-2.25857400	10.92635400
H	-1	5.62953200	-2.39142700	3.36858000
H	-1	7.37186300	-5.28364100	-0.17575800
H	-1	4.91015100	-4.82869400	-0.08729800
H	-1	11.79786000	-4.37035400	3.51349700
H	-1	11.82533900	-4.21217800	-0.77466900
H	-1	9.32378100	-4.07394100	-0.70678000
H	-1	5.72125900	-3.00090300	-1.69573700
H	-1	11.99781800	-3.70594700	-3.42455100
H	-1	12.90373700	-0.20340100	-1.11419600
H	-1	10.43479400	0.22530200	-0.95530700
H	-1	8.64421800	0.87116600	-2.33304000
H	-1	6.17803500	1.24035700	-2.13595700
H	-1	1.98931500	5.21859900	-3.00545500
H	-1	0.90736800	10.16961100	-7.18989200
H	-1	-3.29832100	9.60117600	-6.55983600
H	-1	-2.75006200	7.44547900	-5.39158500
H	-1	-1.93395100	5.32899100	-5.92926600
H	-1	-1.36511600	3.19670900	-4.74723300
H	-1	-3.54060100	5.60228300	0.75874200
H	-1	-4.18782400	7.80100600	-0.23989300
H	-1	-3.12832700	4.07303500	-3.22509600
H	-1	-5.75816800	9.40053000	-5.66123000
H	-1	-3.82642000	11.74490100	-2.62351600

H	-1	-3.32005000	9.61000900	-1.41846000
H	-1	-3.51987500	2.15959500	5.63258100
H	-1	-5.71754500	-1.18618700	4.08924600
H	-1	-7.30579800	-0.92160100	5.99623200
H	-1	-7.97689100	3.38456200	9.99862900
H	-1	-9.26649900	-0.71483100	10.07916500
H	-1	-7.78372400	-1.12996200	8.11360400
H	-1	0.58674700	-4.66346400	-4.20210500
H	-1	-0.68889000	-6.40059300	-5.47880300
H	-1	-2.55260500	-7.80491500	-5.17393200
H	-1	-4.08614800	-9.44808100	-6.28023000
H	-1	-5.58477300	-6.22754200	-8.68820700
H	-1	-2.78207900	-2.05234800	-4.66433400
H	-1	-0.45512200	-6.01714300	-2.33969200
H	-1	-4.76395300	-7.29763800	-0.40337800
H	-1	-3.36549500	-5.59624200	0.78159900
H	-1	-6.03120300	-7.44501000	-2.39812200
H	-1	-7.40129900	-9.16718500	-3.60531200
H	-1	-3.76379100	-11.29789000	-4.41015400
H	-1	-4.89890200	-1.30781300	-3.68049200
H	-1	-6.37385600	-2.86851400	-4.96240200
H	-1	-4.97836600	-4.11838600	-0.44405100
H	-1	-9.55303900	-7.54100100	-3.41383000
H	-1	-7.67592900	-6.70601300	-7.18651500
H	-1	-6.33237800	-4.94115400	-6.03051400
H	-1	6.43130300	1.67839200	0.31019400
H	-1	12.79339500	1.75792200	0.70683800
H	-1	12.73719200	-1.91016200	2.94143200
H	-1	10.28203200	-1.57155700	3.27196100
H	-1	8.54773200	-0.38269200	4.21043100
H	-1	6.06584000	-0.08490400	4.20206800
H	-1	2.30347500	8.05976200	-1.81391800
H	-1	2.75227200	5.86725400	-0.68851000
H	-1	-1.12554200	6.16059400	1.11579000
H	-1	0.90879800	8.90124900	-3.52783000
H	-1	0.16117500	10.98305900	-4.70995900
H	-1	-1.74676500	12.20348200	-1.06415800
N	-1	-2.14058300	-7.19511200	-2.54033300
N	-1	-3.54875100	-9.56105100	-3.32050800
N	-1	-2.99713900	-3.92357000	-5.51195500
N	-1	-4.09379900	-5.72155000	-7.36017900
N	-1	-6.05474500	-4.67072800	-2.11505800
N	-1	-8.14018500	-6.04306000	-3.38894100
N	-1	10.96056900	1.21083900	1.46650200
N	-1	8.20456200	1.06401300	1.16815500
N	-1	-0.75073900	10.40270500	-0.98225500
N	-1	-0.60977300	7.73478900	-0.11891900
N	-1	-5.16063500	1.58882100	6.74994700
N	-1	-7.17378700	2.17233900	8.54000200
N	-1	-3.57996200	-1.96233200	7.05682900
N	-1	-4.77946300	-1.79667500	9.60669400
N	-1	7.31040600	-3.25725800	2.53651400
N	-1	9.94496000	-4.26301200	2.62009900
N	-1	7.66483500	-2.34449500	-1.93667600
N	-1	10.36660100	-2.60117000	-2.81863500
N	-1	0.38824800	8.43802900	-6.19770300
N	-1	0.82735800	6.36817000	-4.27056700
N	-1	-3.69034100	6.05436000	-3.09642900
N	-1	-4.96460400	8.33377000	-4.08895500
O	0	1.67994500	0.59709300	4.79377100

C	0	0.68399000	1.42071200	5.25884100
C	0	0.67141200	1.69076400	6.76035100
O	0	-0.18010600	2.36748800	7.30989300
O	0	1.67375800	1.09364000	7.43691900
H	0	1.55200000	1.32175600	8.37952600
H	0	-0.04429300	1.85007500	4.60298100

Sum of electronic and thermal Free Energies = -13351.322795 (Hartree/Particle).

Table S21: DFT-optimized geometry of **f-[Ce^{III}(OH$_2$C-COOH)-Ce^{III}]$^{2-}$** (doublet), computed at the UB3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.37712300	-2.20046200	-0.61528800
Ce	0	-0.97785400	1.83128500	1.77005500
Ce	-1	-1.74492900	-1.64249300	1.49208200
Ce	-1	2.16332700	1.54180400	-0.20540800
Ce	-1	-1.25626200	0.41888900	-1.46840500
Ce	0	1.69739300	-0.60336700	2.91695200
O	-1	-4.64506300	13.09087300	-4.68298400
C	-1	-4.14705900	10.78599900	-3.02787800
C	-1	-3.88169700	9.59902100	-2.35408500
O	-1	-6.13398100	-10.05131200	-7.66646000
C	-1	-4.06811200	-8.41357500	-6.57846600
C	-1	-3.20440900	-7.50297800	-5.98408500
O	-1	14.12271000	-4.04816400	0.28249600
C	-1	11.28507000	-4.24169400	0.16226900
C	-1	9.89886100	-4.18746800	0.20433300
O	-1	14.81260800	0.40849000	0.42869500
C	-1	12.26396900	1.00388800	1.28063300
O	-1	-6.76922500	1.28153300	12.69845700
C	-1	-4.72332900	0.75267500	10.77946100
C	-1	-3.84541200	0.43036800	9.75197200
O	-1	-9.28235200	-8.73279400	-7.20495600
C	-1	-7.80771900	-6.50947700	-6.12795800
C	-1	-7.07418900	-5.51996200	-5.48477300
C	-1	-2.27557300	9.25609600	-6.46246600
C	-1	-1.96843600	8.06029300	-5.82815400
O	-1	-2.33442900	13.58364100	-3.00048300
C	-1	-1.15021400	11.49274700	-1.64367600
C	-1	12.18446600	-0.86470700	-1.59127600
C	-1	10.81842500	-0.62132900	-1.52228300
O	-1	-7.71424000	-11.26673000	-4.99392900
C	-1	-6.32887100	-9.26915200	-3.50693600
C	-1	-5.56788000	-8.32600900	-2.82923100
O	-1	-9.94355000	0.73815300	12.15669900
C	-1	-8.69158000	0.09571400	9.62890400
C	-1	-7.86976500	-0.12876600	8.53131100
O	-1	14.38851500	-3.43793800	-2.93408800
C	-1	11.68130700	-2.82624400	-2.87955000
O	-1	-5.76646100	-12.33379300	-5.39533900
C	-1	-4.29711400	-10.46287000	-3.96187300
O	-1	-9.72504800	2.92652000	11.66761900
C	-1	-7.96635800	2.38458000	9.58593900
O	-1	-1.33119600	13.03600700	-4.94917600

C	-1	-0.07087500	10.81147700	-3.67643100
C	-1	0.35944100	9.67105200	-3.01105400
O	-1	15.00186900	-1.36404800	1.81273200
C	-1	12.23353800	-1.03701000	2.54246900
C	-1	10.87189600	-0.83480400	2.73704400
C	-1	0.07603600	9.57949100	-6.81581600
O	-1	-10.20352200	-9.09031000	-5.18067100
C	-1	-8.84720000	-6.98425500	-4.01748900
O	-1	-7.56447600	-0.81340300	12.43825100
C	-1	-5.60511000	-1.47385300	10.60248600
O	-1	14.03217700	-4.04746700	2.53935200
C	-1	11.27523300	-4.31659000	2.56114300
O	-1	-5.56422600	11.75368800	-6.24539000
C	-1	-5.21603000	9.47569100	-4.73112500
O	-1	-6.89842800	-8.29621400	-8.86603300
C	-1	-4.91775000	-6.61385500	-7.91920300
O	-1	0.14057800	-4.30294500	-0.53860600
C	-1	-1.40824300	-6.28795400	-1.89011700
O	-1	-2.82126100	1.40144500	3.32535900
C	-1	-4.34479800	1.45904400	5.70066500
O	-1	0.10449000	4.09236900	1.69671600
C	-1	1.81888200	6.39501000	-0.54295900
C	-1	1.56322900	7.60645500	-1.17238500
O	-1	3.55520400	-1.69814500	-1.60559900
C	-1	6.34994100	-2.13117800	-1.83904000
O	-1	-3.46883900	-0.72487000	2.95576200
C	-1	-5.56745100	-0.41292500	4.83594400
C	-1	-6.44057900	-0.26953000	5.90730900
O	-1	2.01433200	3.81366600	0.53607400
C	-1	-0.35083400	6.56873600	0.46667300
O	-1	3.89369300	0.52569000	-1.50299400
C	-1	6.60164800	0.24104800	-2.07842700
C	-1	7.97036400	0.03265200	-2.18124300
O	-1	-1.55325800	-3.97032400	0.90912500
C	-1	-3.03603500	-6.04446800	-0.14686100
C	-1	-3.81172700	-6.98464700	-0.80952900
O	-1	-0.89914700	-1.06427300	-3.37545300
C	-1	-2.30191700	-3.01350600	-4.83648300
O	-1	3.23954100	-2.48261400	2.65775000
C	-1	5.99579300	-3.03591000	2.57447600
O	-1	-2.61689200	2.40982700	-1.45369200
C	-1	-3.35543600	4.88527900	-2.55101600
O	-1	-2.51655300	3.30229500	0.61210500
C	-1	-3.57732700	5.73778700	-0.32275800
C	-1	-3.93033400	6.96036800	-0.88260900
O	-1	0.72324700	-2.54748700	-2.88440000
C	-1	-0.41566600	-4.47200900	-4.57040900
C	-1	-1.12951500	-5.43569300	-5.27132600
O	-1	2.95341200	-3.47202900	0.65280900
C	-1	5.58779000	-4.39702300	0.63937100
C	-1	6.95366200	-4.63926300	0.58792500
O	-1	-3.59871700	-2.11868100	0.00619800
C	-1	-5.27744900	-3.82259600	-1.44373400
O	-1	1.69715600	2.77577500	-2.27367700
C	-1	1.11669200	5.21657400	-3.65645500
O	-1	4.12470700	1.65881700	1.17609100
C	-1	6.66979400	0.23108000	3.35441700
C	-1	8.04978300	0.06066200	3.35196500
O	-1	-1.36878900	-2.68728500	3.66219400
C	-1	-2.81884600	-2.25897900	6.00339700

O	-1	-3.33951900	-0.76549100	-1.77554100
C	-1	-5.22536000	-2.25131600	-3.25254700
C	-1	-6.03819600	-3.12607000	-3.96426200
O	-1	0.53469400	-1.91677100	4.59261900
C	-1	-0.90371000	-1.14645000	6.91668400
C	-1	-1.69359500	-0.79082400	8.00372600
O	-1	3.86342800	0.37813900	3.01077700
C	-1	6.88230300	1.22153500	1.18137800
O	-1	-0.21628700	1.88656400	-3.06530000
C	-1	-0.76247300	4.08448500	-4.62319700
C	-1	-1.07747600	5.26849900	-5.27347100
O	-1	2.11647200	-0.51544900	0.71502000
O	-1	-0.00314100	1.76254300	-0.13111800
O	-1	-0.45214300	-0.14897200	2.58203800
O	-1	-0.70030600	-1.52393800	-0.49147300
O	-1	0.58154700	-2.40951700	1.66220500
O	-1	1.15889000	-0.05778900	-1.68057400
O	-1	1.41420700	1.60221300	2.16149400
O	-1	-2.09390300	0.39277300	0.62247300
C	-1	-4.98694400	11.97910700	-5.05128000
C	-1	-4.80854000	10.73394600	-4.25842200
C	-1	-4.29013000	8.38568000	-2.92981300
C	-1	-6.02770500	-8.89164100	-8.02459500
C	-1	-4.97076000	-7.96490400	-7.54585400
C	-1	-3.26474400	-6.15904200	-6.38864500
C	-1	13.47810100	-4.13593700	1.31241000
C	-1	12.00071000	-4.27713800	1.36080400
C	-1	9.26528200	-4.18044500	1.45743500
C	-1	14.35013600	-0.43023600	1.37789700
C	-1	12.94853700	-0.12281000	1.76494700
C	-1	10.26128000	0.28649600	2.15518400
C	-1	-6.67360400	0.16880500	12.20768600
C	-1	-5.63215600	-0.21319000	11.21929200
C	-1	-3.91390300	-0.84878400	9.17872300
C	-1	-9.40866900	-8.41815600	-6.03260300
C	-1	-8.70387300	-7.28123200	-5.38316900
C	-1	-7.25254800	-5.32932900	-4.10631700
C	-1	-1.23889700	10.04606000	-6.96457000
C	-1	-0.62017200	7.68224200	-5.72218600
C	-1	-1.49922400	12.84244600	-3.75825500
C	-1	-0.86900700	11.73502800	-2.99615900
C	-1	-0.02219100	9.49200100	-1.67154000
C	-1	12.63822900	-1.99663300	-2.27295200
C	-1	9.93824300	-1.51650300	-2.15113600
C	-1	-6.50517400	-11.34007500	-4.86461300
C	-1	-5.68967700	-10.36314600	-4.09666800
C	-1	-4.17711600	-8.51246700	-2.75335500
C	-1	-9.52303700	1.62059200	11.42281100
C	-1	-8.74115800	1.37912300	10.18379100
C	-1	-7.11641200	0.93765400	8.01267200
C	-1	-1.00440600	-4.57469700	-0.06416500
C	-1	-1.80964400	-5.66451800	-0.70149400
C	-1	-3.33901700	-7.52725400	-2.01411500
C	-1	-3.53052800	0.37392200	3.57584500
C	-1	-4.49955100	0.47707700	4.71096700
C	-1	-6.20237100	0.74313000	6.84987400
C	-1	0.99694700	4.49440700	0.89600300
C	-1	0.83466100	5.84506200	0.28304000
C	-1	0.32786800	8.23610400	-0.95487700
C	-1	4.29420300	-0.67054800	-1.65784700

C	-1	5.76211200	-0.85939500	-1.88164800
C	-1	8.46809200	-1.27647800	-2.08886700
C	-1	-0.34949300	-2.19969500	-3.47909800
C	-1	-1.01503400	-3.23287100	-4.32635700
C	-1	-2.42932600	-5.13299500	-5.70733800
C	-1	3.65594100	-3.15279800	1.66165200
C	-1	5.09035100	-3.55861200	1.64113400
C	-1	7.78696100	-4.02806400	1.53825400
C	-1	-2.77658200	3.36023100	-0.62977700
C	-1	-3.26372200	4.67034500	-1.16845400
C	-1	-3.96001200	7.08508000	-2.28018600
C	-1	-3.85718600	-1.76131900	-1.18375000
C	-1	-4.81568500	-2.60552400	-1.96429900
C	-1	-6.42324200	-4.33635300	-3.36646700
C	-1	0.64512400	2.81613600	-2.98134100
C	-1	0.34891300	4.05049800	-3.77630000
C	-1	-0.26801000	6.39419400	-5.06172100
C	-1	4.57561000	0.96609500	2.14082600
C	-1	6.05955800	0.81643900	2.24209800
C	-1	8.78551100	0.48201600	2.23300000
C	-1	-0.71145300	-2.19767100	4.62636500
C	-1	-1.47272900	-1.88188600	5.87445800
C	-1	-3.03184300	-1.21141500	8.03518500
H	-1	1.43067000	-0.02256200	-2.61191700
H	-1	1.86654700	2.35866000	2.56593500
H	-1	0.61926700	-3.30506700	2.03491600
C	-1	14.09560300	-2.29340800	-2.28697100
O	-1	14.94518800	-1.58664200	-1.77311100
H	-1	15.35366600	-3.56973800	-2.86952400
H	-1	-7.70211700	-8.85224900	-8.90478200
H	-1	-6.37247600	-12.90731000	-5.90191200
H	-1	-10.56325700	-9.86078400	-5.66040000
H	-1	15.63262200	0.02279700	0.06464400
H	-1	-2.91790900	14.08041600	-3.60763800
C	-1	-1.57818100	11.34887000	-7.59456200
O	-1	-2.71468300	11.77063100	-7.71522000
O	-1	-0.49396900	12.01449000	-8.03815600
H	-1	-0.80517000	12.86315000	-8.40655500
H	-1	-5.57158200	12.60003700	-6.73207100
H	-1	-10.20451800	2.99835300	12.51591000
H	-1	-8.35750200	-0.40871000	12.84963100
H	-1	14.93881000	-3.70195700	2.42581700
H	-1	0.13968600	-0.86383800	6.87120400
H	-1	-1.27402100	-0.22427400	8.82779600
H	-1	-3.28941900	-2.82519600	5.20555600
H	-1	-3.15358700	1.17086400	9.36749800
H	-1	-4.73604700	1.74260300	11.22283600
H	-1	-6.29149900	-2.25111700	10.92557300
H	-1	5.62924000	-2.39085900	3.36684300
H	-1	7.37083100	-5.28573300	-0.17568700
H	-1	4.90919400	-4.83036200	-0.08731900
H	-1	11.79728800	-4.37060200	3.51255900
H	-1	11.82441300	-4.21533600	-0.77571600
H	-1	9.32288100	-4.07668300	-0.70770100
H	-1	5.72043100	-3.00378100	-1.69706800
H	-1	11.99673400	-3.71092700	-3.42595600
H	-1	12.90337500	-0.20695000	-1.11805500
H	-1	10.43450900	0.22222600	-0.95923900
H	-1	8.64390800	0.86742100	-2.33725300
H	-1	6.17779700	1.23711100	-2.14020300

H	-1	1.98959000	5.21538400	-3.01202900
H	-1	0.90800800	10.16371900	-7.19972600
H	-1	-3.29771000	9.59633400	-6.56891500
H	-1	-2.74966700	7.44134800	-5.39925200
H	-1	-1.93391700	5.32437600	-5.93557000
H	-1	-1.36529400	3.19281100	-4.75214200
H	-1	-3.53993800	5.60243900	0.75239300
H	-1	-4.18692300	7.80058000	-0.24767500
H	-1	-3.12824100	4.07043000	-3.23044400
H	-1	-5.75750700	9.39666200	-5.66995700
H	-1	-3.82514500	11.74280500	-2.63400300
H	-1	-3.31898500	9.60865500	-1.42754500
H	-1	-3.51929300	2.16305200	5.62856200
H	-1	-5.71759500	-1.18345000	4.08768900
H	-1	-7.30564100	-0.91733600	5.99463500
H	-1	-7.97574300	3.39163900	9.99417100
H	-1	-9.26595200	-0.70750800	10.07759900
H	-1	-7.78341100	-1.12419100	8.11218900
H	-1	0.58545300	-4.66728000	-4.20185700
H	-1	-0.69055400	-6.40508500	-5.47726600
H	-1	-2.55445000	-7.80892400	-5.17127900
H	-1	-4.08833400	-9.45261200	-6.27632800
H	-1	-5.58669400	-6.23348400	-8.68635600
H	-1	-2.78302700	-2.05597900	-4.66556000
H	-1	-0.45645300	-6.01954200	-2.33843600
H	-1	-4.76530300	-7.29808600	-0.40087500
H	-1	-3.36648900	-5.59609400	0.78282500
H	-1	-6.03275100	-7.44662200	-2.39540800
H	-1	-7.40320800	-9.16941100	-3.60131000
H	-1	-3.76608600	-11.30120100	-4.40502700
H	-1	-4.89965300	-1.31046300	-3.68203700
H	-1	-6.37495100	-2.87181400	-4.96275900
H	-1	-4.97924900	-4.11883000	-0.44368500
H	-1	-9.55469000	-7.54277900	-3.41074100
H	-1	-7.67778900	-6.71062700	-7.18415600
H	-1	-6.33387400	-4.94518400	-6.02947000
H	-1	6.43134500	1.67676700	0.30562800
H	-1	12.79348400	1.75562300	0.70165900
H	-1	12.73693400	-1.91093700	2.93874400
H	-1	10.28185300	-1.57174500	3.26925900
H	-1	8.54781200	-0.38198700	4.20707500
H	-1	6.06596300	-0.08383700	4.19872900
H	-1	2.30427600	8.05730700	-1.82244600
H	-1	2.75284700	5.86549600	-0.69559200
H	-1	-1.12476500	6.16063400	1.10885000
H	-1	0.90957200	8.89783900	-3.53680500
H	-1	0.16215400	10.97895800	-4.72027900
H	-1	-1.74528500	12.20213500	-1.07513900
N	-1	-2.14210600	-7.19739700	-2.53813000
N	-1	-3.55069300	-9.56365500	-3.31657700
N	-1	-2.99843900	-3.92774300	-5.51189400
N	-1	-4.09552800	-5.72681300	-7.35880200
N	-1	-6.05585700	-4.67214500	-2.11422200
N	-1	-8.14161200	-6.04503100	-3.38699100
N	-1	10.96064300	1.20932600	1.46185500
N	-1	8.20458900	1.06270700	1.16385000
N	-1	-0.74951800	10.40126600	-0.99210300
N	-1	-0.60887100	7.73391500	-0.12697100
N	-1	-5.16003900	1.59327900	6.74645900
N	-1	-7.17294700	2.17830800	8.53629500

Atom		x	y	z
N	-1	-3.57986500	-1.95790000	7.05560900
N	-1	-4.77911700	-1.79033700	9.60546700
N	-1	7.30991300	-3.25750300	2.53521600
N	-1	9.94432500	-4.26359100	2.61925100
N	-1	7.66408300	-2.34782500	-1.93862300
N	-1	10.36573400	-2.60549800	-2.82064500
N	-1	0.38871900	8.43288700	-6.20631800
N	-1	0.82769200	6.36426900	-4.27781800
N	-1	-3.68995000	6.05192500	-3.10307000
N	-1	-4.96396300	8.33085000	-4.09702900
O	0	1.68022200	0.59921100	4.79035500
C	0	0.68442900	1.42329300	5.25495400
H	0	0.71283300	2.42944500	4.78877300
H	0	-0.32924900	1.03493200	5.04324200
C	0	0.67202400	1.69436400	6.75628200
O	0	-0.17934600	2.37158700	7.30544000
O	0	1.67434100	1.09755100	7.43316600
H	0	1.55269900	1.32632400	8.37562900

Sum of electronic and thermal Free Energies = -13351.893112 (Hartree/Particle).

Table S22: DFT-optimized geometry of **f-[Ce^{III}(HOH$_2$C-COOH)-Ce^{III}]$^{2-}$** (singlet), computed at the B3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.37511800	-2.20108000	-0.61851000
Ce	0	-0.97791000	1.83153400	1.76729100
Ce	-1	-1.74561000	-1.64220700	1.49058100
Ce	-1	2.16206100	1.54117700	-0.20996600
Ce	-1	-1.25842500	0.41842200	-1.47067500
Ce	0	1.69769400	-0.60320600	2.91316800
O	-1	-4.64745200	13.09010800	-4.68619100
C	-1	-4.14877300	10.78555300	-3.03084400
C	-1	-3.88316800	9.59869600	-2.35693300
O	-1	-6.14120500	-10.05257200	-7.66340200
C	-1	-4.07447500	-8.41485700	-6.57701400
C	-1	-3.21029900	-7.50423600	-5.98335700
O	-1	14.12099000	-4.05026400	0.27214700
C	-1	11.28325400	-4.24344500	0.15364800
C	-1	9.89707700	-4.18902600	0.19652100
O	-1	14.81156500	0.40633300	0.41690100
C	-1	12.26351100	1.00226700	1.27021100
O	-1	-6.76287400	1.28509100	12.69925200
C	-1	-4.71818600	0.75551500	10.77916700
C	-1	-3.84092100	0.43285300	9.75123200
O	-1	-9.28912700	-8.73353000	-7.20033800
C	-1	-7.81356200	-6.51015800	-6.12473200
C	-1	-7.07951900	-5.52059100	-5.48221200
C	-1	-2.27952600	9.25460300	-6.46618500
C	-1	-1.97217100	8.05890700	-5.83177800
O	-1	-2.33575600	13.58296000	-3.00517500
C	-1	-1.15101400	11.49222500	-1.64858400
C	-1	12.18205700	-0.86698500	-1.60121500

C	-1	10.81609000	-0.62341000	-1.53146900
O	-1	-7.72004100	-11.26716000	-4.98965200
C	-1	-6.33352600	-9.26942000	-3.50394500
C	-1	-5.57200800	-8.32622000	-2.82691100
O	-1	-9.93759100	0.74200600	12.15950200
C	-1	-8.68720500	0.09881300	9.63111500
C	-1	-7.86607100	-0.12603100	8.53308700
O	-1	14.38496900	-3.44082100	-2.94473500
C	-1	11.67787500	-2.82875500	-2.88873500
O	-1	-5.77264100	-12.33457400	-5.39196900
C	-1	-4.30219700	-10.46351300	-3.95980900
O	-1	-9.71909000	2.93023000	11.66978400
C	-1	-7.96170600	2.38757300	9.58718800
O	-1	-1.33375100	13.03474000	-4.95433500
C	-1	-0.07297000	10.81033900	-3.68182000
C	-1	0.35758900	9.67001200	-3.01643300
O	-1	15.00141200	-1.36590900	1.80123800
C	-1	12.23355700	-1.03833400	2.53254000
C	-1	10.87205800	-0.83590200	2.72787500
C	-1	0.07191600	9.57760400	-6.82100500
O	-1	-10.20914400	-9.09045300	-5.17542400
C	-1	-8.85185400	-6.98430700	-4.01353600
O	-1	-7.55855700	-0.80980000	12.44000500
C	-1	-5.60036700	-1.47093700	10.60323200
O	-1	14.03179500	-4.04903000	2.52905700
C	-1	11.27482900	-4.31778200	2.55254500
O	-1	-5.56771900	11.75268200	-6.24774100
C	-1	-5.21892700	9.47499000	-4.73315300
O	-1	-6.90613100	-8.29765200	-8.86293000
C	-1	-4.92466900	-6.61533600	-7.91766500
O	-1	0.13834000	-4.30338100	-0.54060600
C	-1	-1.41154500	-6.28849900	-1.89073700
O	-1	-2.82045200	1.40230000	3.32378800
C	-1	-4.34257300	1.46065300	5.69998300
O	-1	0.10469000	4.09245700	1.69278500
C	-1	1.81805900	6.39435000	-0.54844200
C	-1	1.56219300	7.60568300	-1.17799800
O	-1	3.55267800	-1.69928200	-1.61022900
C	-1	6.34721900	-2.13274000	-1.84522600
O	-1	-3.46853000	-0.72401500	2.95506900
C	-1	-5.56598600	-0.41135500	4.83642200
C	-1	-6.43846000	-0.26759500	5.90827100
O	-1	2.01380600	3.81323100	0.53107500
C	-1	-0.35103500	6.56859900	0.46243600
O	-1	3.89152200	0.52453200	-1.50834200
C	-1	6.59909800	0.23939700	-2.08531400
C	-1	7.96772500	0.03079600	-2.18889300
O	-1	-1.55459300	-3.97019900	0.90805200
C	-1	-3.03827100	-6.04439100	-0.14657300
C	-1	-3.81448000	-6.98462200	-0.80856200
O	-1	-0.90263700	-1.06523100	-3.37758900
C	-1	-2.30653200	-3.01461700	-4.83733400
O	-1	3.23943900	-2.48271800	2.65348900
C	-1	5.99556800	-3.03639900	2.56871000
O	-1	-2.61878200	2.40954400	-1.45561800
C	-1	-3.35764900	4.88483900	-2.55308000
O	-1	-2.51710000	3.30247900	0.60991100
C	-1	-3.57810600	5.73789400	-0.32488900
C	-1	-3.93128300	6.96039200	-0.88481500
O	-1	0.71985100	-2.54854600	-2.88715300

C	-1	-0.42031700	-4.47330800	-4.57203900
C	-1	-1.13470900	-5.43706100	-5.27230900
O	-1	2.95199000	-3.47256100	0.64894800
C	-1	5.58623700	-4.39790800	0.63416300
C	-1	6.95204600	-4.64034100	0.58196400
O	-1	-3.60034200	-2.11849400	0.00590700
C	-1	-5.28015900	-3.82252400	-1.44263400
O	-1	1.69482700	2.77472900	-2.27824600
C	-1	1.11386700	5.21528300	-3.66124700
O	-1	4.12427500	1.65825100	1.17034200
C	-1	6.67046400	0.23068300	3.34749100
C	-1	8.05042800	0.06008100	3.34426100
O	-1	-1.36832200	-2.68654400	3.66071200
C	-1	-2.81693400	-2.25750200	6.00267500
O	-1	-3.34202100	-0.76575300	-1.77630000
C	-1	-5.22893400	-2.25167100	-3.25184200
C	-1	-6.04230800	-3.12648300	-3.96287200
O	-1	0.53581400	-1.91606600	4.58982900
C	-1	-0.90110900	-1.14501400	6.91456800
C	-1	-1.69030300	-0.78903100	8.00199500
O	-1	3.86391400	0.37803400	3.00548100
C	-1	6.88181600	1.22060400	1.17409600
O	-1	-0.21920300	1.88558800	-3.06852700
C	-1	-0.76602100	4.08321900	-4.62661100
C	-1	-1.08125300	5.26712400	-5.27697400
O	-1	2.11547900	-0.51585600	0.71096800
O	-1	-0.00433400	1.76222100	-0.13444300
O	-1	-0.45198000	-0.14860400	2.57942300
O	-1	-0.70214800	-1.52425200	-0.49362100
O	-1	0.58086500	-2.40950000	1.65950300
O	-1	1.15653700	-0.05862600	-1.68416500
O	-1	1.41435200	1.60223600	2.15736500
O	-1	-2.09483000	0.39290300	0.62070500
C	-1	-4.98969900	11.97830200	-5.05402600
C	-1	-4.81099000	10.73330100	-4.26098400
C	-1	-4.29210300	8.38527500	-2.93213600
C	-1	-6.03498800	-8.89299900	-8.02187000
C	-1	-4.97763700	-7.96629100	-7.54397100
C	-1	-3.27069600	-6.16038600	-6.38819300
C	-1	13.47698000	-4.13771200	1.30246400
C	-1	11.99959900	-4.27870600	1.35176700
C	-1	9.26424200	-4.18162700	1.44999700
C	-1	14.34954500	-0.43211100	1.36657200
C	-1	12.94821600	-0.12440900	1.75438100
C	-1	10.26124500	0.28534400	2.14611600
C	-1	-6.66769100	0.17223600	12.20868300
C	-1	-5.62688000	-0.21012700	11.21976100
C	-1	-3.90992100	-0.84642300	9.17832100
C	-1	-9.41470800	-8.41860200	-6.02798400
C	-1	-8.70937600	-7.28162100	-5.37923200
C	-1	-7.25703600	-5.32961400	-4.10369500
C	-1	-1.24304300	10.04431300	-6.96908800
C	-1	-0.62389500	7.68070200	-5.72652100
C	-1	-1.50109900	12.84147900	-3.76326900
C	-1	-0.87057700	11.73415400	-3.00129000
C	-1	-0.02327300	9.49132300	-1.67665100
C	-1	12.63526600	-1.99913000	-2.28289700
C	-1	9.93541600	-1.51861300	-2.15959200
C	-1	-6.51090800	-11.34063500	-4.86103600
C	-1	-5.69482600	-10.36363600	-4.09380200

C	-1	-4.18122400	-8.51284500	-2.75181600
C	-1	-9.51739700	1.62421800	11.42516000
C	-1	-8.73628400	1.38235800	10.18573300
C	-1	-7.11288400	0.94016800	8.01375400
C	-1	-1.00639800	-4.57487100	-0.06542300
C	-1	-1.81215900	-5.66473300	-0.70202100
C	-1	-3.34255600	-7.52757100	-2.01330200
C	-1	-3.52970600	0.37492900	3.57493300
C	-1	-4.49804200	0.47847700	4.71060500
C	-1	-6.19955900	0.74525300	6.85045900
C	-1	0.99672500	4.49419100	0.89144900
C	-1	0.83425500	5.84472500	0.27826900
C	-1	0.32704500	8.23554600	-0.95990400
C	-1	4.29178200	-0.67179500	-1.66315400
C	-1	5.75953300	-0.86088900	-1.88778100
C	-1	8.46533400	-1.27837900	-2.09650700
C	-1	-0.35319500	-2.20075000	-3.48129600
C	-1	-1.01937600	-3.23403400	-4.32792000
C	-1	-2.43473800	-5.13429200	-5.70762000
C	-1	3.65515900	-3.15318900	1.65730000
C	-1	5.08950300	-3.55919800	1.63602600
C	-1	7.78598900	-4.02903100	1.53165700
C	-1	-2.77785800	3.36016100	-0.63183000
C	-1	-3.26514400	4.67021400	-1.17052200
C	-1	-3.96177300	7.08478300	-2.28240300
C	-1	-3.85946900	-1.76137500	-1.18397100
C	-1	-4.81854200	-2.60563400	-1.96375500
C	-1	-6.42716000	-4.33657600	-3.36456700
C	-1	0.64238100	2.81506500	-2.98529500
C	-1	0.34586200	4.04928100	-3.78036500
C	-1	-0.27151200	6.39276000	-5.06596500
C	-1	4.57565800	0.96569300	2.13497100
C	-1	6.05964600	0.81586400	2.23539800
C	-1	8.78554900	0.48107800	2.22476200
C	-1	-0.71035000	-2.19679300	4.62438000
C	-1	-1.47084400	-1.88061700	5.87285000
C	-1	-3.02858800	-1.20943700	8.03434500
H	-1	1.42777000	-0.02365100	-2.61567700
H	-1	1.86703200	2.35871700	2.56136200
H	-1	0.61868700	-3.30496800	2.03240000
C	-1	14.09259200	-2.29610100	-2.29771100
O	-1	14.94257500	-1.58932900	-1.78451900
H	-1	15.35014100	-3.57273400	-2.88071300
H	-1	-7.70991600	-8.85358900	-8.90107300
H	-1	-6.37903300	-12.90812900	-5.89804900
H	-1	-10.56926600	-9.86099100	-5.65476100
H	-1	15.63131200	0.02044600	0.05245400
H	-1	-2.91953000	14.07967200	-3.61209900
C	-1	-1.58252800	11.34702100	-7.59918100
O	-1	-2.71904500	11.76890500	-7.71926400
O	-1	-0.49849100	12.01239400	-8.04357300
H	-1	-0.80979800	12.86101000	-8.41198500
H	-1	-5.57525100	12.59891800	-6.73461400
H	-1	-10.19804700	3.00232400	12.51834200
H	-1	-8.35128500	-0.40490700	12.85176100
H	-1	14.93840600	-3.70366700	2.41490400
H	-1	0.14229700	-0.86255100	6.86840300
H	-1	-1.27016500	-0.22234500	8.82568400
H	-1	-3.28805500	-2.82384200	5.20524500
H	-1	-3.14922600	1.17316800	9.36617600

H	-1	-4.73051000	1.74554800	11.22231900
H	-1	-6.28666700	-2.24803500	10.92690700
H	-1	5.62957000	-2.39111500	3.36114400
H	-1	7.36867700	-5.28704400	-0.18174500
H	-1	4.90715300	-4.83132600	-0.09202300
H	-1	11.79744100	-4.37164200	3.50366300
H	-1	11.82204400	-4.21737700	-0.78466300
H	-1	9.32057100	-4.07837600	-0.71519700
H	-1	5.71767700	-3.00522600	-1.70267800
H	-1	11.99286100	-3.71360700	-3.43512200
H	-1	12.90133400	-0.20921400	-1.12857400
H	-1	10.43261900	0.22032700	-0.96839400
H	-1	8.64128700	0.86543900	-2.34549600
H	-1	6.17534300	1.23550200	-2.14707000
H	-1	1.98714700	5.21412700	-3.01733800
H	-1	0.90373800	10.16163200	-7.20554400
H	-1	-3.30168100	9.59495200	-6.57210800
H	-1	-2.75323000	7.44016500	-5.40226900
H	-1	-1.93807900	5.32296000	-5.93857800
H	-1	-1.36903600	3.19159500	-4.75499100
H	-1	-3.54009700	5.60279100	0.75027100
H	-1	-4.18738400	7.80078500	-0.24992400
H	-1	-3.13096500	4.06980200	-3.23245300
H	-1	-5.76097100	9.39581500	-5.67164500
H	-1	-3.82649800	11.74240700	-2.63738300
H	-1	-3.31990600	9.60847100	-1.43072900
H	-1	-3.51701700	2.16453500	5.62722700
H	-1	-5.71667600	-1.18203400	4.08843600
H	-1	-7.30355600	-0.91526600	5.99626100
H	-1	-7.97071500	3.39472800	9.99519100
H	-1	-9.26141800	-0.70422800	10.08033700
H	-1	-7.78009700	-1.12156500	8.11414600
H	-1	0.58099500	-4.66862700	-4.20403500
H	-1	-0.69599800	-6.40655900	-5.47828300
H	-1	-2.55989900	-7.81007900	-5.17086500
H	-1	-4.09465500	-9.45382100	-6.27462200
H	-1	-5.59401700	-6.23505400	-8.68451000
H	-1	-2.78741300	-2.05698700	-4.66634800
H	-1	-0.45998500	-6.02031700	-2.33968200
H	-1	-4.76785500	-7.29783900	-0.39927000
H	-1	-3.36811400	-5.59575800	0.78320500
H	-1	-6.03650500	-7.44667100	-2.39301700
H	-1	-7.40790500	-9.16955800	-3.59770500
H	-1	-3.77154300	-11.30201700	-4.40308300
H	-1	-4.90335700	-1.31096100	-3.68174400
H	-1	-6.37962100	-2.87241400	-4.96122800
H	-1	-4.98140500	-4.11856500	-0.44269300
H	-1	-9.55905800	-7.54259600	-3.40623900
H	-1	-7.68428400	-6.71157100	-7.18096000
H	-1	-6.33945100	-4.94603800	-6.02748100
H	-1	6.43039900	1.67569300	0.29850800
H	-1	12.79278200	1.75379700	0.69074900
H	-1	12.73707200	-1.91223500	2.92871900
H	-1	10.28223300	-1.57264100	3.26061100
H	-1	8.54890600	-0.38243500	4.19917800
H	-1	6.06709200	-0.08395800	4.19223400
H	-1	2.30291400	8.05628500	-1.82860300
H	-1	2.75186300	5.86467700	-0.70150500
H	-1	-1.12464000	6.16074900	1.10516700
H	-1	0.90730600	8.89660400	-3.54233000

H	-1	0.15946200	10.97754700	-4.72584500
H	-1	-1.74565400	12.20182400	-1.07985900
N	-1	-2.14591200	-7.19799500	-2.53810300
N	-1	-3.55527400	-9.56424700	-3.31516500
N	-1	-3.00357500	-3.92891900	-5.51211900
N	-1	-4.10199700	-5.72827200	-7.35795800
N	-1	-6.05907700	-4.67212500	-2.11246200
N	-1	-8.14576800	-6.04503000	-3.38367500
N	-1	10.96031900	1.20792000	1.45215800
N	-1	8.20407000	1.06159700	1.15582100
N	-1	-0.75007600	10.40084200	-0.99699500
N	-1	-0.60927000	7.73367400	-0.13132600
N	-1	-5.15717600	1.59523900	6.74622900
N	-1	-7.16894500	2.18095200	8.53712200
N	-1	-3.57728900	-1.95607700	7.05526800
N	-1	-4.77500700	-1.78776200	9.60579700
N	-1	7.30963500	-3.25817500	2.52872200
N	-1	9.94396300	-4.26459300	2.61142900
N	-1	7.66127300	-2.34958400	-1.94553800
N	-1	10.36236600	-2.60782100	-2.82910100
N	-1	0.38480800	8.43110000	-6.21142600
N	-1	0.82465100	6.36287200	-4.28270500
N	-1	-3.69233600	6.05140100	-3.10520700
N	-1	-4.96663600	8.33026300	-4.09894000
O	0	1.68179300	0.59980900	4.78630100
C	0	0.68638500	1.42413200	5.25129900
H	0	0.71464500	2.43017100	4.78486700
H	0	-0.32747000	1.03585600	5.04027800
C	0	0.67490600	1.69555300	6.75257100
O	0	-0.17604900	2.37301700	7.30207600
O	0	1.67754500	1.09876500	7.42899900
H	0	1.55649200	1.32777300	8.37148100
H	0	2.46615000	0.53447600	5.33595100

Sum of electronic and thermal Free Energies = -13352.466364 (Hartree/Particle).

Table S23: DFT-optimized geometry of **f-[Ce^{III}(H₂C-COOH)-Ce^{III}]²⁻** (doublet), computed at the UB3LYP-D3/ 6-31G* (HCNO)/ MWB28 (Ce) level in water solvent using PCM.

Atom		x	y	z
Ce	-1	1.38445400	-2.18427600	-0.58906200
Ce	0	-0.98218100	1.82337300	1.86966100
Ce	-1	-1.74409600	-1.65144400	1.51517400
Ce	-1	2.16541200	1.55438900	-0.13832700
Ce	-1	-1.24939600	0.44094600	-1.42246900
Ce	0	1.68351300	-0.66709800	2.89422700
O	-1	-4.64304500	13.14186100	-4.51545600
C	-1	-4.14715600	10.82053500	-2.88286100
C	-1	-3.88238400	9.62694000	-2.22062600
O	-1	-6.09827800	-9.96982400	-7.74206900
C	-1	-4.03725800	-8.34122000	-6.63140700
C	-1	-3.17621900	-7.43589600	-6.02522300
O	-1	14.12949100	-4.02758000	0.32541400
C	-1	11.29241200	-4.22288000	0.19521600
C	-1	9.90603300	-4.17056800	0.23394000

O	-1	14.81410000	0.42805700	0.51959400
C	-1	12.26243500	1.01190300	1.37047000
O	-1	-6.80295200	1.15124600	12.73699300
C	-1	-4.75111300	0.64443000	10.81839500
C	-1	-3.86997000	0.33369600	9.79010300
O	-1	-9.24937000	-8.65950100	-7.27582000
C	-1	-7.78019300	-6.44586400	-6.17176500
C	-1	-7.04955000	-5.46226900	-5.51633000
C	-1	-2.26438600	9.32820800	-6.32779800
C	-1	-1.95771800	8.12624000	-5.70501500
O	-1	-2.33767300	13.61967400	-2.82146400
C	-1	-1.15497400	11.51613100	-1.48301000
C	-1	12.19302000	-0.82699300	-1.52080600
C	-1	10.82652600	-0.58579600	-1.45314300
O	-1	-7.68468500	-11.21448200	-5.08669300
C	-1	-6.30567200	-9.23090600	-3.57525000
C	-1	-5.54761400	-8.29400700	-2.88569900
O	-1	-9.97515100	0.61011300	12.18072600
C	-1	-8.71540400	-0.00483100	9.64995800
C	-1	-7.89027400	-0.21707900	8.55241900
O	-1	14.40363500	-3.38385900	-2.88393300
C	-1	11.69561800	-2.77564500	-2.83068900
O	-1	-5.73462300	-12.27526400	-5.49362900
C	-1	-4.27134400	-10.41769300	-4.03678300
O	-1	-9.75767500	2.80365000	11.71490000
C	-1	-7.99257100	2.28512800	9.63268500
O	-1	-1.32838800	13.09328000	-4.77288300
C	-1	-0.06920300	10.85705800	-3.51965300
C	-1	0.36049600	9.71027500	-2.86488700
O	-1	15.00142400	-1.35848900	1.88576900
C	-1	12.23070400	-1.04196000	2.61106000
C	-1	10.86830200	-0.84322600	2.80388400
C	-1	0.08784800	9.65774300	-6.67117400
O	-1	-10.17581400	-9.03890100	-5.25793500
C	-1	-8.82506000	-6.94353800	-4.06924600
O	-1	-7.59517800	-0.94173500	12.45291900
C	-1	-5.62995700	-1.58108800	10.61594500
O	-1	14.03263800	-4.05030700	2.58189400
C	-1	11.27594000	-4.32257700	2.59315100
O	-1	-5.55636500	11.81991800	-6.09417400
C	-1	-5.20991900	9.52676400	-4.60255500
O	-1	-6.86128300	-8.20323600	-8.92558900
C	-1	-4.88510600	-6.52864400	-7.95586000
O	-1	0.15000000	-4.28875500	-0.53758600
C	-1	-1.39285600	-6.26133900	-1.91388500
O	-1	-2.82888800	1.37223500	3.37677100
C	-1	-4.35913300	1.40365800	5.74825300
O	-1	0.09846700	4.08296300	1.78425200
C	-1	1.81660400	6.41045500	-0.42668100
C	-1	1.56138800	7.62806800	-1.04427300
O	-1	3.56475000	-1.66943000	-1.56800300
C	-1	6.36060100	-2.09705000	-1.79804700
O	-1	-3.47310100	-0.75083600	2.98340500
C	-1	-5.57731000	-0.46057500	4.86080100
C	-1	-6.45359200	-0.32919200	5.93113100
O	-1	2.01185500	3.81830600	0.62616800
C	-1	-0.35612100	6.57142500	0.57858700
O	-1	3.90051600	0.55358500	-1.44147400
C	-1	6.61038200	0.27779000	-2.01220100
C	-1	7.97960700	0.07192600	-2.11331600

O	-1	-1.54824500	-3.97292000	0.90873700
C	-1	-3.02578900	-6.03761700	-0.17279000
C	-1	-3.79859300	-6.97172300	-0.84731600
O	-1	-0.88531900	-1.02204500	-3.34372900
C	-1	-2.28185800	-2.95756600	-4.82876100
O	-1	3.23800600	-2.49825800	2.68610900
C	-1	5.99508400	-3.04772700	2.60487200
O	-1	-2.61223900	2.43017500	-1.39101200
C	-1	-3.35041600	4.91604900	-2.46477100
O	-1	-2.51866300	3.30135000	0.68417000
C	-1	-3.57947800	5.74524300	-0.22845600
C	-1	-3.93225400	6.97316900	-0.77663400
O	-1	0.73731600	-2.50852500	-2.86346800
C	-1	-0.39476400	-4.41673100	-4.57246800
C	-1	-1.10559300	-5.37387900	-5.28531000
O	-1	2.95857700	-3.46720200	0.67025500
C	-1	5.59399200	-4.38920100	0.65466700
C	-1	6.96026700	-4.62944100	0.60456100
O	-1	-3.59319300	-2.11422300	0.01924200
C	-1	-5.26599200	-3.80484900	-1.45293200
O	-1	1.70368500	2.80917400	-2.19503800
C	-1	1.12442500	5.26351500	-3.55415000
O	-1	4.12278700	1.65920600	1.24981600
C	-1	6.66332300	0.21174300	3.42042100
C	-1	8.04349900	0.04282900	3.42008700
O	-1	-1.37289200	-2.71820900	3.67542300
C	-1	-2.82996700	-2.31566800	6.01684100
O	-1	-3.33048700	-0.74241500	-1.74768300
C	-1	-5.21055700	-2.21490200	-3.24526000
C	-1	-6.02043900	-3.08311800	-3.96825800
O	-1	0.52713400	-1.95532500	4.61910900
C	-1	-0.91861500	-1.21059900	6.94695600
C	-1	-1.71192900	-0.86706900	8.03538900
O	-1	3.85777100	0.35935600	3.07043000
C	-1	6.88083300	1.22483100	1.25833800
O	-1	-0.20655900	1.92615500	-3.00118400
C	-1	-0.75078500	4.13947700	-4.53781700
C	-1	-1.06526100	5.32981300	-5.17670500
O	-1	2.11823100	-0.51231600	0.76065800
O	-1	-0.00149500	1.77204000	-0.06785300
O	-1	-0.45600200	-0.16789200	2.62413500
O	-1	-0.69405300	-1.51128100	-0.46410500
O	-1	0.58273200	-2.41770600	1.68390300
O	-1	1.16686100	-0.03094000	-1.63276200
O	-1	1.40960100	1.58953300	2.22695600
O	-1	-2.09285900	0.39232800	0.66566300
C	-1	-4.98267700	12.03359800	-4.89618000
C	-1	-4.80513100	10.78049900	-4.11573200
C	-1	-4.28787500	8.41918000	-2.81000600
C	-1	-5.99226900	-8.80640100	-8.08790300
C	-1	-4.93768400	-7.88353600	-7.59664100
C	-1	-3.23689200	-6.08791500	-6.41604300
C	-1	13.48209700	-4.12668000	1.35255000
C	-1	12.00473200	-4.26994700	1.39532800
C	-1	9.26894000	-4.17717200	1.48526200
C	-1	14.34988900	-0.42092800	1.45877500
C	-1	12.94687700	-0.11901100	1.84503900
C	-1	10.25809100	0.28337700	2.23192700
C	-1	-6.70473900	0.04375300	12.23502100
C	-1	-5.66011100	-0.32689700	11.24566500

C	-1	-3.93545500	-0.93953600	9.20347700
C	-1	-9.37931400	-8.35713100	-6.10063900
C	-1	-8.67758400	-7.22623100	-5.43751300
C	-1	-7.23197700	-5.28608500	-4.13648400
C	-1	-1.22717300	10.12442300	-6.81879600
C	-1	-0.60934400	7.74855100	-5.59916900
C	-1	-1.49953900	12.88724100	-3.58450300
C	-1	-0.87024700	11.77267700	-2.83212100
C	-1	-0.02469000	9.51698200	-1.52837300
C	-1	12.64992900	-1.95132900	-2.21286300
C	-1	9.94908800	-1.47536100	-2.09368400
C	-1	-6.47590500	-11.28787300	-4.95474300
C	-1	-5.66363200	-10.31806500	-4.17445500
C	-1	-4.15686500	-8.47975800	-2.80784400
C	-1	-9.55355000	1.50053700	11.45718000
C	-1	-8.76794100	1.27272100	10.21793500
C	-1	-7.13663900	0.85544700	8.04694700
C	-1	-0.99601000	-4.56661600	-0.06920000
C	-1	-1.79826600	-5.65064800	-0.72001700
C	-1	-3.32191900	-7.50134700	-2.05610900
C	-1	-3.53772900	0.34142300	3.61463200
C	-1	-4.51003900	0.43180800	4.74803000
C	-1	-6.21913300	0.67392500	6.88477500
C	-1	0.99272200	4.49420700	0.99024900
C	-1	0.83067500	5.85095100	0.39082000
C	-1	0.32473500	8.25411900	-0.82374400
C	-1	4.30276600	-0.64056200	-1.60755200
C	-1	5.77150300	-0.82552200	-1.82916400
C	-1	8.47850700	-1.23755800	-2.03307300
C	-1	-0.33413400	-2.15574900	-3.45755500
C	-1	-0.99617000	-3.18082100	-4.31731300
C	-1	-2.40450800	-5.06807600	-5.72182400
C	-1	3.65792700	-3.15766700	1.68431400
C	-1	5.09283200	-3.56171900	1.66363700
C	-1	7.79023200	-4.02721000	1.56349400
C	-1	-2.77527600	3.37184200	-0.55777200
C	-1	-3.26233800	4.68693400	-1.08425100
C	-1	-3.95815400	7.11228800	-2.17292600
C	-1	-3.84871900	-1.74485700	-1.16767200
C	-1	-4.80410400	-2.58197000	-1.95959400
C	-1	-6.40583300	-4.29992600	-3.38408500
C	-1	0.65359600	2.85572600	-2.90520300
C	-1	0.35826100	4.09792300	-3.68819500
C	-1	-0.25762300	6.45412100	-4.95106000
C	-1	4.57174400	0.95703100	2.20860500
C	-1	6.05556500	0.80791700	2.31249800
C	-1	8.78189700	0.47650900	2.30760900
C	-1	-0.71879500	-2.23788600	4.64644700
C	-1	-1.48390800	-1.93582900	5.89559000
C	-1	-3.04980000	-1.28938800	8.05873700
H	-1	1.44121000	0.01420000	-2.56292300
H	-1	1.85997900	2.34224100	2.64046200
H	-1	0.62038900	-3.31702100	2.04744500
C	-1	14.10766000	-2.24639100	-2.22585000
O	-1	14.95502900	-1.54406900	-1.70232800
H	-1	15.36874500	-3.51529000	-2.81802100
H	-1	-7.66425200	-8.75969800	-8.97234000
H	-1	-6.33858800	-12.84416000	-6.00780400
H	-1	-10.53336100	-9.80475800	-5.74660900
H	-1	15.63555200	0.04702100	0.15388500

H	-1	-2.91999300	14.12207600	-3.42509100
C	-1	-1.56611700	11.43331200	-7.43624400
O	-1	-2.70273800	11.85508700	-7.55573300
O	-1	-0.48139500	12.10463600	-7.86988700
H	-1	-0.79249300	12.95672700	-8.23037100
H	-1	-5.56328400	12.67124400	-6.57210300
H	-1	-10.23959700	2.86620000	12.56253700
H	-1	-8.38979600	-0.54216100	12.86622800
H	-1	14.93920700	-3.70267500	2.47448400
H	-1	0.12459400	-0.92642000	6.90733200
H	-1	-1.29528600	-0.30862000	8.86644500
H	-1	-3.29768400	-2.87411000	5.21187200
H	-1	-3.17788100	1.07886200	9.41524700
H	-1	-4.76615500	1.62970900	11.27193800
H	-1	-6.31639800	-2.36238000	10.92905200
H	-1	5.62560800	-2.41129100	3.40282800
H	-1	7.38028100	-5.26754000	-0.16451300
H	-1	4.91790900	-4.81572900	-0.07836700
H	-1	11.79538700	-4.38586300	3.54542200
H	-1	11.83435100	-4.18625500	-0.74092600
H	-1	9.33248800	-4.05097600	-0.67851600
H	-1	5.73165100	-2.97174400	-1.66686900
H	-1	12.01354100	-3.65429700	-3.38531700
H	-1	12.90988100	-0.17339700	-1.03879500
H	-1	10.44011200	0.25148400	-0.88249500
H	-1	8.65267200	0.90898000	-2.25879700
H	-1	6.18561600	1.27398600	-2.06487200
H	-1	1.99551600	5.25659500	-2.90731900
H	-1	0.92025200	10.24679300	-7.04668600
H	-1	-3.28659300	9.66843800	-6.43360000
H	-1	-2.73947000	7.50206300	-5.28472900
H	-1	-1.91990500	5.39161800	-5.84059700
H	-1	-1.35226600	3.24854200	-4.67766300
H	-1	-3.54495200	5.59883000	0.84534000
H	-1	-4.19153900	7.80650000	-0.13377700
H	-1	-3.12042700	4.10850800	-3.15194000
H	-1	-5.74867700	9.45686500	-5.54367200
H	-1	-3.82739400	11.77356200	-2.47821700
H	-1	-3.32227900	9.62759600	-1.29245700
H	-1	-3.53420000	2.10925100	5.68574900
H	-1	-5.72451500	-1.22348600	4.10420500
H	-1	-7.31818600	-0.97878700	6.00932600
H	-1	-8.00420000	3.28790400	10.05127200
H	-1	-9.29015200	-0.81325900	10.08871300
H	-1	-7.80165700	-1.20802600	8.12327800
H	-1	0.60553200	-4.61473400	-4.20314100
H	-1	-0.66499700	-6.34062200	-5.50002100
H	-1	-2.52820500	-7.74953300	-5.21379800
H	-1	-4.05718800	-9.38334500	-6.34007900
H	-1	-5.55231500	-6.14107800	-8.72092000
H	-1	-2.76449200	-2.00237000	-4.64930700
H	-1	-0.44010900	-5.98729300	-2.35672900
H	-1	-4.75296700	-7.29038400	-0.44460400
H	-1	-3.35933600	-5.59922800	0.76054600
H	-1	-6.01466000	-7.41964700	-2.44412100
H	-1	-7.37984900	-9.13133900	-3.67160900
H	-1	-3.73816000	-11.25083300	-4.48708000
H	-1	-4.88467800	-1.26931400	-3.66408700
H	-1	-6.35467500	-2.81891500	-4.96501700
H	-1	-4.97027100	-4.11108500	-0.45516300

H	-1	-9.53363500	-7.50905600	-3.47029200
H	-1	-7.64708600	-6.63594900	-7.22961500
H	-1	-6.30834200	-4.88110400	-6.05297600
H	-1	6.43183200	1.68861000	0.38607400
H	-1	12.79274700	1.77014500	0.80078500
H	-1	12.73394500	-1.91939900	2.99969700
H	-1	10.27757700	-1.58625700	3.32679500
H	-1	8.53961600	-0.40810300	4.27197500
H	-1	6.05747600	-0.11252700	4.25973200
H	-1	2.30376000	8.08640400	-1.68755400
H	-1	2.75157100	5.88354200	-0.58215100
H	-1	-1.13140000	6.15588400	1.21433500
H	-1	0.91294300	8.94312400	-3.39705100
H	-1	0.16656500	11.03556700	-4.56105500
H	-1	-1.75241200	12.21897000	-0.90884900
N	-1	-2.12390600	-7.16481600	-2.57332100
N	-1	-3.52771700	-9.52440100	-3.38013300
N	-1	-2.97548500	-3.86551500	-5.51553800
N	-1	-4.06542800	-5.64656700	-7.38401400
N	-1	-6.04159000	-4.64825000	-2.13434800
N	-1	-8.12226800	-6.01012900	-3.42709500
N	-1	10.95838300	1.21406800	1.55014000
N	-1	8.20333600	1.06760100	1.24288700
N	-1	-0.75491100	10.41840100	-0.84162600
N	-1	-0.61376900	7.74240200	-0.00370900
N	-1	-5.17744600	1.52620800	6.79308200
N	-1	-7.19599800	2.09056100	8.58320000
N	-1	-3.59425900	-2.02629200	7.06996400
N	-1	-4.80083000	-1.88637000	9.61803500
N	-1	7.30955100	-3.26750200	2.56702000
N	-1	9.94481600	-4.27159900	2.64806100
N	-1	7.67525400	-2.31125700	-1.89616700
N	-1	10.37964400	-2.55692200	-2.77320500
N	-1	0.40007700	8.50523400	-6.07267900
N	-1	0.83591100	6.41726200	-4.16443100
N	-1	-3.68465900	6.08798100	-3.00567900
N	-1	-4.95837600	8.37569900	-3.97961600
C	0	1.85614800	0.20870700	4.90498900
C	0	0.87959200	1.35770100	5.34819200
O	0	0.02937400	1.76221900	4.58035700
O	0	0.98435000	1.88915500	6.56835700
H	0	0.45191900	2.51560100	6.80999700
H	0	1.74463800	-0.58989000	5.60834400
H	0	2.85273800	0.58620000	5.00095200

Sum of electronic and thermal Free Energies = -13276.650649 (Hartree/Particle).

Table S24: DFT-optimized geometry of **CO$_2$** (singlet), computed at the B3LYP-D3/ 6-31G* (CO) level in water solvent using PCM.

Atom	x	y	z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16909400
O	0.00000000	0.00000000	-1.16909400

Sum of electronic and thermal Free Energies = -188.592753 (Hartree/Particle).

Table S25: DFT-optimized geometry of **H₂O** (singlet), computed at the B3LYP-D3/ 6-31G* (HO) level in water solvent using PCM.

Atom	x	y	z
O	0.00000000	0.00000000	0.12073800
H	0.00000000	0.75883000	-0.48295200
H	0.00000000	-0.75883000	-0.48295200

Sum of electronic and thermal Free Energies = -76.412854 (Hartree/Particle).

Table S26: DFT-optimized geometry of **H₂O·⁺** (doublet), computed at the UB3LYP-D3/ 6-31G* (HO) level in water solvent using PCM.

Atom	x	y	z
O	0.00000000	0.00000000	0.11866100
H	0.00000000	0.81561500	-0.47464200
H	0.00000000	-0.81561500	-0.47464200

Sum of electronic and thermal Free Energies = -76.088041 (Hartree/Particle).

Table S27: DFT-optimized geometry of **OH·** (doublet), computed at the UB3LYP-D3/ 6-31G* (HO) level in water solvent using PCM.

Atom	x	y	z
O	0.00000000	0.00000000	0.10922700
H	0.00000000	0.00000000	-0.87381300

Sum of electronic and thermal Free Energies = -75.736849 (Hartree/Particle).

Table S28: DFT-optimized geometry of **CH₃COOH** (singlet), computed at the B3LYP-D3/ 6-31G* (HCO) level in water solvent using PCM.

Atom	x	y	z
C	-1.04953300	-0.92686300	0.00000000
H	-2.04231600	-0.47652700	0.00000000
H	-0.92743400	-1.56240900	0.88304500
H	-0.92743400	-1.56240900	-0.88304500
C	0.00000000	0.15461300	0.00000000

O	-0.20817800	1.35120300	0.00000000
O	1.24794300	-0.36915600	0.00000000
H	1.87626900	0.37846700	0.00000000

Sum of electronic and thermal Free Energies = -229.056692 (Hartree/Particle).

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