Supporting Information for

Redox Control of a Polymerization Catalyst by Changing the Oxidation State of the Metal Center

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Experimental

All experiments were performed under a dry nitrogen atmosphere using standard Schlenk techniques or an MBraun inert-gas glovebox. Solvents were purified using a two-column solid-state purification system by the method of Grubbs[1] and transferred to the glove box without exposure to air. $CeCl_3$ and L-lactide were purchased from Alfa Aesar, and KO^{t}Bu was purchased from Sigma-Aldrich. L-lactide was recrystallized three times from toluene prior to use. ε-caprolactone was distilled and dried over sieves in the glovebox before use. All other reagents were used as received. Ferrocenium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate ($FcBAr^F$),[2] trimethylene carbonate,[3] **1-H$_2$**,[4] **2-H$_2$**,[5] **1-Ce(O^{t}Bu)**,[4] and **1-Ce(O^{t}Bu)I**[4] were synthesized according to published procedures. NMR solvents were obtained from Cambridge Isotope Laboratories, degassed, and stored over activated molecular sieves prior to use. ^{1}H NMR spectra were recorded on Bruker300 or Bruker500 spectrometers at room temperature in C_6D_6 (the UCLA NMR spectrometers are supported by the NSF grant CHE-9974928). Chemical shifts are reported with respect to internal solvent, 7.16 ppm (C_6D_6) for ^{1}H NMR spectra. For ^{31}P and ^{19}F NMR and spectra, chemical shifts are reported with respect to an external standard, 121 ppm (1% trimethylphosphite in C_6D_6) and -68.22 and -72.50 ppm (1% Freon-113 in C_6D_6). XANES experiments at both Fe K-edge and Ce L_3-edge were performed at the Materials Research Collaborative Access Team (MRCAT) beamline (10-BM) at the Advanced Photon Source, Argonne National Laboratory. CHN analyses were performed by Midwest Microlabs, LLC, 7212 N. Shadeland Ave Suite 110, Indianapolis, IN 46250.

[1-Ce(O^{t}Bu)][BAr^F]. In diethyl ether, FcBArF (0.084 g, 0.080 mmol) was added to a toluene solution of **1-Ce(O^{t}Bu)** (0.093 g, 0.080 mmol). Upon addition, the color of the reaction turned from yellow to red brown. After stirring for 0.5 h at room temperature, the volatiles were removed. The product was washed with hexanes and extracted with ether and precipitated by dissolving it in concentrated diethyl ether, followed by layering with pentane at -36 ^{o}C. Yield: 0.132 g, 81.5%. ^{1}H NMR (300 MHz, 25 ^{o}C, C_6D_6), δ (ppm): 8.41 (s, 10H, B(C_6H_3) and P(C_6H_5)$_2$), 7.63 (s, 10H, B(C_6H_3) and P(C_6H_5)$_2$), 7.42 (d, 2H, P(C_6H_5)$_2$), 7.07 (br s, 12H, P(C_6H_5)$_2$), 6.55 (m, 2H, OC$_6H_3$), 6.43 (m, 2H, OC$_6H_3$), 3.99 (s, 4H, C_5H_4), 3.84 (s, 2H, C_5H_4), 3.52 (s, 2H, C_5H_4), 1.17 (s, 18H, CCH_3), 0.99 (s, 9H, CCH_3). ^{13}C NMR (75 MHz, 25 ^{o}C, C_6D_6), δ (ppm): 138.4, 135.9, 135.0, 134.2, 133.4, 132.2, 130.6, 130.4, 129.8, 126.7, 124.7, 122.6, 120.1, 118.6, 114.0, 113.1, 90.4, 72.6, 72.2, 69.1, 35.5, 33.7, 30.6, 23.3, 14.6. ^{19}F NMR (282 MHz, 25 ^{o}C, C_6D_6), δ (ppm): -62.4. ^{31}P NMR (121 MHz, 25 ^{o}C, C_6D_6), δ (ppm): 7.9. Anal. for $BC_{90}CeH_{73}F_{24}FeN_2O_3P_2$ Calcd.: C, 55.29%; H, 3.76%; N, 1.43%. Found: C, 55.61%; H, 4.09 %; N, 1.41 %.

2-CeCl(THF). In THF, at -78 ^{o}C, the sodium salt of the salen ligand, **2-Na$_2$(THF)$_2$**, (0.780 g, 1.14 mmol) was added to $CeCl_3(THF)_3$ (0.525 g, 1.14 mmol). After 1 h of stirring at -78 ^{o}C, the volatiles were removed. The product was extracted with toluene. The volatiles were removed and the product was recrystallized from a concentrated toluene solution layered with *n*-pentane at -36 ^{o}C. Yield: 0.510 g, 67.2%. ^{1}H NMR (300 MHz, 25 ^{o}C, C_6D_6), δ (ppm): 16.69 (s, 2H, OC$_6H_2$ or NC*H*), 16.26 (s, 2H, OC$_6H_2$ or NC*H*), 15.78 (s, 2H, OC$_6H_2$ or NC*H*), 5.39 (s, 18H, CCH_3), 4.42 (s, 18H, CCH_3), 1.83 (br s, 4H, C_4H_8O), 0.30 (br s, 4H, C_4H_8O), -7.51 (br s, 2H C_2H_4), -21.67 (br s, 2H C_2H_4). Anal. for $C_{36}H_{54}CeN_2O_3Cl$ (0.25 C_6H_{14}) Calcd.: C, 59.30%; H, 7.63%; N, 3.69%. Found: C, 59.20%; H, 7.15%; N, 3.79%.

[2-Ce(O^{t}Bu)]$_2$. A diethyl ether solution of KO^{t}Bu (0.086 g, 0.754 mmol) was added to an ether slurry of **2-CeCl(THF)** (0.502 g, 0.754 mmol) at -78 ^{o}C. After 1 h of stirring at -78 ^{o}C, the volatiles were removed. The product was extracted with hexanes, and volatiles were removed. The product was precipitated from concentrated *n*-pentane to yield an orange powder at -36 ^{o}C. Yield: 0.230 g, 43.4%. ^{1}H NMR (300 MHz, 25 ^{o}C, C_6D_6), δ (ppm): 19.99 (s, 1H,CH_2CH_2), 13.09 (s, 1H, OC$_6H_2$), 9.23 (s, 3H, OC$_6H_2$), 5.89 (d, 2H, N=C*H*), 2.87 (br s, 9H, CCH_3), 1.80 (br s, 9H, CCH_3), 1.28 (br s, 9H, CCH_3), 0.17 (br s, 9H, CCH_3), -3.10 (br s, 1H, CH_2CH_2), -5.50 (br s, 9H, CCH_3), -8.73 (br s, 1H, CH_2CH_2), -15.34 (br s, 1H, CH_2CH_2). Anal. for $C_{72}H_{110}N_4O_8Ce$. Calcd.: C, 61.42%; H, 7.88%; N, 3.98%. Found: C, 61.53%; H, 7.88%; N, 3.33%.

[2-Ce(O^{t}Bu)][BAr^F]. In diethyl ether, FcBAr^F was added to a tetrahydrofuran or diethyl ether solution of **[2- Ce(O^{t}Bu)]$_2$**. Upon addition, the reaction solution turned from orange to a purple black. After stirring for 0.5 h, the volatiles were removed. The product was washed with hexanes and extracted with diethyl ether. The product could be precipitated from concentrated diethyl ether layered with pentane at -36^{o}C. Yield: 0.110 g, 73.8%. ^{1}H NMR (300 MHz, 25 ^{o}C, C_6D_6), δ (ppm): 8.29 (s, 8H, B(C$_6H_3$)), 7.92 (s, 2H, N=C*H*), 7.69 (d, 2H, OC$_6H_2$) 7.60 (s, 4H, B(C$_6H_3$)), 7.11 (d, 2H, OC$_6H_2$), 4.13 (m, 2H, CH_2CH_2), 3.14 (m, 2H, CH_2CH_2), 3.00 (s, 4H, C$_4H_8$O), 1.36 (s, 18H, CCH_3), 1.26 (s, 18H, CCH_3), 0.78 (s, 9H, CCH_3), 0.57 (s, 4H, C$_4H_8$O). ^{13}C NMR (75 MHz, 25 ^{o}C, C_6D_6), δ (ppm):135.9, 129.8, 129.1, 126.5, 66.1, 35.6, 35.0, 34.8, 31.9, 30.3, 23.3, 21.9, 15.4, 14.8. ^{19}F NMR (282 MHz, 25 ^{o}C, C_6D_6), δ (ppm): -62.6. Anal. for. $C_{72}H_{77}BCeF_{24}N_2O_4$ Calcd.: C, 52.69%; H, 4.37%; N, 1.71%. Found: C, 52.34%; H, 4.50%; N, 1.86%.

J. Young tube scale polymerization reactions

In a J. Young tube in C_6D_6, the catalyst was added to L-lactide (0.2 M) in a 1:100 ratio. The reaction was monitored by ^{1}H NMR spectroscopy.

Large scale polymerization reactions

In a vial in the glovebox in tetrahydrofuran, the catalyst was added to a stirring solution of L-lactide (0.2 M). The reaction was monitored by ^{1}H NMR spectroscopy of aliquots that were quenched through exposure to air. Once the polymerization was complete, the reaction was exposed to air and volatiles were removed. The product was dissolved in minimal dichloromethane, and the polymer was precipitated by addition of cold MeOH. The polymer was washed with cold MeOH, and then collected by dissolving the polymer in dichloromethane. This procedure was repeated two more times.

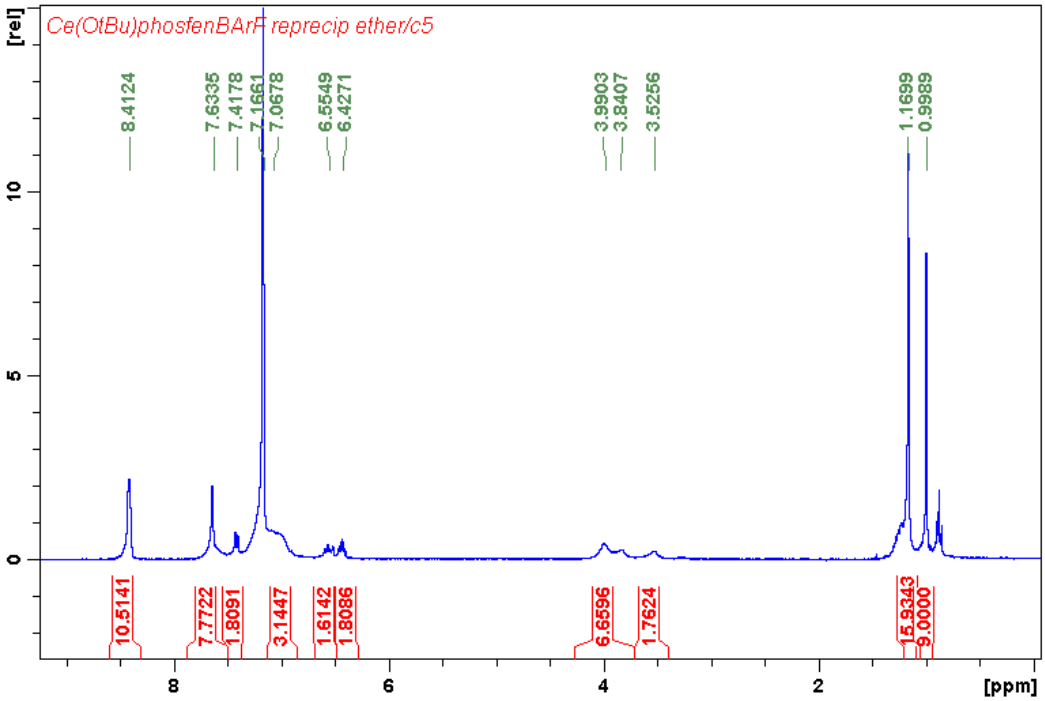
Diffusion-Coefficient Experiment

The pulse-gradient, spin−echo (SE: 90°−t_1−180°−t_1−echo) technique was used to measure the self-diffusion coefficient of **[2- Ce(O^{t}Bu)]$_2$**in C_6D_6 at room temperature on a Bruker DRX-500 NMR spectrometer. The gradient strength was measured running the pulse-gradient spin−echo experiment on H_2O and using the literature value of 2.3 × 10^{-9} m^2/s for the self-diffusion coefficient. The gradient strength was found to be 51.0 G/cm. The time during which the diffusion process occurred was varied from 50 μs to 5 ms. The duration of the gradient pulse (δ) was set to 1 ms. The hydrodynamic radius was obtained by using the Stokes−Einstein equation.[6]

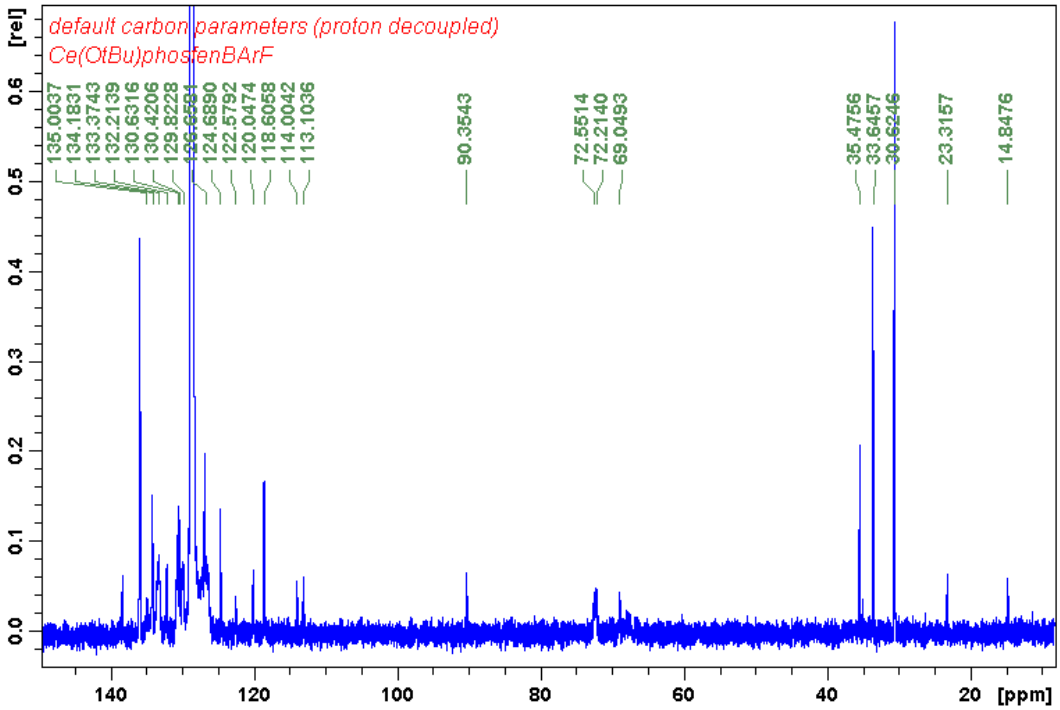
NMR Spectra

[1-Ce(O^{t}Bu)][BAr^F]

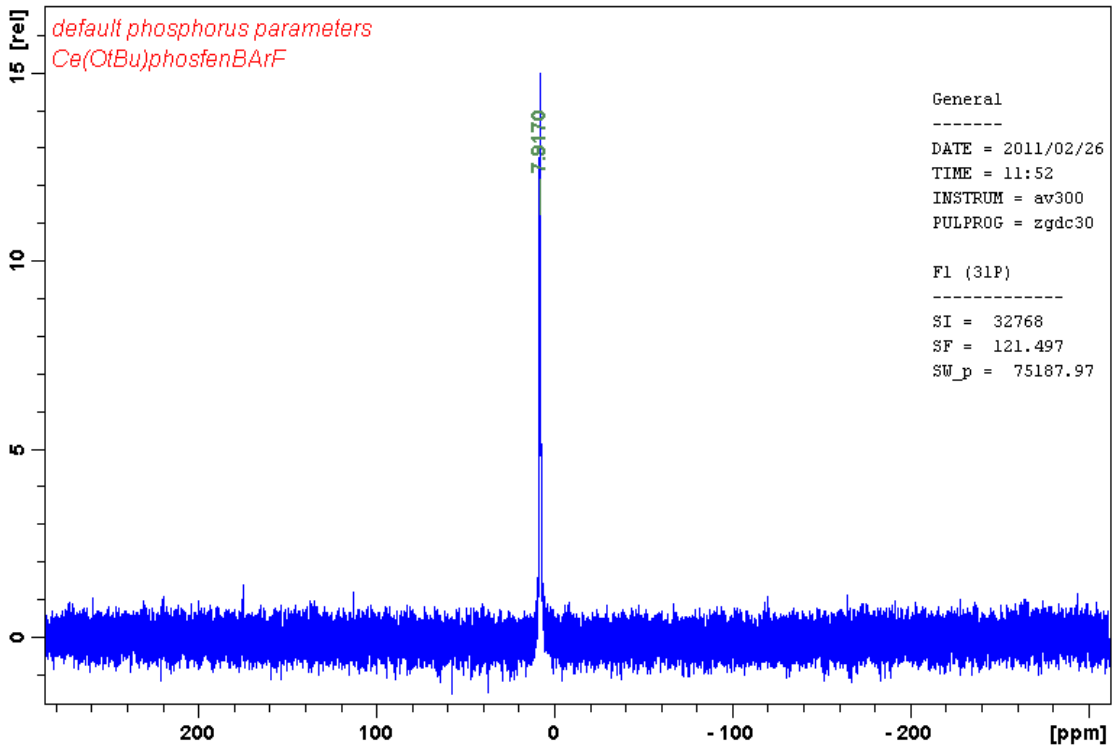
^{1}H NMR Spectrum (300 MHz, 25 °C, C_6D_6)



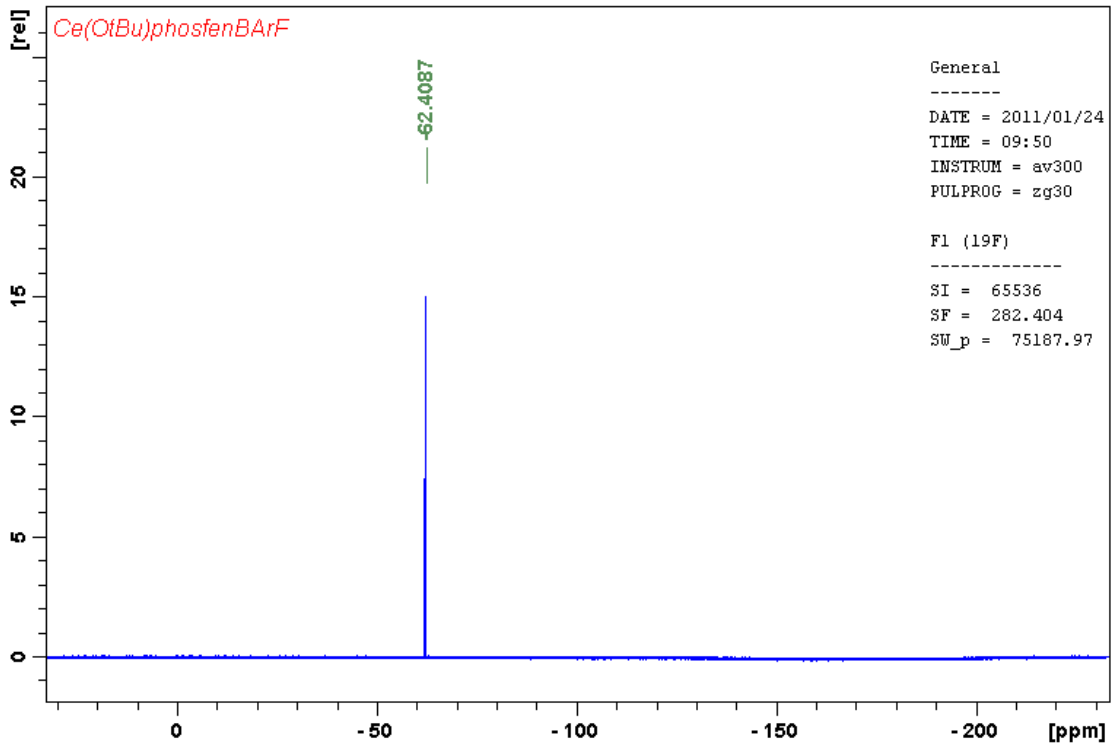
^{13}C NMR Spectrum (75 MHz, 25 °C, C_6D_6)



^{31}P NMR Spectrum (121 MHz, 25 °C, C_6D_6)

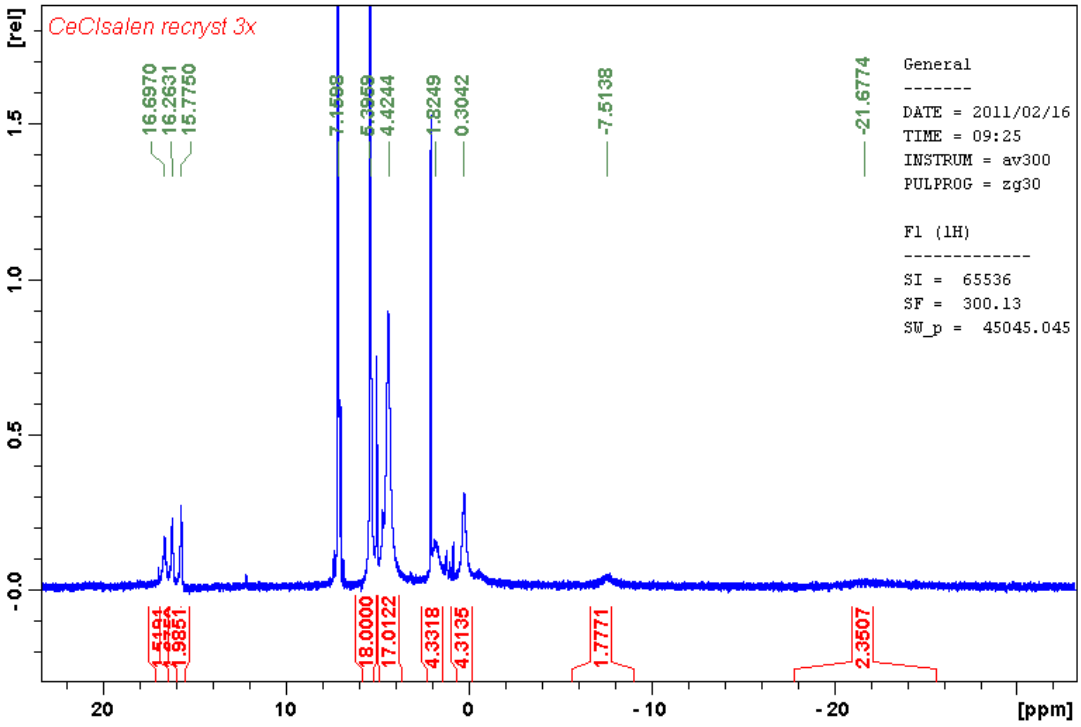


^{19}F NMR Spectrum (282 MHz, 25 °C, C_6D_6)



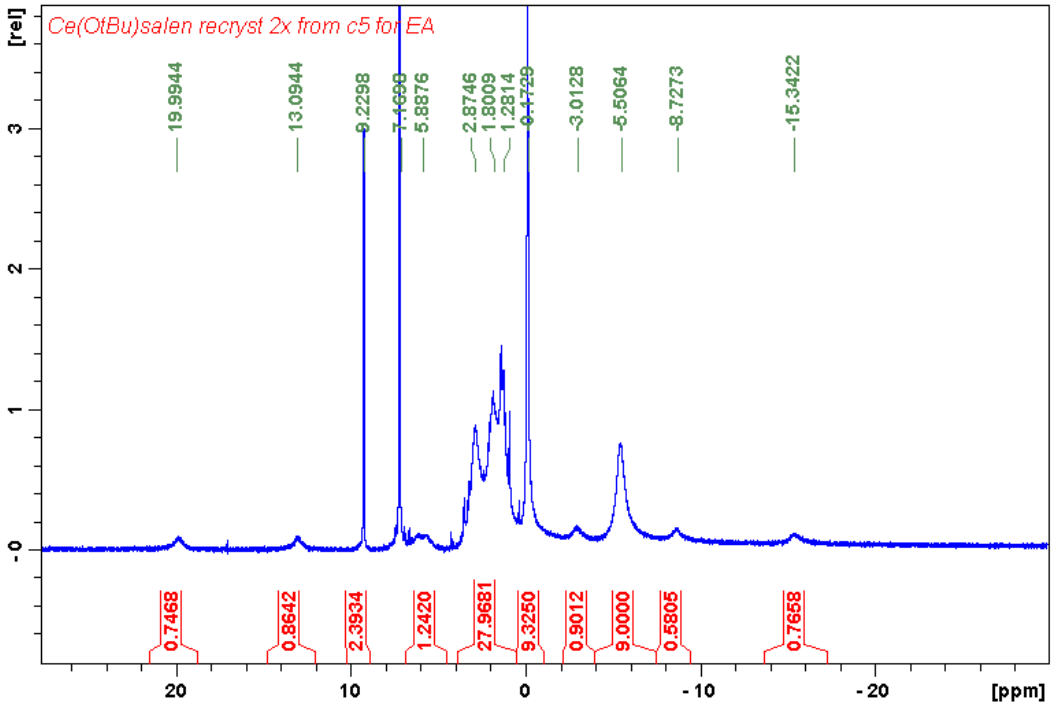
2-CeCl(THF)

^{1}H NMR Spectrum (300 MHz, 25 °C, C_6D_6)



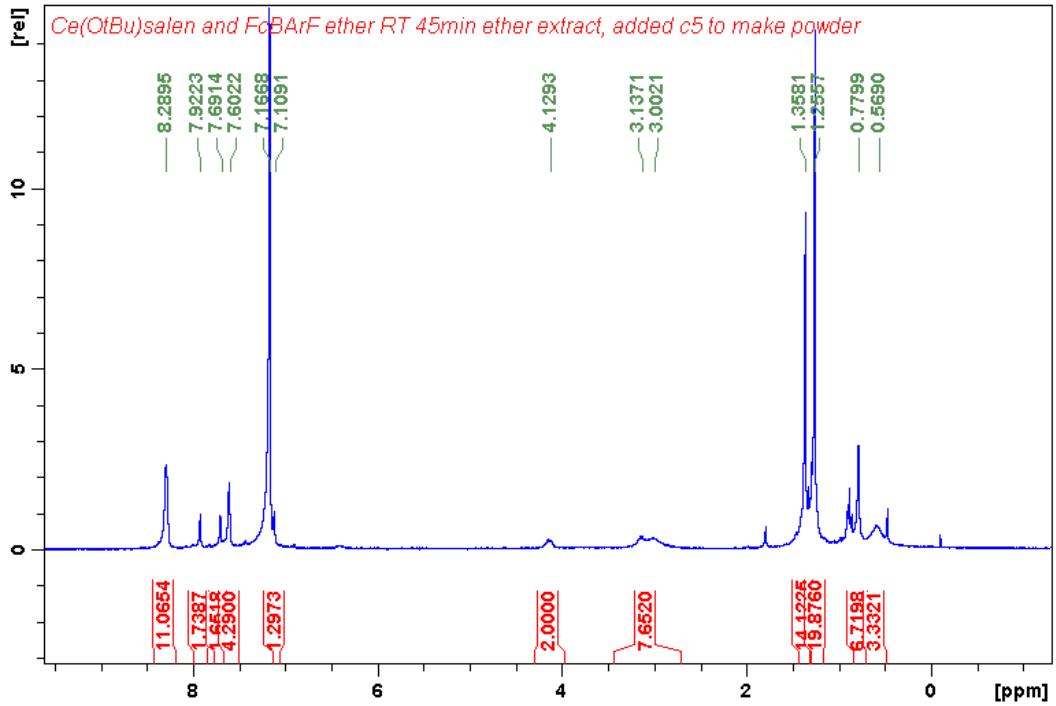
2-Ce(O^{t}Bu)

^{1}H NMR Spectrum (300 MHz, 25 °C, C_6D_6)

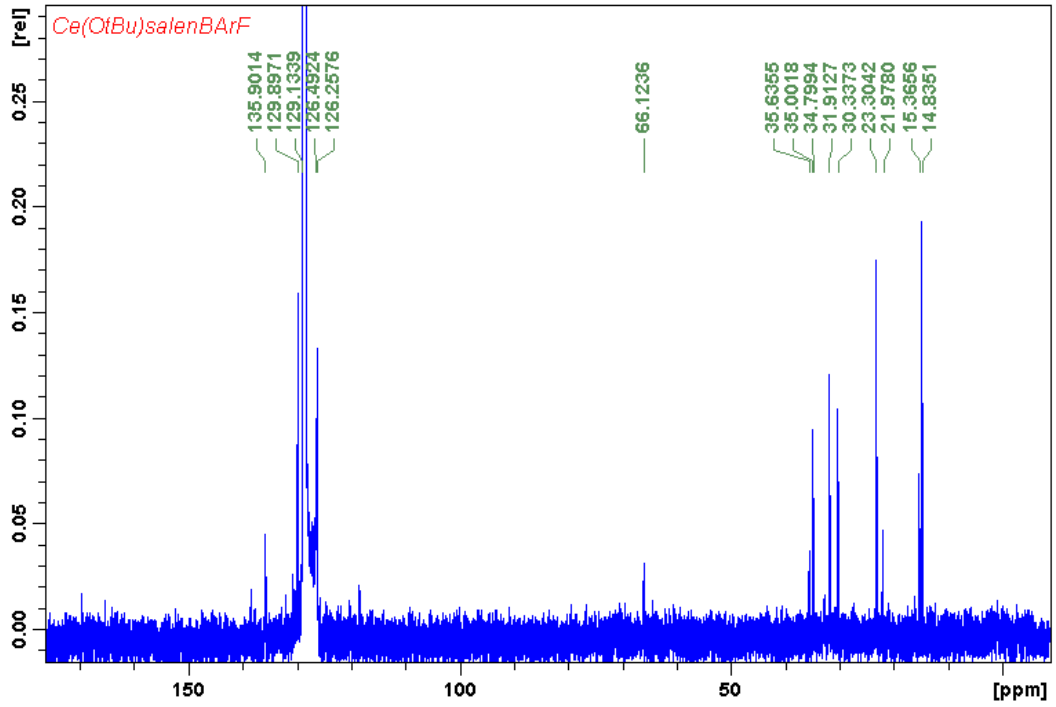


[2-Ce(O^{t}Bu)][BAr^F]

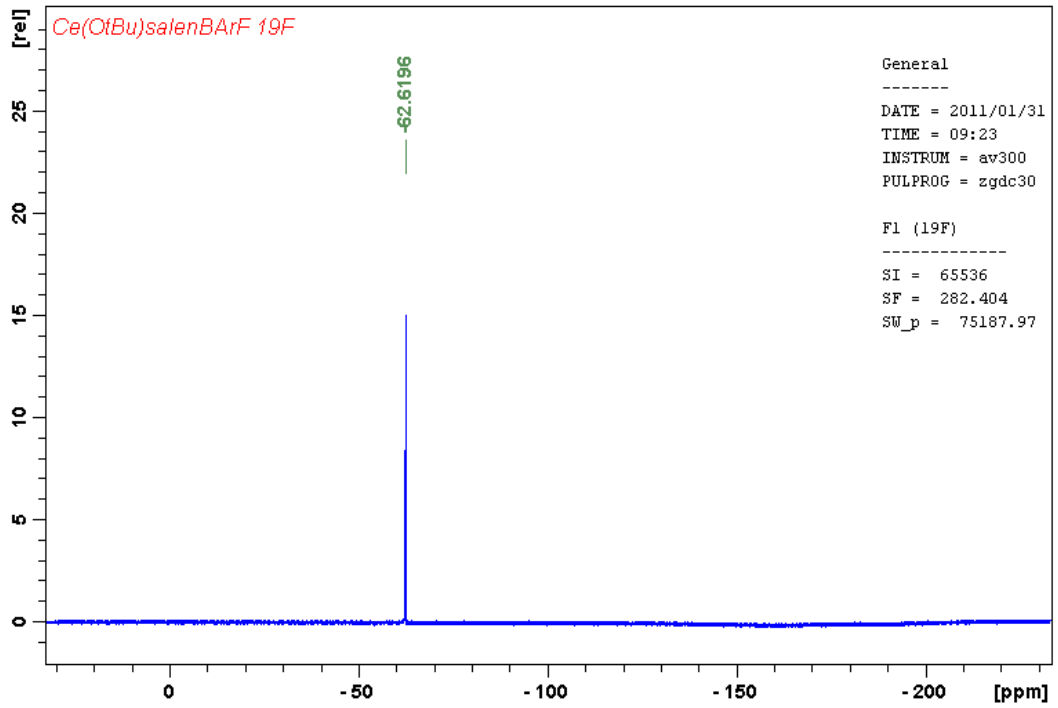
^{1}H NMR Spectrum (300 MHz, 25 °C, C_6D_6)



^{13}C NMR Spectrum (75 MHz, 25 °C, C_6D_6)

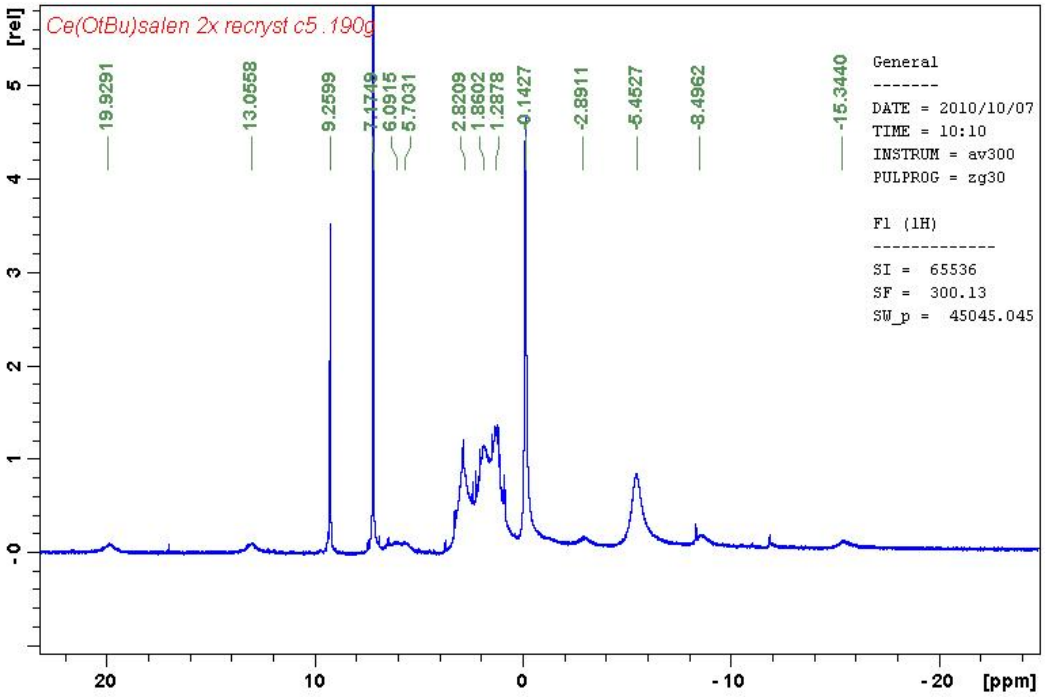


^{19}F NMR Spectrum (282 MHz, 25 °C, C_6D_6)

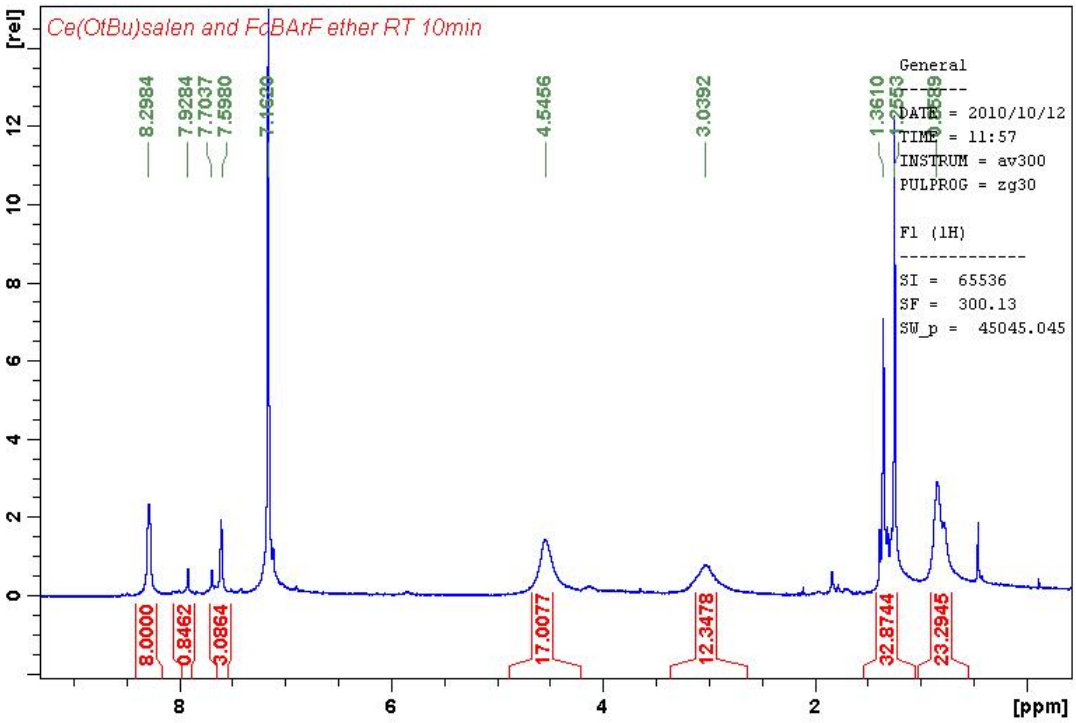


Oxidation and Reduction Reactions

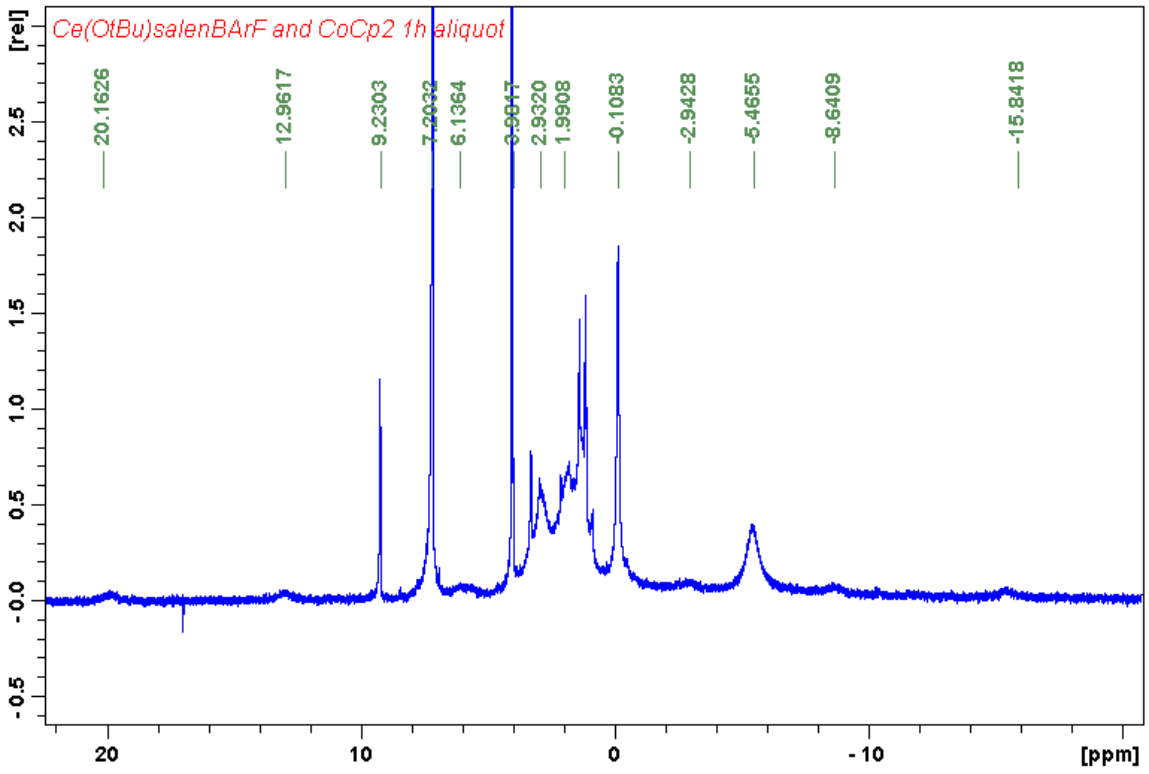
2-Ce(O^{t}Bu)



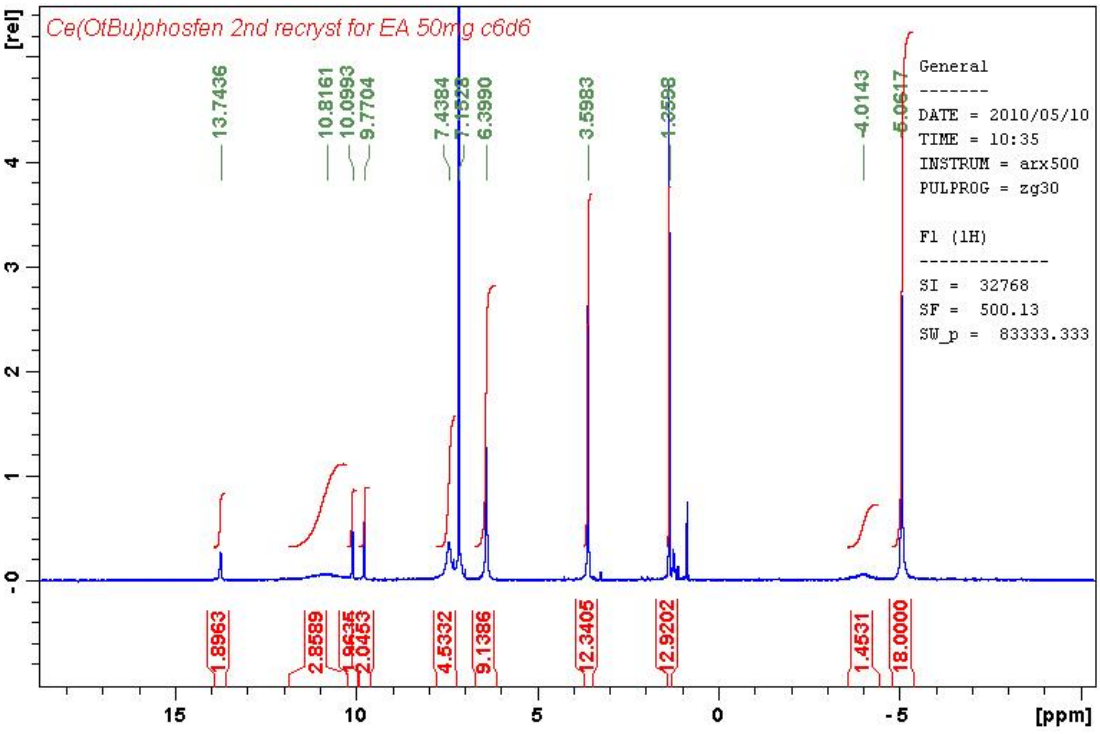
2-Ce(O^{t}Bu) and FcBAr^F



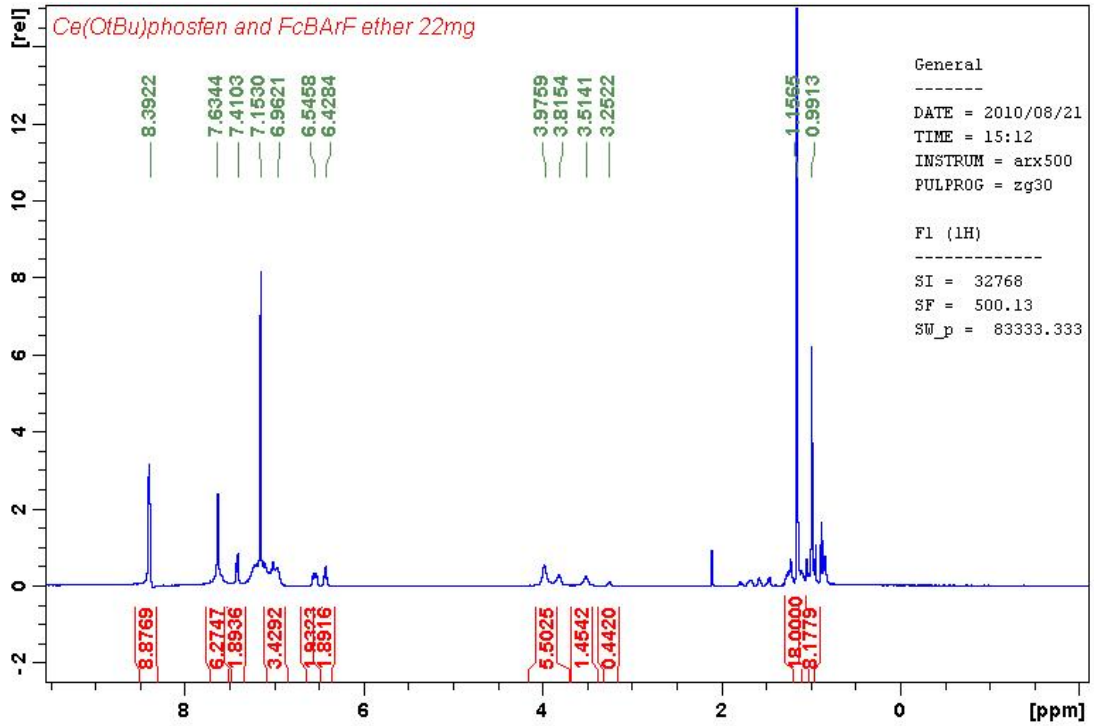
[2-Ce(O^{t}Bu)][BAr^F] and $CoCp_2$



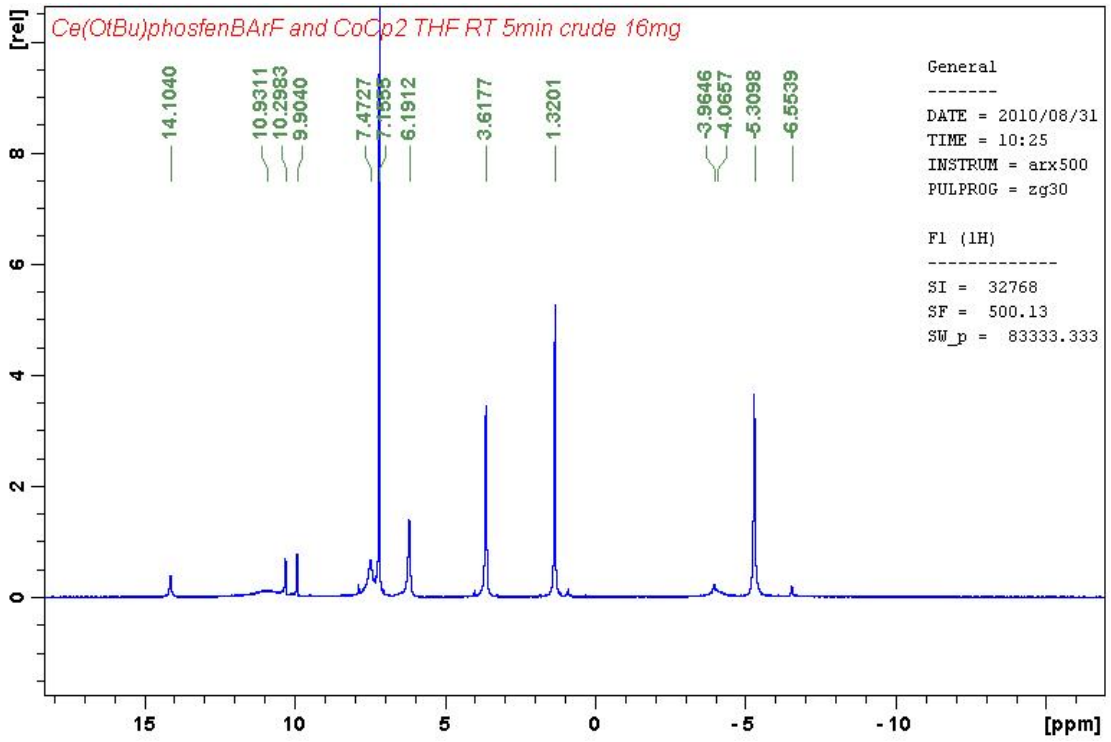
1-Ce(O^{t}Bu)



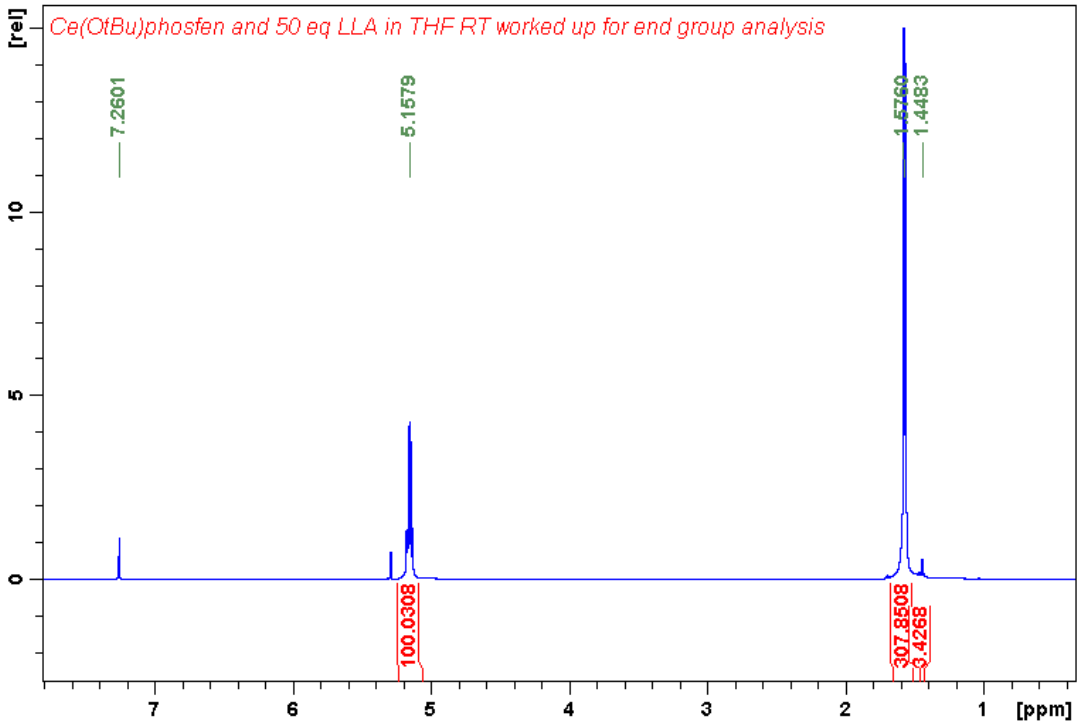
1-Ce(O^{t}Bu) and FcBAr^F



[1-Ce(O^{t}Bu)][BAr^F] and $CoCp_2$

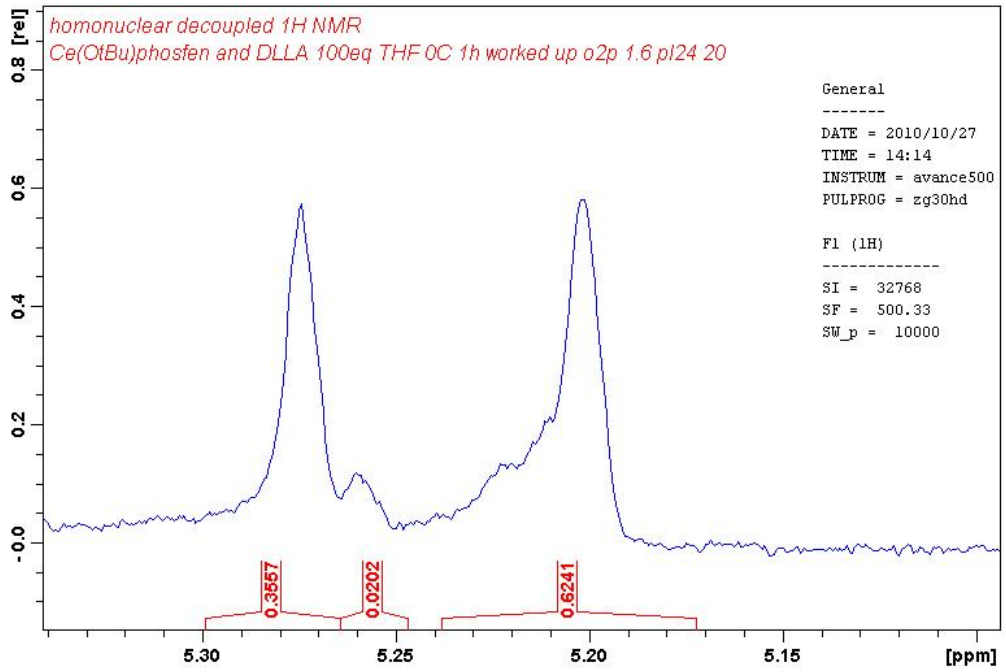


^{1}H NMR Spectrum for end-group analysis of poly(lactide) from 1-Ce(O^{t}Bu) with 50 equivalents of L-lactide

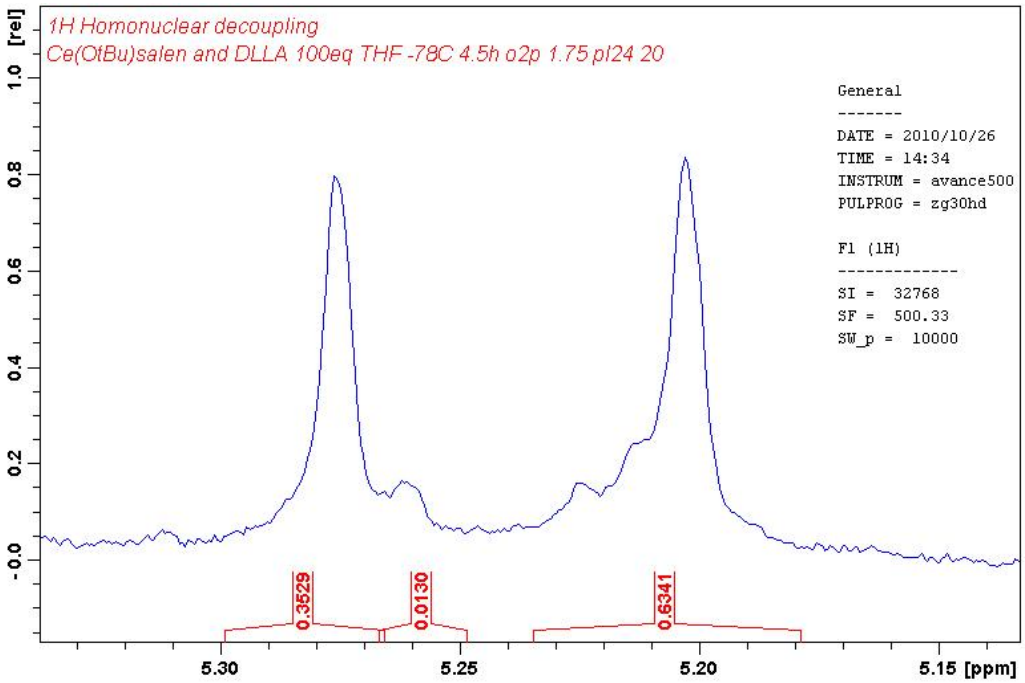


Heteronuclear decoupled ^{1}H NMR spectra of poly(D,L-lactide)

1-Ce(O^{t}Bu) and 100 equivalents of D,L-lactide at 0 °C in THF

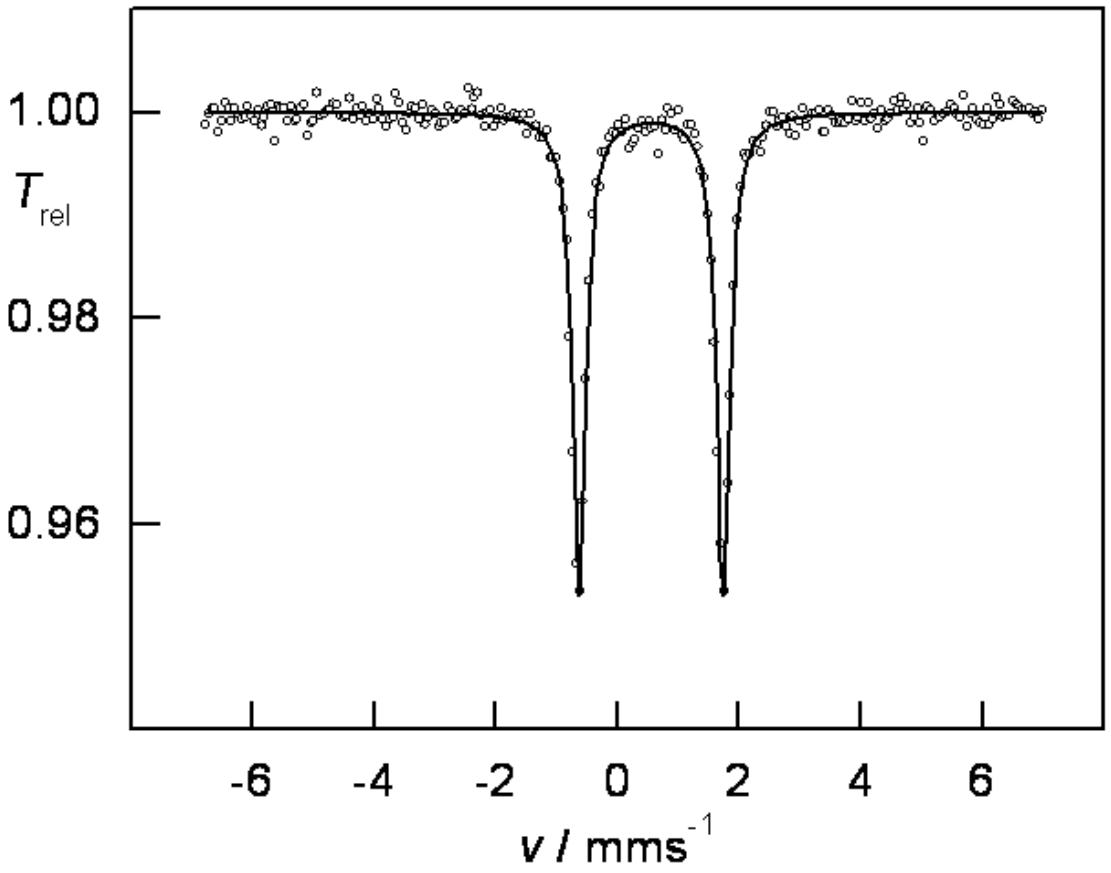


2-Ce(O^{t}Bu) and 100 equivalents of D,L-lactide at 0 °C in THF



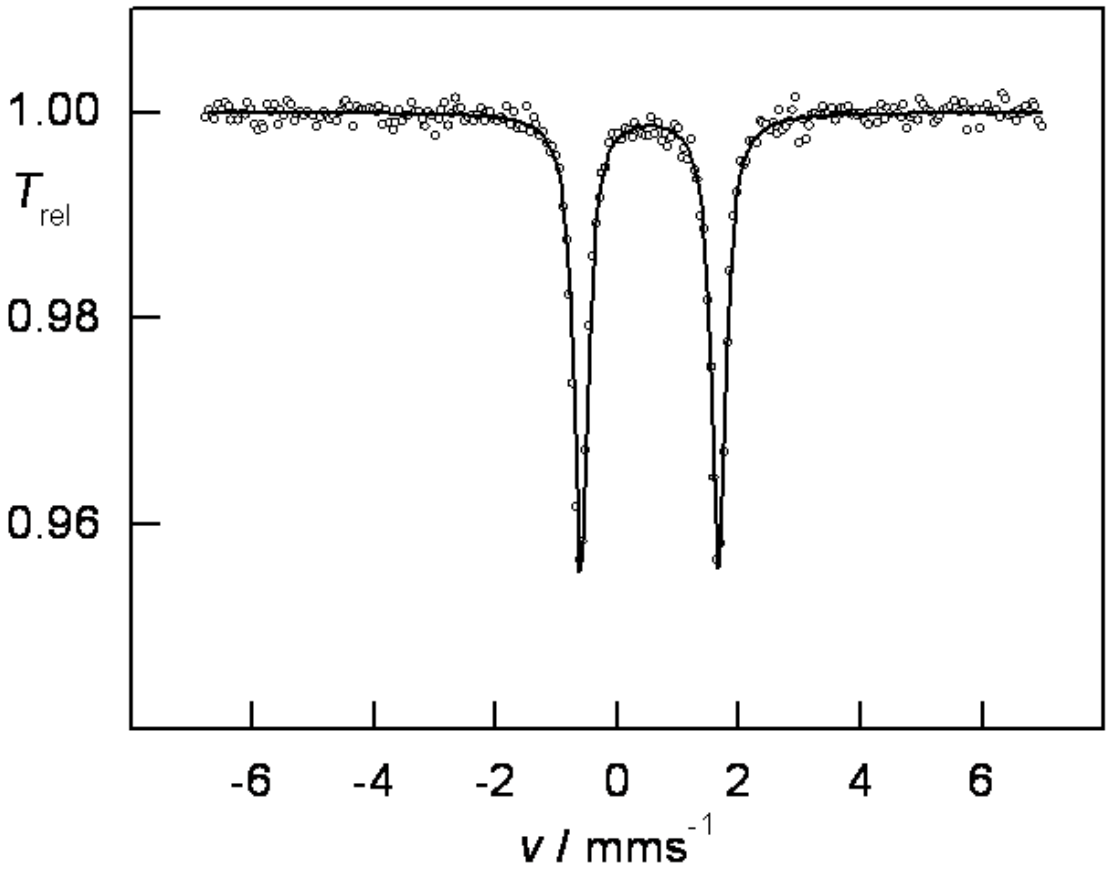
Mössbauer Spectroscopy

[1-Ce(O^{t}Bu)][BAr^F]



Spectrum
Type: doublet
$\delta = 0.55(1)$ mms^{-1}
$\Delta E_Q = 2.37(1)$ mms^{-1}
$\Gamma_{FWHM} = 0.26(1)$ mms^{-1}

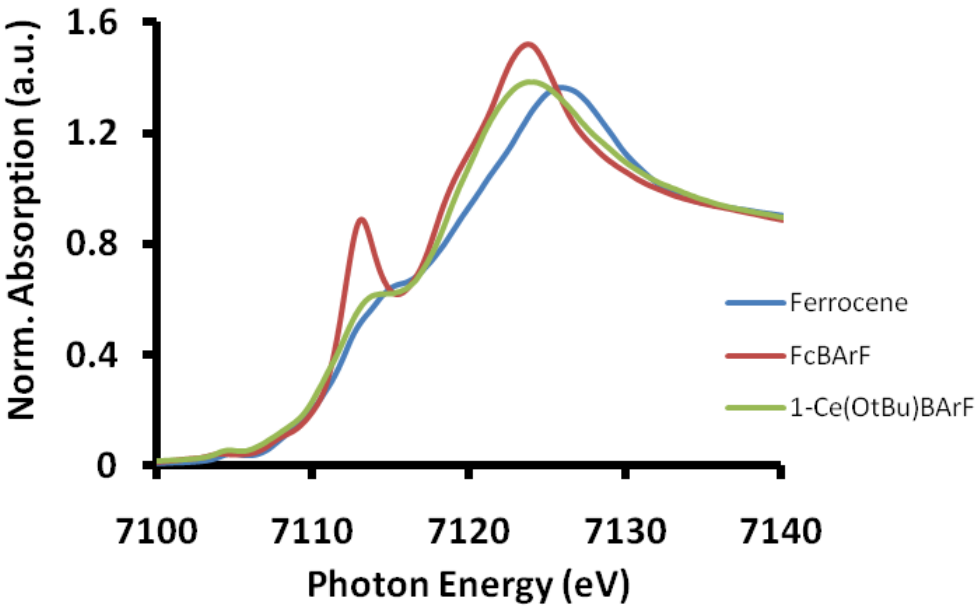
1-Ce(O^{t}Bu)I



Spectrum
Type: doublet
$\delta = 0.53(1)$ mms^{-1}
$\Delta E_Q = 2.27(1)$ mms^{-1}
$\Gamma_{FWHM} = 0.28(1)$ mms^{-1}

XANES Spectroscopy

Fe K-Edge



Ce L3-Edge

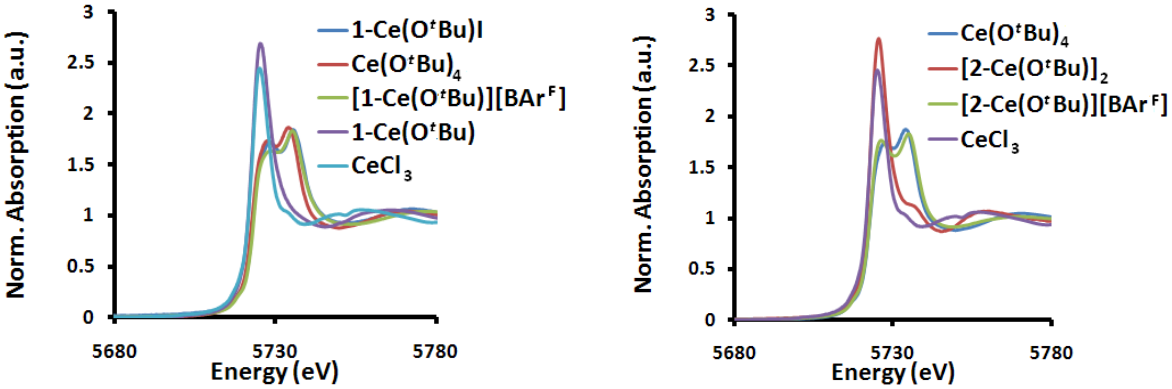
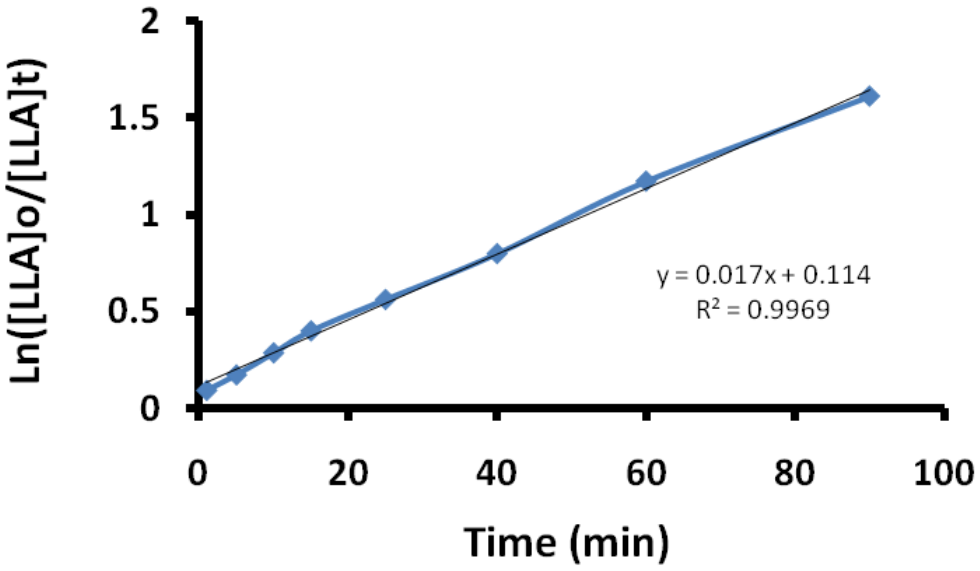


Table S1. Gel permeation chromatography data for **1-Ce(O^{t}Bu)** and **2-Ce(O^{t}Bu)** with L-lactide (0.2 M in THF) at ambient temperature.

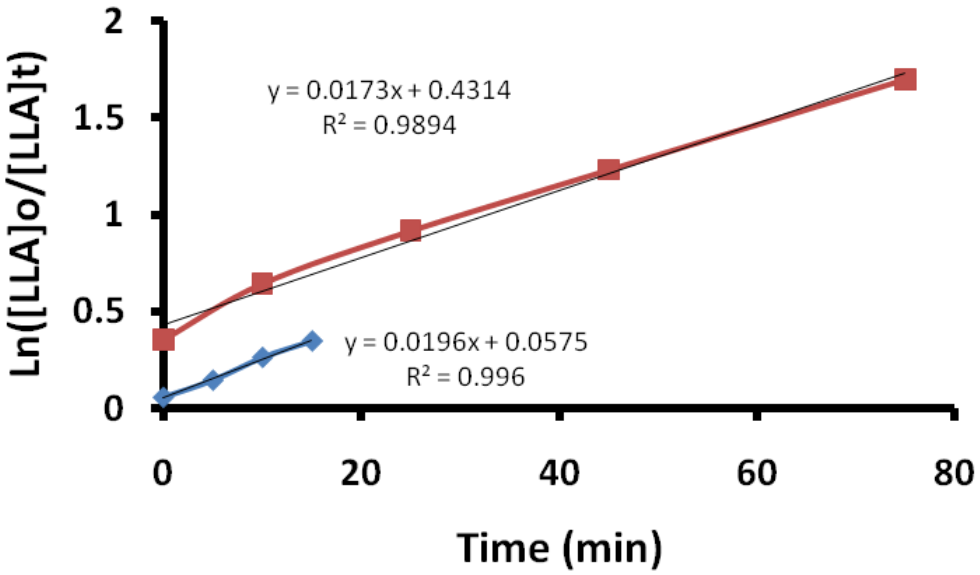
complex	equiv. LLA	time (h)	conv.	M_n[a,b] (kg/mol)	PDI
1-Ce(O^{t}Bu)	100	0.5	96%	16.3	1.11
	200	0.5	94%	35.1	1.14
	300	0.5	85%	41.4	1.07
	400	0.5	87%	46.1	1.05
	500	2	81%	55.6	1.11
2-Ce(O^{t}Bu)	100	4	93%	11.1	1.34
	200	4	92%	23.3	1.22
	300	4	84%	29.2	1.15
	400	7	81%	33.7	1.16
	500	9	76%	32.1	1.12
2-Ce(O^{t}Bu) add $FcBAr^F$	100	0.75	70%	9.09	1.60
add $CoCp_2$		0.33	70%	10.8	1.53
		1.5	90%	11.5	1.73

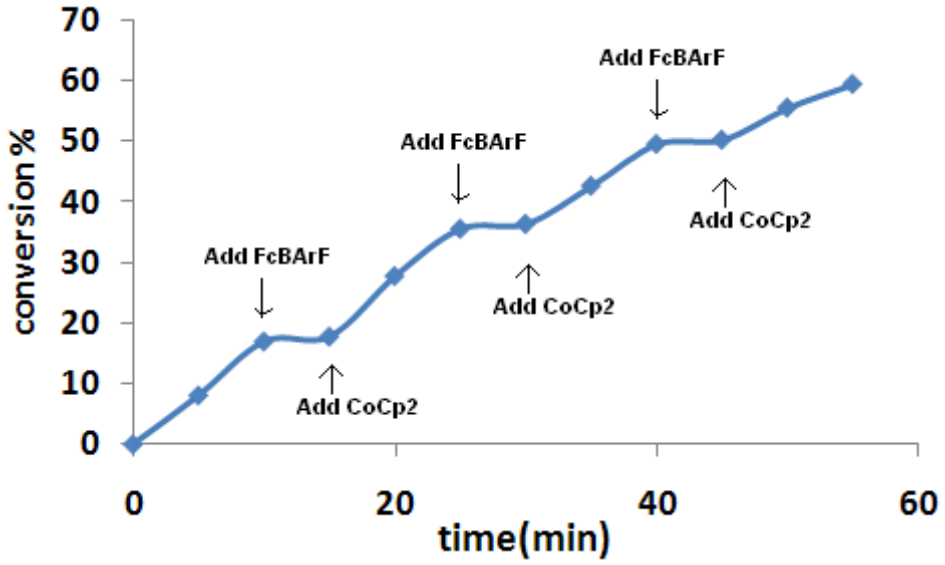
[a] Samples were run in THF with polystyrene standards.
[b] A Mark Houwink factor of 0.58 was applied to the experimental molecular weights.

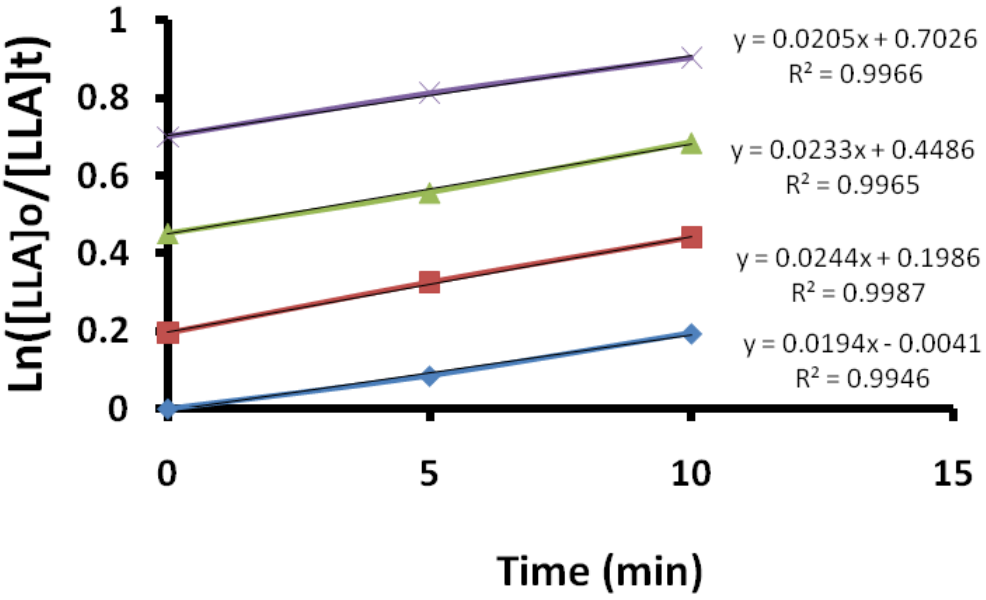
Kinetic Data without Switching



Kinetic Data for In Situ Switching

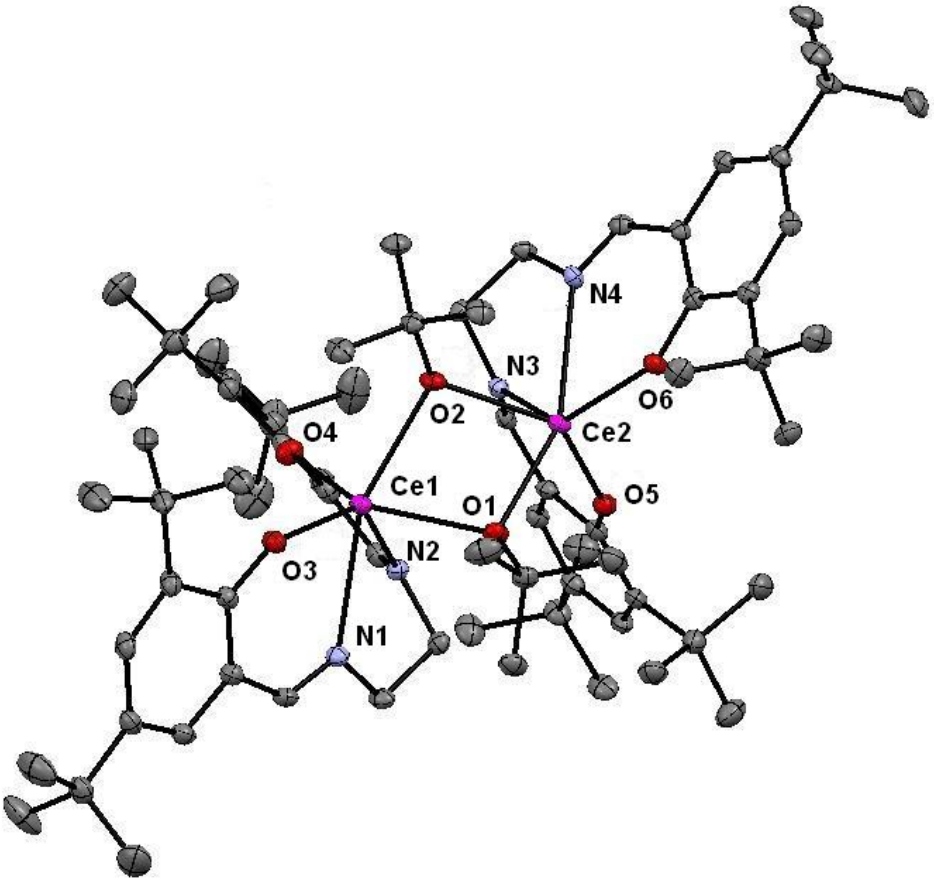


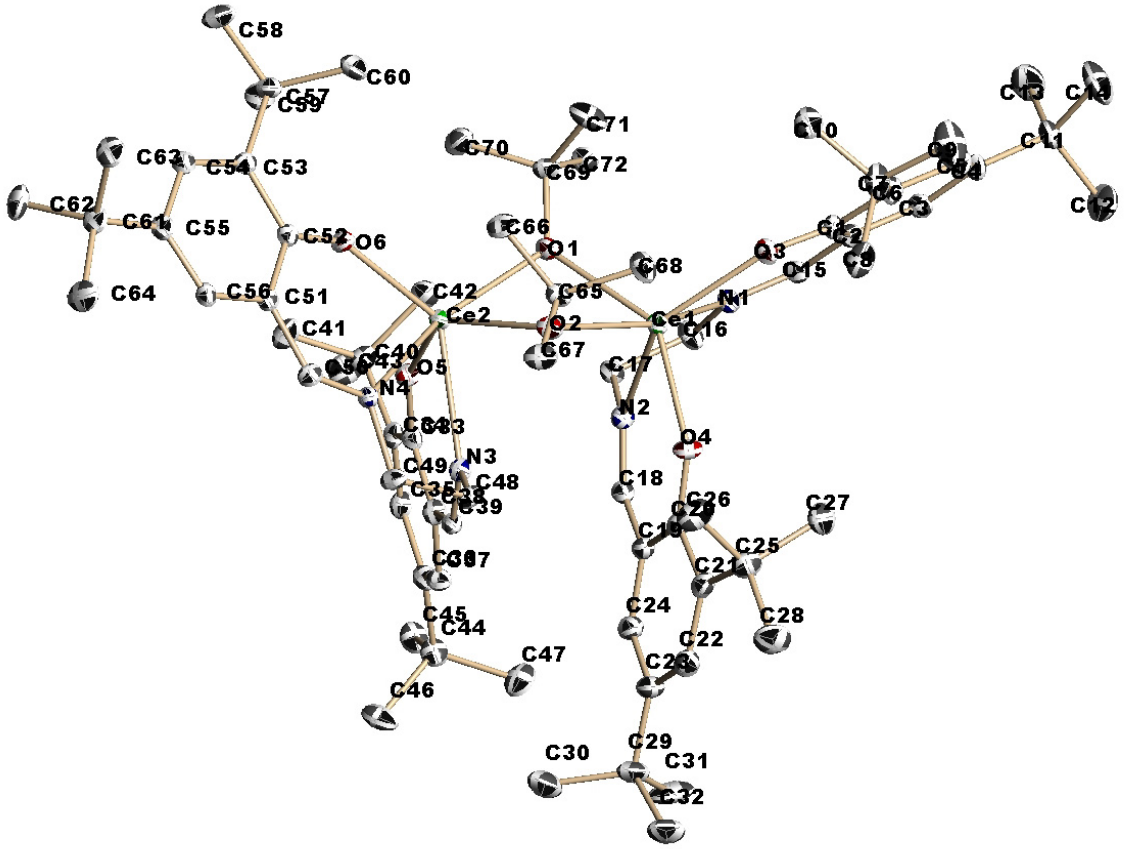




X-Ray Data

Thermal-ellipsoid (50% probability) representation of **[2-Ce(O^{t}Bu)]$_2$**. Hydrogen and solvent atoms were omitted for clarity.





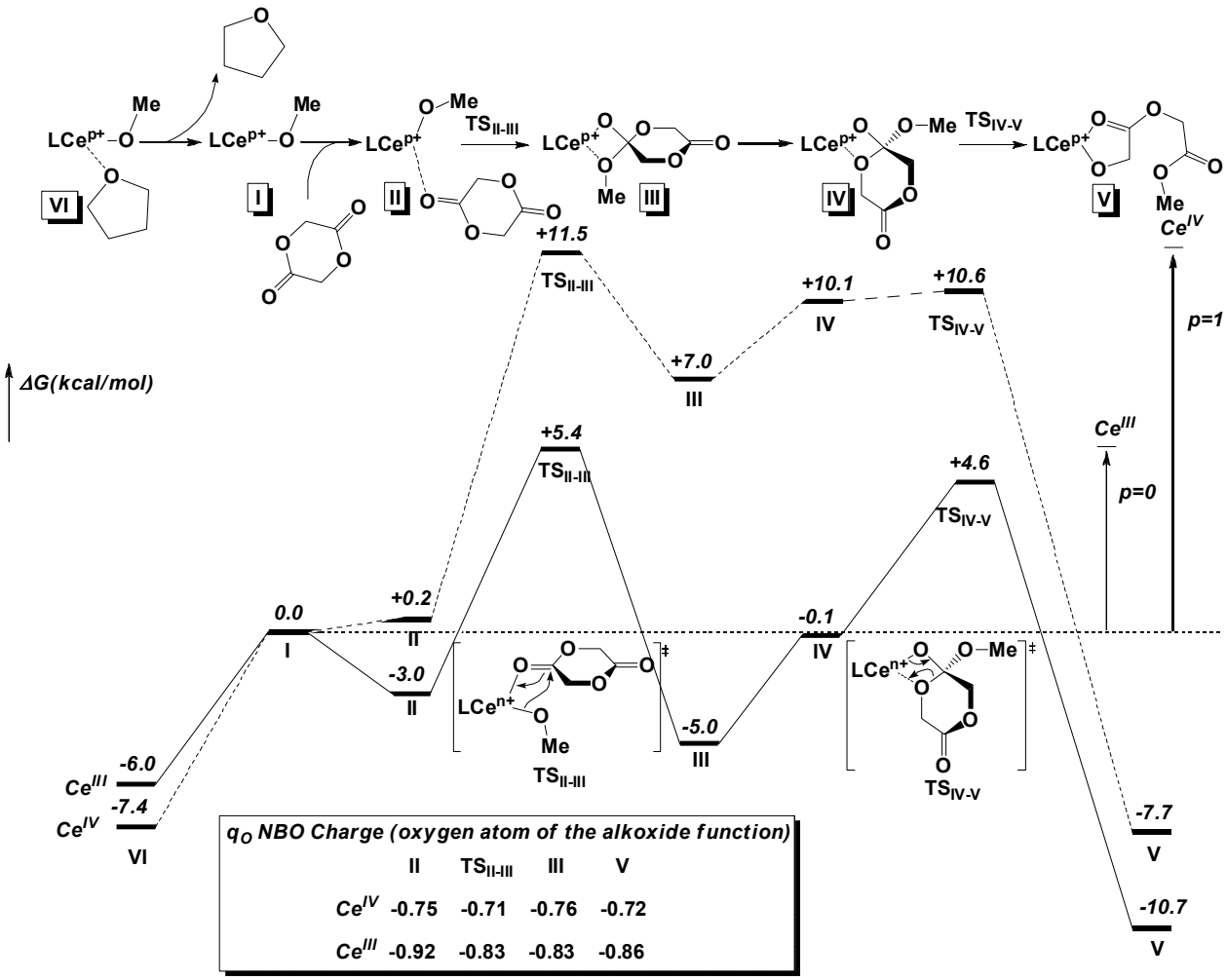
X-ray quality crystals were obtained from a concentrated pentane solution placed in a -35 °C freezer in the glove box. A total of 41565 reflections ($-19 \le h \le 20$, $-23 \le k \le 23$, $-25 \le l \le 24$) were collected at T = 100(2) K with $2\theta_{max}$ = 61.69°, of which 23106 were unique. The residual peak and hole electron density were 0.77 and -0.55 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0265 and GOF = 0.995. Crystal and refinement data for **[2-Ce(O^{t}Bu)]$_2$**: formula $C_{72}H_{110}N_4O_6Ce_2$ (C_5H_{12}, C_4H_{10}), space group $P2_1$, a = 14.471(3), b = 16.704(3), c = 17.748(4), β = 102.508(2)°, V = 4188.4(14) Å^3, Z = 2, μ = 1.123 mm^{-1}, F(000) = 1636, R_1 = 0.0271 and wR_2 = 0.0569 (based on all 23106 data, I > 2σ(I)).

DFT Calculations

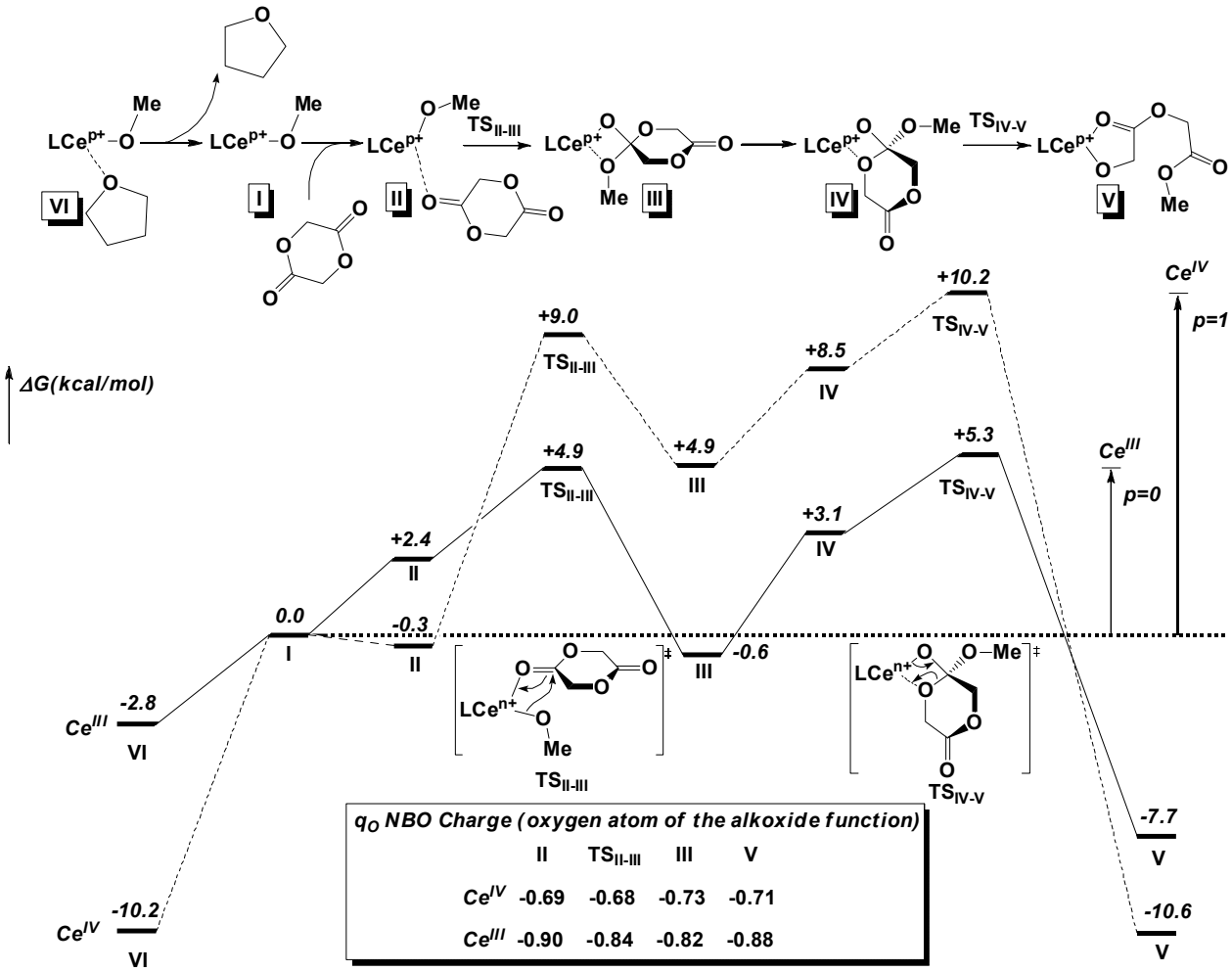
Computational Details

The B3LYP[7,8] hybrid density functional was employed to optimize the equilibrium molecular structure of the model complexes. The small core relativistic effective core potential developed by the Stuttgart-Dresden group was used for cerium, it incorporates scalar relativistic effects.[9] The RECP was used in combination with its optimized basis set with the valence electrons represented as [5s/5p/4d/3f] (the 4f electrons are treated as part of the valence shell). 6-31G* basis sets were used for carbon, hydrogen, nitrogen, phosphorus and sulfur. The LANL2DZ[10] effective core potential and valence double zeta basis set was used for iron. Harmonic vibrational analyses were performed to confirm to characterize the structures as minima or transition states. All calculations were carried out using the *Gaussian09*[11] suite of codes; NBO[12] analysis was employed for charges determination.

Free energy surfaces for ligand set L = 1 (cerium(III) is represented as a solid line and cerium(IV) as a dotted line)



Free energy surfaces for ligand set L = 2 (cerium(III) is represented as a solid line and cerium(IV) as a dotted line)



Optimized structure and free energy for glycolide

8	3.062289000	1.319692000	-0.443549000
6	3.030091000	1.993219000	-1.464594000
8	4.098728000	2.001590000	-2.341607000
6	1.843912000	2.845610000	-1.869256000
1	1.156599000	2.265855000	-2.498224000
1	1.315336000	3.177441000	-0.978562000
6	3.929415000	2.658196000	-3.647646000
1	4.935448000	2.814587000	-4.030085000
1	3.390219000	1.983242000	-4.324278000
6	3.211971000	3.989994000	-3.553191000
8	2.232851000	4.073379000	-2.580741000
8	3.450858000	4.940867000	-4.285274000

Sum of electronic and thermal Free Energies= -455.500623

Optimized structure and free energy for THF

6	-1.364582000	0.462029000	-0.159295000
8	0.097964000	0.434997000	0.004558000
6	0.600740000	1.811270000	0.151656000
6	-0.578030000	2.733374000	-0.202794000
6	-1.803435000	1.887504000	0.212852000
1	-1.609726000	0.224234000	-1.202943000
1	-1.790364000	-0.309849000	0.487766000
1	0.930298000	1.956634000	1.188688000
1	1.462043000	1.930486000	-0.511788000
1	-0.529770000	3.696210000	0.314891000
1	-0.601926000	2.929202000	-1.281593000
1	-1.970374000	1.967961000	1.293775000
1	-2.723333000	2.191592000	-0.295782000

Sum of electronic and thermal Free Energies= -232.292921

*Optimized structures and free energies for ligand set **1***

*Optimized structure and free energy for **1**-Ce^{III}-**I***

Ce	0.126772000	-0.115629000	-0.230664000
Fe	-0.161531000	0.014093000	3.988531000
P	3.416279000	-0.687592000	1.325131000
P	-1.574416000	3.018475000	0.643305000
N	1.739937000	-0.926071000	1.584810000
N	-0.709141000	1.685328000	1.341543000
O	2.202233000	-0.294240000	-1.293241000
O	-0.651518000	1.557012000	-1.667151000
C	1.283994000	-1.167514000	2.895789000
C	0.098561000	-1.932363000	3.187538000
H	-0.528741000	-2.396906000	2.441904000
C	-0.067367000	-1.984335000	4.612631000
H	-0.861126000	-2.493514000	5.136851000
C	0.994424000	-1.232489000	5.214952000
H	1.142522000	-1.072477000	6.272211000

C	1.812418000	-0.701934000	4.157823000
H	2.671950000	-0.059799000	4.289277000
C	-0.939190000	1.535627000	2.745579000
C	-2.019908000	0.800244000	3.370553000
H	-2.768649000	0.229636000	2.841360000
C	-1.889801000	0.927638000	4.790386000
H	-2.529038000	0.471166000	5.530879000
C	-0.734467000	1.738656000	5.062103000
H	-0.362074000	1.999513000	6.041327000
C	-0.150984000	2.116832000	3.808131000
H	0.739652000	2.710360000	3.662176000
C	4.051097000	-1.371100000	-0.246896000
C	5.201817000	-2.172160000	-0.291526000
H	5.739550000	-2.418627000	0.619581000
C	5.642109000	-2.649040000	-1.524013000
H	6.529436000	-3.269100000	-1.585394000
C	4.920793000	-2.325827000	-2.687680000
H	5.267410000	-2.704481000	-3.645784000
C	3.766096000	-1.540221000	-2.660771000
C	3.307081000	-1.044550000	-1.406137000
C	-0.830986000	3.778366000	-0.844249000
C	-0.649461000	5.163791000	-0.969802000
H	-0.917794000	5.833774000	-0.158043000
C	-0.122101000	5.666156000	-2.157626000
H	0.026541000	6.733062000	-2.282048000
C	0.218879000	4.778132000	-3.194741000
H	0.629563000	5.178485000	-4.118166000
C	0.056330000	3.395614000	-3.082334000
C	-0.477590000	2.870560000	-1.870471000
C	0.433564000	2.444288000	-4.187240000
H	1.199919000	1.735508000	-3.850474000
H	-0.427950000	1.841448000	-4.499209000
H	0.815847000	2.983091000	-5.059899000
C	2.989708000	-1.211514000	-3.909319000
H	1.965455000	-1.601346000	-3.854774000
H	2.899913000	-0.127143000	-4.045464000
H	3.471130000	-1.634338000	-4.796634000
H	4.222830000	-1.275179000	2.353256000
H	3.807492000	0.701300000	1.379667000
H	-1.730616000	4.100591000	1.570291000
H	-2.942169000	2.693624000	0.316657000
O	-1.228868000	-1.759425000	-0.391291000
C	-2.135558000	-2.834667000	-0.634449000
H	-2.693438000	-3.092979000	0.277923000
H	-2.865350000	-2.567811000	-1.412606000
H	-1.599789000	-3.734961000	-0.968370000

Sum of electronic and thermal Free Energies= -2584.694548

*Optimized structure and free energy for **1**-Ce^{III}-**II***

O	4.417278000	1.786805000	0.270386000
C	5.470377000	2.682103000	-0.094764000

H	6.405849000	2.426497000	0.423458000
H	5.672601000	2.641033000	-1.177099000
H	5.216667000	3.722972000	0.157641000
O	2.222771000	0.512210000	-1.389788000
C	2.407326000	1.661050000	-1.821033000
O	3.232176000	1.857028000	-2.883929000
C	1.688432000	2.857743000	-1.256045000
H	0.711585000	2.971172000	-1.744809000
H	1.545897000	2.695764000	-0.181287000
C	3.277643000	3.190668000	-3.514217000
H	4.233602000	3.233231000	-4.030268000
H	2.466238000	3.253263000	-4.249072000
C	3.183566000	4.340594000	-2.529660000
O	2.437786000	4.115742000	-1.397789000
O	3.713157000	5.426121000	-2.734747000
Ce	3.381348000	-0.022004000	0.943497000
Fe	-0.511883000	-0.822761000	2.470108000
P	2.977477000	-3.694775000	1.103536000
P	2.219984000	2.619147000	2.948640000
N	2.119085000	-2.212861000	1.321475000
N	1.465879000	1.654285000	1.731670000
O	4.821319000	-1.653440000	0.123649000
O	3.891963000	0.250492000	3.185803000
C	0.962025000	-2.322239000	2.152877000
C	-0.345505000	-2.794524000	1.747612000
H	-0.613593000	-3.087148000	0.743405000
C	-1.206203000	-2.768869000	2.892083000
H	-2.251138000	-3.040237000	2.907521000
C	-0.452669000	-2.266038000	4.007162000
H	-0.830264000	-2.106644000	5.005977000
C	0.883180000	-1.998768000	3.558013000
H	1.692736000	-1.593422000	4.146015000
C	0.155240000	1.185120000	1.957749000
C	-0.651558000	0.603438000	0.913056000
H	-0.323802000	0.434037000	-0.101330000
C	-1.949113000	0.305693000	1.453923000
H	-2.774507000	-0.130099000	0.911566000
C	-1.944001000	0.661065000	2.842311000
H	-2.762683000	0.539020000	3.534907000
C	-0.640342000	1.176052000	3.162599000
H	-0.309830000	1.488156000	4.142346000
C	3.994852000	-3.821244000	-0.411913000
C	3.949652000	-4.956174000	-1.235667000
H	3.273817000	-5.776254000	-1.010026000
C	4.787513000	-5.016358000	-2.346975000
H	4.772798000	-5.883629000	-2.997736000
C	5.651063000	-3.939816000	-2.620598000
H	6.302502000	-3.992593000	-3.489105000
C	5.699908000	-2.796462000	-1.820001000
C	4.844930000	-2.723480000	-0.683130000
C	2.810653000	1.896288000	4.534224000

C	2.470317000	2.431859000	5.784749000
H	1.829225000	3.307415000	5.854179000
C	2.975298000	1.833681000	6.937869000
H	2.733206000	2.235432000	7.915752000
C	3.806861000	0.704665000	6.821705000
H	4.201093000	0.244134000	7.723884000
C	4.146109000	0.146439000	5.586846000
C	3.629032000	0.745995000	4.402333000
C	5.033854000	-1.064665000	5.466064000
H	4.503107000	-1.902070000	4.995194000
H	5.901261000	-0.855240000	4.829069000
H	5.391164000	-1.392186000	6.447282000
C	6.611689000	-1.636770000	-2.124101000
H	6.036064000	-0.725619000	-2.330925000
H	7.255380000	-1.406242000	-1.266924000
H	7.245439000	-1.849977000	-2.990777000
H	2.109107000	-4.835108000	1.052510000
H	3.835004000	-4.022893000	2.220896000
H	1.425729000	3.743338000	3.361911000
H	3.342853000	3.128624000	2.246219000

Sum of electronic and thermal Free Energies= -3040.199979

*Optimized structure and free energy for **1**-Ce^{III}-**$TS_{II\text{-}III}$***

O	0.047030000	-0.236496000	0.110999000
C	1.111080000	0.711338000	0.302340000
H	0.762219000	1.580267000	0.880004000
H	1.957604000	0.254407000	0.832424000
H	1.473633000	1.084782000	-0.665945000
O	-2.463087000	-0.515957000	0.838521000
C	-1.469003000	-0.395455000	1.613289000
O	-1.273762000	0.808393000	2.252925000
C	-0.866089000	-1.616522000	2.263633000
H	-1.543056000	-1.972840000	3.052698000
H	-0.738479000	-2.389336000	1.508218000
C	-0.447228000	0.823866000	3.471817000
H	-0.030244000	1.826248000	3.536202000
H	-1.104993000	0.654522000	4.333893000
C	0.686581000	-0.185882000	3.493209000
O	0.456540000	-1.380562000	2.858883000
O	1.743872000	0.025891000	4.079475000
Ce	-1.532928000	-0.747528000	-1.515045000
Fe	-3.905782000	-4.137684000	-2.128731000
P	-4.218419000	0.300497000	-3.774925000
P	0.481282000	-3.660104000	-1.322205000
N	-3.655493000	-1.025529000	-2.818785000
N	-1.085819000	-3.219973000	-0.765217000
O	-2.006672000	1.400086000	-2.229312000
O	-0.043625000	-1.471304000	-3.124929000
C	-4.240336000	-2.289832000	-3.134516000
C	-5.479331000	-2.811877000	-2.598607000
H	-6.087014000	-2.317256000	-1.855805000

C	-5.722973000	-4.089855000	-3.196962000
H	-6.556238000	-4.742514000	-2.983703000
C	-4.638208000	-4.378363000	-4.093880000
H	-4.523502000	-5.279261000	-4.677502000
C	-3.726967000	-3.272181000	-4.061733000
H	-2.801296000	-3.184320000	-4.611521000
C	-2.135477000	-4.153904000	-0.842406000
C	-3.353330000	-4.008873000	-0.084801000
H	-3.575703000	-3.180229000	0.569991000
C	-4.176173000	-5.161014000	-0.327936000
H	-5.144422000	-5.349720000	0.110016000
C	-3.498028000	-6.002409000	-1.270130000
H	-3.864139000	-6.935301000	-1.670997000
C	-2.255630000	-5.366568000	-1.616074000
H	-1.537161000	-5.733974000	-2.334379000
C	-4.207149000	1.939781000	-2.960014000
C	-5.310755000	2.804551000	-3.022849000
H	-6.216430000	2.509188000	-3.545149000
C	-5.225573000	4.049675000	-2.403538000
H	-6.063510000	4.737033000	-2.440498000
C	-4.047563000	4.404661000	-1.721289000
H	-3.991446000	5.374686000	-1.234447000
C	-2.945107000	3.551459000	-1.635692000
C	-3.019417000	2.280759000	-2.271941000
C	0.904442000	-3.658218000	-3.112918000
C	1.507441000	-4.743806000	-3.763083000
H	1.745604000	-5.652757000	-3.216309000
C	1.808402000	-4.635179000	-5.120025000
H	2.282455000	-5.457958000	-5.643828000
C	1.496466000	-3.446251000	-5.804353000
H	1.738054000	-3.366881000	-6.861028000
C	0.883271000	-2.357815000	-5.177504000
C	0.565123000	-2.463892000	-3.794902000
C	0.547727000	-1.086690000	-5.912901000
H	-0.533894000	-0.899744000	-5.912107000
H	1.008169000	-0.217695000	-5.428154000
H	0.888785000	-1.129055000	-6.951890000
C	-1.696281000	3.918067000	-0.877679000
H	-1.532474000	3.231566000	-0.037134000
H	-0.809296000	3.843755000	-1.518053000
H	-1.758833000	4.937562000	-0.484347000
H	-5.567887000	0.118853000	-4.221718000
H	-3.498356000	0.436635000	-5.019801000
H	0.916891000	-4.948128000	-0.859124000
H	1.302289000	-2.689819000	-0.688702000

Sum of electronic and thermal Free Energies= -3040.186565

*Optimized structure and free energy for **1**-Ce^{III}-**III***

O	1.358268000	2.745563000	0.961399000
C	1.426132000	3.470455000	2.231772000
H	0.438386000	3.360217000	2.680987000

H	2.189567000	3.027356000	2.872976000
H	1.647082000	4.526847000	2.056077000
O	2.236677000	1.712281000	-0.840531000
C	2.579216000	2.608275000	0.105153000
O	3.614200000	2.144627000	1.040950000
C	2.988104000	3.957043000	-0.499852000
H	3.589087000	3.765857000	-1.393182000
H	2.107727000	4.537103000	-0.767096000
C	4.939148000	2.724487000	0.847950000
H	5.574899000	2.306979000	1.626420000
H	5.349202000	2.447389000	-0.133262000
C	4.878433000	4.232486000	1.002050000
O	3.757774000	4.812650000	0.427381000
O	5.704989000	4.917470000	1.595268000
Ce	0.175983000	0.723631000	-0.171949000
Fe	-0.271119000	-0.070481000	-4.264811000
P	0.043543000	-2.861542000	-0.450494000
P	-2.591496000	2.740333000	-1.414710000
N	-0.016460000	-1.418851000	-1.407136000
N	-1.179927000	1.919399000	-1.934947000
O	0.860968000	-0.873081000	1.375558000
O	-1.833483000	1.247553000	0.889768000
C	0.083055000	-1.582182000	-2.819344000
C	1.271278000	-1.367127000	-3.614612000
H	2.222625000	-1.038169000	-3.223893000
C	0.949860000	-1.635024000	-4.983691000
H	1.622192000	-1.543839000	-5.823390000
C	-0.434072000	-2.017748000	-5.052509000
H	-0.976678000	-2.266659000	-5.952027000
C	-0.972224000	-1.981515000	-3.723767000
H	-1.992698000	-2.185670000	-3.435538000
C	-0.954910000	1.737403000	-3.319173000
C	0.318420000	1.948071000	-3.961146000
H	1.217701000	2.254151000	-3.448275000
C	0.168974000	1.664573000	-5.359768000
H	0.947940000	1.727195000	-6.104341000
C	-1.190099000	1.267201000	-5.594500000
H	-1.613053000	0.979869000	-6.545048000
C	-1.879729000	1.283387000	-4.333663000
H	-2.907444000	0.995923000	-4.165539000
C	1.450283000	-3.070437000	0.704744000
C	2.254036000	-4.216635000	0.772572000
H	2.071133000	-5.064143000	0.117807000
C	3.292042000	-4.246979000	1.702473000
H	3.928303000	-5.121444000	1.783612000
C	3.514691000	-3.131729000	2.531954000
H	4.331098000	-3.163428000	3.248691000
C	2.732965000	-1.974673000	2.466404000
C	1.668845000	-1.938563000	1.524394000
C	-3.775549000	1.834807000	-0.348132000
C	-5.157161000	1.791729000	-0.578293000

H	-5.592011000	2.289916000	-1.440555000
C	-5.965156000	1.102777000	0.325414000
H	-7.038077000	1.056322000	0.174927000
C	-5.378527000	0.468639000	1.436147000
H	-6.016585000	-0.063662000	2.136756000
C	-4.001402000	0.492566000	1.675280000
C	-3.169592000	1.186648000	0.753741000
C	-3.374505000	-0.188227000	2.863810000
H	-2.630613000	-0.931853000	2.552125000
H	-2.836499000	0.531691000	3.492771000
H	-4.130207000	-0.688124000	3.477483000
C	2.991156000	-0.771240000	3.334539000
H	3.227614000	0.108630000	2.723057000
H	2.103005000	-0.514083000	3.925304000
H	3.823021000	-0.953887000	4.022246000
H	0.016411000	-4.042330000	-1.258287000
H	-1.145031000	-2.947172000	0.344664000
H	-3.366295000	3.256825000	-2.502198000
H	-2.207134000	3.900393000	-0.663202000

Sum of electronic and thermal Free Energies= -3040.203137

*Optimized structure and free energy for **1**-Ce^{III}-**IV***

O	2.172242000	3.632589000	-0.945304000
C	2.200653000	5.016028000	-0.467435000
H	1.865308000	5.609296000	-1.318286000
H	1.514111000	5.147685000	0.373577000
H	3.207906000	5.322775000	-0.172876000
O	2.335274000	1.392025000	-0.669418000
C	2.481304000	2.569421000	-0.050504000
O	1.350844000	2.645819000	1.062835000
C	3.821423000	2.704517000	0.677254000
H	4.071624000	1.741772000	1.129766000
H	4.602117000	2.990002000	-0.025830000
C	1.779014000	2.647664000	2.460034000
H	0.906216000	2.900539000	3.061577000
H	2.137273000	1.651971000	2.759314000
C	2.862736000	3.679382000	2.702772000
O	3.832315000	3.751977000	1.718134000
O	2.915983000	4.416579000	3.681938000
Ce	0.206077000	0.514692000	-0.133603000
Fe	-0.058047000	-0.010053000	-4.229196000
P	0.020409000	-3.036552000	-0.585332000
P	-2.450943000	2.710744000	-1.276830000
N	0.042097000	-1.554291000	-1.464929000
N	-1.166240000	1.719600000	-1.826722000
O	0.919271000	-1.134364000	1.373916000
O	-1.751019000	1.045777000	0.993412000
C	0.263544000	-1.611019000	-2.870319000
C	1.497787000	-1.279017000	-3.545658000
H	2.395471000	-0.931831000	-3.056390000
C	1.299394000	-1.455548000	-4.952469000

H	2.030910000	-1.269393000	-5.724232000
C	-0.051516000	-1.898100000	-5.163409000
H	-0.507983000	-2.101518000	-6.120309000
C	-0.695405000	-1.987137000	-3.884938000
H	-1.723452000	-2.260154000	-3.698940000
C	-0.866694000	1.683931000	-3.212486000
C	0.411192000	2.023394000	-3.789896000
H	1.266842000	2.363773000	-3.225170000
C	0.327577000	1.816301000	-5.205462000
H	1.127245000	1.967937000	-5.914686000
C	-0.996945000	1.356519000	-5.518591000
H	-1.364763000	1.103360000	-6.501454000
C	-1.731886000	1.254169000	-4.289660000
H	-2.745624000	0.899190000	-4.175314000
C	1.361268000	-3.352999000	0.624881000
C	2.072996000	-4.559336000	0.681775000
H	1.860989000	-5.360668000	-0.020880000
C	3.053690000	-4.715804000	1.659537000
H	3.616025000	-5.640251000	1.729057000
C	3.308547000	-3.662422000	2.555607000
H	4.073046000	-3.791601000	3.317141000
C	2.620023000	-2.447304000	2.503541000
C	1.620470000	-2.273982000	1.505571000
C	-3.654781000	1.921025000	-0.141881000
C	-5.041094000	2.061098000	-0.298334000
H	-5.449331000	2.634271000	-1.126297000
C	-5.888480000	1.456602000	0.628685000
H	-6.964115000	1.553541000	0.531388000
C	-5.336933000	0.719631000	1.691940000
H	-6.003272000	0.253716000	2.413105000
C	-3.958703000	0.558954000	1.857191000
C	-3.086194000	1.168494000	0.912792000
C	-3.370060000	-0.234056000	2.994700000
H	-2.774894000	-1.079347000	2.626726000
H	-2.686679000	0.381086000	3.592550000
H	-4.153604000	-0.622902000	3.652294000
C	2.913730000	-1.322328000	3.461101000
H	3.348799000	-0.460439000	2.936849000
H	1.997310000	-0.967436000	3.947094000
H	3.620499000	-1.635883000	4.235331000
H	-0.015349000	-4.186292000	-1.436697000
H	-1.202722000	-3.101936000	0.157192000
H	-3.234073000	3.256244000	-2.343551000
H	-1.955104000	3.875388000	-0.589616000

Sum of electronic and thermal Free Energies= -3040.195738

*Optimized structure and free energy for **1**-Ce^{III}-**$TS_{IV\text{-}V}$***

O	-1.474540000	2.981902000	2.752887000
C	-1.810678000	4.307074000	2.217955000
H	-2.616108000	4.777087000	2.785081000
H	-0.888340000	4.878069000	2.316448000

H	-2.093887000	4.215324000	1.168017000
O	-1.899414000	0.823028000	3.194696000
C	-2.397545000	1.954059000	2.811299000
O	-2.738801000	1.673914000	0.969977000
C	-3.821964000	2.255003000	3.254597000
H	-4.371861000	1.311412000	3.263990000
H	-3.812644000	2.674473000	4.262905000
C	-4.120974000	1.735573000	0.545316000
H	-4.166852000	1.807533000	-0.544838000
H	-4.670548000	0.829967000	0.849212000
C	-4.807083000	2.962237000	1.111703000
O	-4.533188000	3.248877000	2.446100000
O	-5.553230000	3.706073000	0.482836000
Ce	-1.378196000	-0.385409000	1.104800000
Fe	2.100314000	-0.975945000	3.233268000
P	-1.886338000	-3.507335000	2.881736000
P	1.309809000	0.841636000	-0.948586000
N	-0.674792000	-2.370416000	2.399298000
N	0.904413000	0.589738000	0.697543000
O	-3.330980000	-1.671111000	1.133422000
O	-0.968854000	-0.847022000	-1.139410000
C	0.475209000	-2.348780000	3.251093000
C	0.586991000	-1.675550000	4.527933000
H	-0.167360000	-1.028763000	4.950851000
C	1.876370000	-1.971120000	5.075684000
H	2.270575000	-1.595431000	6.007722000
C	2.575690000	-2.815548000	4.145337000
H	3.581872000	-3.187486000	4.265482000
C	1.717189000	-3.050094000	3.022156000
H	1.947016000	-3.631173000	2.141772000
C	1.934969000	0.491352000	1.658716000
C	1.884466000	1.125824000	2.951436000
H	1.058597000	1.724542000	3.305320000
C	3.102346000	0.820098000	3.644224000
H	3.363400000	1.147650000	4.639006000
C	3.908178000	-0.012098000	2.796164000
H	4.877153000	-0.420704000	3.039490000
C	3.178813000	-0.240685000	1.579993000
H	3.492721000	-0.856595000	0.749521000
C	-3.078731000	-3.996413000	1.584100000
C	-3.383422000	-5.343559000	1.334419000
H	-2.882654000	-6.134826000	1.884964000
C	-4.341805000	-5.650222000	0.371064000
H	-4.596445000	-6.683264000	0.162025000
C	-4.975992000	-4.608191000	-0.329586000
H	-5.724168000	-4.854043000	-1.078597000
C	-4.676280000	-3.262273000	-0.104583000
C	-3.693555000	-2.937083000	0.873721000
C	1.183190000	-0.568590000	-2.114782000
C	2.201307000	-0.953307000	-2.997610000
H	3.144650000	-0.414333000	-3.024968000

C	1.978720000	-2.037282000	-3.845419000
H	2.746998000	-2.354850000	-4.541824000
C	0.748396000	-2.717809000	-3.791464000
H	0.583020000	-3.561673000	-4.456180000
C	-0.274187000	-2.355856000	-2.909592000
C	-0.052307000	-1.255209000	-2.036807000
C	-1.584904000	-3.095203000	-2.848702000
H	-1.746453000	-3.542948000	-1.860465000
H	-2.428991000	-2.416084000	-3.019451000
H	-1.623697000	-3.892005000	-3.597933000
C	-5.347399000	-2.151288000	-0.868711000
H	-5.843957000	-1.447105000	-0.189700000
H	-4.615828000	-1.568851000	-1.442677000
H	-6.096222000	-2.545291000	-1.562605000
H	-2.647164000	-3.057227000	4.021469000
H	-1.326061000	-4.738546000	3.354741000
H	2.627451000	1.375031000	-1.128632000
H	0.416979000	1.842400000	-1.441267000

Sum of electronic and thermal Free Energies= -3040.187834

*Optimized structure and free energy for **1**-Ce^{III}-**V***

O	5.823266000	3.636965000	1.228249000
C	4.702196000	4.498911000	0.805688000
H	4.994803000	5.079543000	-0.070811000
H	3.899212000	3.804294000	0.572270000
H	4.426334000	5.172447000	1.619300000
O	7.189783000	5.463993000	1.504772000
C	7.005609000	4.244622000	1.523453000
O	5.736339000	0.210642000	3.891662000
C	8.084025000	3.258398000	1.932713000
H	9.028027000	3.582645000	1.495258000
H	8.186791000	3.262750000	3.023270000
C	6.535417000	1.285733000	3.479877000
H	5.984436000	2.240002000	3.467295000
H	7.416791000	1.432850000	4.133945000
C	7.051687000	1.017044000	2.064994000
O	7.861967000	1.914794000	1.417593000
O	6.786415000	-0.042900000	1.472923000
Ce	5.206316000	-1.718753000	2.845631000
Fe	3.719454000	-2.175819000	-1.221050000
P	6.378591000	-4.901432000	1.584182000
P	1.822260000	-0.626013000	2.596402000
N	5.485893000	-3.505018000	1.073250000
N	3.207600000	-0.654182000	1.578786000
O	6.920982000	-3.066470000	3.679147000
O	3.355515000	-2.541860000	4.008099000
C	4.976697000	-3.582537000	-0.259300000
C	5.620012000	-3.069621000	-1.448612000
H	6.548512000	-2.519170000	-1.456379000
C	4.795408000	-3.382989000	-2.576780000
H	4.993117000	-3.111685000	-3.602991000

C	3.635823000	-4.088511000	-2.102349000
H	2.817923000	-4.442180000	-2.711912000
C	3.744610000	-4.213810000	-0.678171000
H	3.024457000	-4.667000000	-0.012970000
C	3.011416000	-0.690730000	0.183222000
C	3.939183000	-0.119626000	-0.759759000
H	4.871153000	0.355607000	-0.495551000
C	3.405110000	-0.294761000	-2.081631000
H	3.871493000	0.031923000	-2.998614000
C	2.158830000	-0.996235000	-1.972526000
H	1.521300000	-1.295184000	-2.790645000
C	1.927675000	-1.268440000	-0.579070000
H	1.094545000	-1.823022000	-0.171688000
C	8.039465000	-4.653093000	2.319966000
C	9.188177000	-5.338757000	1.903522000
H	9.144337000	-6.048814000	1.082350000
C	10.389876000	-5.095060000	2.568196000
H	11.294561000	-5.613439000	2.269907000
C	10.421218000	-4.170366000	3.628262000
H	11.361863000	-3.988808000	4.141882000
C	9.287485000	-3.467910000	4.046900000
C	8.060412000	-3.704593000	3.368533000
C	1.117507000	-2.166796000	3.306538000
C	-0.228143000	-2.544176000	3.209423000
H	-0.939919000	-1.925482000	2.668825000
C	-0.640770000	-3.722436000	3.830595000
H	-1.677658000	-4.035961000	3.777419000
C	0.298479000	-4.501289000	4.532415000
H	-0.032912000	-5.415865000	5.017578000
C	1.647069000	-4.147570000	4.629486000
C	2.078911000	-2.953138000	3.987925000
C	2.651936000	-4.985377000	5.375510000
H	3.428028000	-5.371648000	4.701654000
H	3.175456000	-4.390777000	6.133393000
H	2.170990000	-5.836161000	5.868245000
C	9.323593000	-2.471879000	5.176168000
H	9.052652000	-1.466775000	4.828585000
H	8.595736000	-2.730957000	5.954366000
H	10.318543000	-2.423906000	5.629816000
H	6.577141000	-5.827265000	0.510901000
H	5.640603000	-5.663738000	2.556002000
H	0.706757000	0.050179000	1.997839000
H	2.220503000	0.161606000	3.714220000

Sum of electronic and thermal Free Energies= -3040.212301

*Optimized structure and free energy for **1**-Ce^{III}-**VI***

O	4.552364000	1.836353000	0.414980000
C	5.527516000	2.816443000	0.065527000
H	6.509322000	2.357294000	-0.123177000
H	5.237122000	3.366941000	-0.844644000
H	5.658492000	3.558414000	0.869706000

Ce	3.422441000	0.076642000	1.006730000
Fe	-0.536966000	-0.754068000	2.485224000
P	2.962542000	-3.607119000	1.100087000
P	2.272159000	2.633712000	3.084141000
N	2.076103000	-2.134139000	1.284604000
N	1.519305000	1.677913000	1.866172000
O	4.841963000	-1.608393000	0.161311000
O	3.924651000	0.257418000	3.285137000
C	0.914754000	-2.259139000	2.111062000
C	-0.397126000	-2.699315000	1.683231000
H	-0.664271000	-2.958700000	0.669605000
C	-1.263710000	-2.706330000	2.823790000
H	-2.311761000	-2.965985000	2.824472000
C	-0.508035000	-2.259609000	3.960901000
H	-0.888200000	-2.134247000	4.963520000
C	0.833195000	-1.991277000	3.527685000
H	1.643947000	-1.615808000	4.134053000
C	0.192874000	1.259863000	2.067391000
C	-0.636506000	0.757326000	1.001015000
H	-0.320768000	0.658473000	-0.025552000
C	-1.940506000	0.469056000	1.531588000
H	-2.782894000	0.093265000	0.971138000
C	-1.919949000	0.751218000	2.936507000
H	-2.739882000	0.619963000	3.625929000
C	-0.598684000	1.207331000	3.275516000
H	-0.253037000	1.454998000	4.268097000
C	3.960744000	-3.738296000	-0.427251000
C	3.880037000	-4.846764000	-1.284583000
H	3.190065000	-5.659118000	-1.072779000
C	4.701893000	-4.891203000	-2.409605000
H	4.660052000	-5.738676000	-3.085108000
C	5.589897000	-3.827843000	-2.659700000
H	6.231756000	-3.871653000	-3.535962000
C	5.679026000	-2.713153000	-1.823136000
C	4.836116000	-2.651624000	-0.673948000
C	2.867990000	1.894932000	4.661812000
C	2.539671000	2.415916000	5.921057000
H	1.908772000	3.297424000	6.005534000
C	3.042389000	1.795957000	7.064104000
H	2.809293000	2.186447000	8.048805000
C	3.859646000	0.658129000	6.927933000
H	4.251647000	0.179687000	7.822081000
C	4.186361000	0.113508000	5.683686000
C	3.672627000	0.736393000	4.508729000
C	5.059084000	-1.106475000	5.542619000
H	4.517375000	-1.930453000	5.060345000
H	5.927475000	-0.898010000	4.906187000
H	5.415049000	-1.453160000	6.518059000
C	6.628533000	-1.574783000	-2.090072000
H	6.089558000	-0.626704000	-2.212167000
H	7.311730000	-1.426892000	-1.244891000

H	7.222214000	-1.756994000	-2.991476000
H	2.114061000	-4.764497000	1.074879000
H	3.846011000	-3.904027000	2.205114000
H	1.483785000	3.758950000	3.509781000
H	3.400005000	3.147170000	2.391187000
O	2.228160000	0.275662000	-1.253788000
C	2.161850000	1.585073000	-1.962799000
C	1.640985000	-0.799037000	-2.102438000
C	1.867254000	1.214727000	-3.418483000
H	1.357526000	2.169704000	-1.505018000
H	3.117854000	2.078579000	-1.790750000
C	1.002629000	-0.060905000	-3.286351000
H	2.457602000	-1.458332000	-2.410088000
H	0.940077000	-1.354172000	-1.477935000
H	2.797139000	0.991337000	-3.954333000
H	1.351461000	2.018302000	-3.952776000
H	1.003863000	-0.667210000	-4.196891000
H	-0.036563000	0.207184000	-3.060056000

Sum of electronic and thermal Free Energies= -2816.99706

*Optimized structure and free energy for **1**-Ce^{IV}-**I***

Ce	0.465829000	0.194807000	-0.081986000
Fe	-0.071580000	0.118954000	3.810726000
P	3.746551000	-0.760251000	1.144599000
P	-1.964542000	2.851425000	0.433465000
N	2.095242000	-0.407123000	1.552460000
N	-0.955927000	1.652080000	1.180430000
O	2.206869000	-0.447979000	-1.276585000
O	0.017563000	1.845169000	-1.455831000
C	1.703720000	-0.590211000	2.908883000
C	0.934870000	-1.707379000	3.415268000
H	0.551815000	-2.519917000	2.816703000
C	0.779750000	-1.532800000	4.825381000
H	0.235822000	-2.186713000	5.489569000
C	1.449269000	-0.320585000	5.206014000
H	1.493894000	0.087759000	6.203959000
C	2.013379000	0.270163000	4.030083000
H	2.559734000	1.199897000	3.975399000
C	-1.257923000	1.307877000	2.528680000
C	-2.023045000	0.160999000	2.972432000
H	-2.444374000	-0.594418000	2.326537000
C	-2.104184000	0.210839000	4.398859000
H	-2.589495000	-0.515929000	5.032056000
C	-1.405342000	1.381730000	4.849941000
H	-1.278164000	1.682218000	5.878610000
C	-0.873100000	2.056667000	3.705638000
H	-0.277496000	2.956920000	3.706426000
C	3.973452000	-1.762869000	-0.371713000
C	4.930208000	-2.783473000	-0.463303000
H	5.564641000	-3.034922000	0.380943000
C	5.053762000	-3.471870000	-1.670346000

H	5.787218000	-4.263383000	-1.770342000
C	4.225230000	-3.138769000	-2.754001000
H	4.334235000	-3.681220000	-3.687946000
C	3.254700000	-2.131822000	-2.675538000
C	3.128534000	-1.432435000	-1.451533000
C	-1.106474000	3.853055000	-0.836767000
C	-1.352893000	5.226069000	-0.982189000
H	-2.045032000	5.743354000	-0.324982000
C	-0.690301000	5.919233000	-1.995221000
H	-0.865717000	6.980122000	-2.130130000
C	0.205377000	5.240753000	-2.836907000
H	0.712852000	5.791650000	-3.622596000
C	0.473861000	3.873231000	-2.698423000
C	-0.198309000	3.168658000	-1.670961000
C	1.438201000	3.146190000	-3.598678000
H	2.253164000	2.688858000	-3.024934000
H	0.938705000	2.330747000	-4.135137000
H	1.874939000	3.825891000	-4.335060000
C	2.360791000	-1.783661000	-3.836891000
H	1.305481000	-1.963006000	-3.596329000
H	2.447245000	-0.722898000	-4.098754000
H	2.614203000	-2.378576000	-4.718259000
H	4.417097000	-1.442225000	2.202662000
H	4.486465000	0.457183000	0.985733000
H	-2.494798000	3.769263000	1.389436000
H	-3.138804000	2.266986000	-0.155880000
O	-0.802957000	-1.401035000	-0.354521000
C	-1.653684000	-2.527192000	-0.645209000
H	-2.166013000	-2.849988000	0.267852000
H	-2.400226000	-2.245835000	-1.395409000
H	-1.052605000	-3.357229000	-1.030689000

Sum of electronic and thermal Free Energies= -2584.488714

*Optimized structure and free energy for **1**-Ce^{IV}-**II***

O	4.354254000	1.633593000	0.555963000
C	5.499476000	2.430130000	0.181576000
H	5.982528000	2.839638000	1.076676000
H	6.225786000	1.812868000	-0.358393000
H	5.180165000	3.257885000	-0.461947000
O	2.090507000	0.486733000	-1.141792000
C	2.113050000	1.494996000	-1.866918000
O	2.445109000	1.375361000	-3.170317000
C	1.785682000	2.881728000	-1.369356000
H	0.737524000	3.129396000	-1.584168000
H	1.953466000	2.928483000	-0.294426000
C	2.354308000	2.577518000	-4.039373000
H	2.964742000	2.345709000	-4.908301000
H	1.310577000	2.704203000	-4.347522000
C	2.878638000	3.825284000	-3.353312000
O	2.666511000	3.884171000	-1.981711000
O	3.447139000	4.729804000	-3.941312000

Ce	3.207445000	-0.013807000	1.117232000
Fe	-0.540984000	-0.653790000	2.331346000
P	2.945259000	-3.637827000	1.098176000
P	2.419989000	2.683500000	3.171501000
N	2.098918000	-2.131664000	1.278806000
N	1.626404000	1.731285000	1.956058000
O	4.675510000	-1.435855000	0.301460000
O	3.785179000	0.098386000	3.233255000
C	0.797765000	-2.223541000	1.850519000
C	-0.437239000	-2.374849000	1.110848000
H	-0.520143000	-2.370324000	0.034578000
C	-1.502580000	-2.515797000	2.053321000
H	-2.549537000	-2.625671000	1.814997000
C	-0.946953000	-2.445177000	3.376845000
H	-1.506452000	-2.496355000	4.298451000
C	0.466936000	-2.264838000	3.260522000
H	1.172456000	-2.160035000	4.070657000
C	0.290920000	1.337128000	2.210245000
C	-0.678889000	1.105168000	1.165402000
H	-0.481009000	1.164612000	0.107250000
C	-1.939009000	0.812170000	1.781121000
H	-2.860726000	0.596719000	1.263176000
C	-1.756024000	0.825796000	3.202911000
H	-2.515783000	0.625140000	3.942608000
C	-0.378073000	1.118412000	3.472860000
H	0.078616000	1.169421000	4.450175000
C	4.141322000	-3.681277000	-0.286127000
C	4.301509000	-4.821680000	-1.086134000
H	3.695194000	-5.707565000	-0.924747000
C	5.262638000	-4.799215000	-2.095882000
H	5.409421000	-5.669472000	-2.724881000
C	6.036727000	-3.645137000	-2.297321000
H	6.783707000	-3.640649000	-3.085192000
C	5.878454000	-2.491637000	-1.519819000
C	4.904761000	-2.513838000	-0.491309000
C	3.064307000	1.855185000	4.684695000
C	2.920689000	2.416381000	5.961513000
H	2.406649000	3.363229000	6.099072000
C	3.460098000	1.741715000	7.056039000
H	3.370105000	2.159931000	8.051766000
C	4.122234000	0.518568000	6.862605000
H	4.541247000	0.003116000	7.721365000
C	4.261137000	-0.067293000	5.598647000
C	3.712473000	0.615617000	4.485496000
C	4.968526000	-1.381991000	5.395762000
H	4.289266000	-2.140697000	4.986637000
H	5.793531000	-1.281032000	4.681218000
H	5.372480000	-1.760049000	6.338638000
C	6.701984000	-1.251075000	-1.747624000
H	6.068417000	-0.403836000	-2.038680000
H	7.230213000	-0.953661000	-0.834267000

H	7.440673000	-1.410657000	-2.537618000
H	2.044780000	-4.726575000	0.891682000
H	3.633605000	-3.998793000	2.307368000
H	1.611397000	3.763568000	3.645149000
H	3.506574000	3.250873000	2.458216000

Sum of electronic and thermal Free Energies= -3039.989021

*Optimized structure and free energy for **1**-Ce^{IV}-**TS_{II-III}***

O	-0.163708000	-0.482912000	-0.011025000
C	0.960456000	0.438990000	0.002415000
H	0.661502000	1.391521000	0.451416000
H	1.789925000	0.007782000	0.571895000
H	1.282993000	0.626261000	-1.027396000
O	-2.552942000	-0.577302000	0.606313000
C	-1.510654000	-0.374583000	1.350667000
O	-1.322247000	0.897937000	1.848234000
C	-1.029709000	-1.494274000	2.244252000
H	-1.746856000	-1.631372000	3.064419000
H	-0.949963000	-2.411891000	1.669403000
C	-0.594957000	1.036541000	3.132824000
H	-0.193325000	2.046885000	3.136276000
H	-1.320868000	0.933432000	3.948051000
C	0.537360000	0.039392000	3.304289000
O	0.300879000	-1.226491000	2.796668000
O	1.593193000	0.305472000	3.860384000
Ce	-1.775394000	-0.987214000	-1.604447000
Fe	-4.035858000	-4.149807000	-2.103674000
P	-4.349505000	0.295699000	-3.778968000
P	0.484650000	-3.608603000	-1.189337000
N	-3.794823000	-1.047994000	-2.826479000
N	-1.186525000	-3.239802000	-0.901055000
O	-2.042849000	1.094189000	-2.223652000
O	-0.221893000	-1.498870000	-3.063010000
C	-4.526791000	-2.261778000	-2.929071000
C	-5.568881000	-2.690827000	-2.020489000
H	-5.872346000	-2.160056000	-1.130805000
C	-6.099032000	-3.923179000	-2.509608000
H	-6.874622000	-4.509639000	-2.041412000
C	-5.396528000	-4.272982000	-3.713509000
H	-5.560202000	-5.162181000	-4.302696000
C	-4.422603000	-3.258859000	-3.976240000
H	-3.726412000	-3.233547000	-4.801411000
C	-2.145332000	-4.262212000	-1.088546000
C	-3.235667000	-4.514840000	-0.174574000
H	-3.445539000	-3.940183000	0.713911000
C	-3.948553000	-5.662898000	-0.644494000
H	-4.817415000	-6.101457000	-0.178684000
C	-3.325864000	-6.116272000	-1.855600000
H	-3.646839000	-6.953416000	-2.456118000
C	-2.230822000	-5.241861000	-2.150946000
H	-1.577502000	-5.301561000	-3.008834000

C	-4.148650000	1.921231000	-2.965089000
C	-5.137369000	2.912814000	-3.032825000
H	-6.068794000	2.740127000	-3.562731000
C	-4.897391000	4.134329000	-2.404221000
H	-5.642123000	4.920531000	-2.444428000
C	-3.691488000	4.341084000	-1.716255000
H	-3.517348000	5.296545000	-1.231394000
C	-2.700806000	3.355191000	-1.622163000
C	-2.940889000	2.117639000	-2.264219000
C	1.094951000	-3.489037000	-2.921235000
C	1.952363000	-4.442692000	-3.487199000
H	2.289224000	-5.300833000	-2.913201000
C	2.377067000	-4.264032000	-4.804147000
H	3.047444000	-4.982715000	-5.260936000
C	1.934552000	-3.150190000	-5.535054000
H	2.274046000	-3.020579000	-6.558035000
C	1.064539000	-2.194942000	-4.993051000
C	0.634773000	-2.375169000	-3.657175000
C	0.585494000	-1.004996000	-5.783214000
H	-0.502266000	-1.034232000	-5.926849000
H	0.808316000	-0.067008000	-5.262152000
H	1.056797000	-0.973642000	-6.769032000
C	-1.421855000	3.575368000	-0.858423000
H	-1.374253000	2.919147000	0.019309000
H	-0.547068000	3.350542000	-1.479159000
H	-1.345341000	4.611315000	-0.517281000
H	-5.728836000	0.166338000	-4.117712000
H	-3.680912000	0.330362000	-5.047685000
H	0.851590000	-4.908345000	-0.726939000
H	1.166686000	-2.657372000	-0.385324000

Sum of electronic and thermal Free Energies= -3039.971040

*Optimized structure and free energy for **1**-Ce^{IV}-**III***

O	1.121395000	2.460394000	0.776483000
C	1.102806000	3.181989000	2.059595000
H	0.101578000	3.025883000	2.460290000
H	1.852816000	2.759929000	2.728977000
H	1.292162000	4.243579000	1.889623000
O	2.065506000	1.391449000	-0.941852000
C	2.382958000	2.359232000	-0.017421000
O	3.401142000	1.956093000	0.916294000
C	2.742039000	3.686181000	-0.681912000
H	3.438663000	3.492859000	-1.503457000
H	1.851884000	4.177261000	-1.067509000
C	4.679979000	2.679845000	0.856465000
H	5.256893000	2.332597000	1.710819000
H	5.218313000	2.428040000	-0.065922000
C	4.457026000	4.176265000	0.967441000
O	3.340147000	4.633692000	0.269020000
O	5.147737000	4.946749000	1.616051000
Ce	0.104896000	0.440922000	-0.358339000

Fe	-0.188533000	-0.077276000	-4.246081000
P	0.358071000	-3.130464000	-0.647017000
P	-2.399177000	2.842263000	-1.311541000
N	0.162248000	-1.627653000	-1.499706000
N	-1.173912000	1.763158000	-1.874000000
O	0.813450000	-0.961803000	1.169614000
O	-1.722262000	0.919319000	0.760039000
C	0.251121000	-1.660378000	-2.920552000
C	1.429013000	-1.336345000	-3.697277000
H	2.366163000	-0.992195000	-3.286268000
C	1.111970000	-1.528301000	-5.077195000
H	1.773221000	-1.347877000	-5.910691000
C	-0.250855000	-1.973998000	-5.170104000
H	-0.782379000	-2.188956000	-6.084460000
C	-0.790681000	-2.050250000	-3.846330000
H	-1.796036000	-2.335909000	-3.575264000
C	-0.943077000	1.643424000	-3.268495000
C	0.291743000	1.969704000	-3.945902000
H	1.189672000	2.317279000	-3.459849000
C	0.110739000	1.707826000	-5.340098000
H	0.857198000	1.831802000	-6.109578000
C	-1.227133000	1.227013000	-5.540683000
H	-1.657171000	0.932442000	-6.485490000
C	-1.877313000	1.165521000	-4.266086000
H	-2.881654000	0.818301000	-4.073285000
C	1.648821000	-3.128160000	0.652501000
C	2.531362000	-4.198229000	0.851329000
H	2.493094000	-5.081662000	0.221647000
C	3.463768000	-4.104291000	1.885057000
H	4.156775000	-4.917752000	2.065578000
C	3.504683000	-2.953679000	2.688466000
H	4.234812000	-2.895597000	3.489624000
C	2.641250000	-1.867395000	2.493173000
C	1.694872000	-1.963907000	1.446576000
C	-3.592317000	2.099286000	-0.133414000
C	-4.958390000	2.411892000	-0.158156000
H	-5.363197000	3.096182000	-0.897529000
C	-5.793775000	1.827708000	0.794622000
H	-6.853151000	2.056054000	0.799753000
C	-5.259212000	0.943796000	1.745025000
H	-5.919460000	0.498694000	2.482793000
C	-3.899300000	0.608748000	1.776145000
C	-3.051165000	1.201270000	0.810363000
C	-3.330316000	-0.346788000	2.792279000
H	-2.909969000	-1.238546000	2.310733000
H	-2.513370000	0.115222000	3.358076000
H	-4.099425000	-0.671420000	3.497850000
C	2.703525000	-0.626583000	3.343695000
H	2.970431000	0.246646000	2.736321000
H	1.731528000	-0.415407000	3.805111000
H	3.444437000	-0.736575000	4.140276000

H	0.651215000	-4.204220000	-1.537278000
H	-0.884638000	-3.491658000	-0.036403000
H	-3.157334000	3.395117000	-2.384760000
H	-1.799624000	3.977866000	-0.672037000

Sum of electronic and thermal Free Energies= -3039.978164

*Optimized structure and free energy for **1**-Ce^{IV}-**IV***

O	1.883096000	3.366598000	-1.045711000
C	1.987500000	4.792553000	-0.697052000
H	1.811870000	5.313463000	-1.637030000
H	1.224519000	5.068755000	0.036110000
H	2.977334000	5.040976000	-0.309737000
O	2.026411000	1.147065000	-0.645855000
C	2.058850000	2.378807000	-0.058417000
O	0.772911000	2.416364000	0.830002000
C	3.259981000	2.559727000	0.867682000
H	3.430626000	1.629380000	1.415009000
H	4.150787000	2.807965000	0.292925000
C	0.939896000	2.563894000	2.284859000
H	-0.033374000	2.842844000	2.685403000
H	1.249173000	1.610700000	2.732926000
C	1.946181000	3.648643000	2.619015000
O	3.076151000	3.670511000	1.814028000
O	1.807677000	4.462520000	3.521024000
Ce	0.052554000	0.132845000	-0.341025000
Fe	-0.033783000	-0.063863000	-4.197794000
P	0.479518000	-3.401357000	-0.845467000
P	-2.165738000	2.800516000	-1.085781000
N	0.251397000	-1.850155000	-1.587074000
N	-1.177732000	1.548486000	-1.750383000
O	0.784428000	-1.310570000	1.163155000
O	-1.734550000	0.572265000	0.826512000
C	0.402984000	-1.748406000	-2.999033000
C	1.601801000	-1.317630000	-3.688714000
H	2.509098000	-0.981824000	-3.209310000
C	1.349807000	-1.394514000	-5.092841000
H	2.037955000	-1.115991000	-5.875949000
C	0.008867000	-1.872415000	-5.286691000
H	-0.475394000	-2.020068000	-6.239766000
C	-0.584532000	-2.084325000	-4.001873000
H	-1.589610000	-2.424896000	-3.803173000
C	-0.880979000	1.555317000	-3.137925000
C	0.363156000	1.980355000	-3.743921000
H	1.217791000	2.348635000	-3.196681000
C	0.236284000	1.806413000	-5.156169000
H	1.001765000	2.009317000	-5.889388000
C	-1.074700000	1.289501000	-5.438268000
H	-1.458842000	1.044284000	-6.416499000
C	-1.766002000	1.117982000	-4.197373000
H	-2.762749000	0.726614000	-4.060339000
C	1.679522000	-3.435701000	0.539775000

C	2.564433000	-4.507293000	0.724372000
H	2.583955000	-5.341979000	0.030400000
C	3.421816000	-4.484496000	1.824023000
H	4.113480000	-5.301821000	1.990752000
C	3.384636000	-3.399488000	2.713053000
H	4.051382000	-3.395502000	3.569653000
C	2.518932000	-2.312909000	2.535070000
C	1.650890000	-2.330410000	1.416922000
C	-3.373208000	2.183187000	0.152169000
C	-4.648977000	2.755710000	0.258707000
H	-4.950969000	3.571024000	-0.391654000
C	-5.530741000	2.261165000	1.219643000
H	-6.519631000	2.692605000	1.321372000
C	-5.135066000	1.201126000	2.049370000
H	-5.829439000	0.823032000	2.793066000
C	-3.871563000	0.605988000	1.949459000
C	-2.972230000	1.111952000	0.979234000
C	-3.453620000	-0.540403000	2.833020000
H	-3.240017000	-1.440267000	2.242937000
H	-2.536827000	-0.304204000	3.385326000
H	-4.237718000	-0.784140000	3.554530000
C	2.496290000	-1.151044000	3.493760000
H	2.876393000	-0.236813000	3.018169000
H	1.477334000	-0.939144000	3.836736000
H	3.119865000	-1.351539000	4.368859000
H	0.898267000	-4.383314000	-1.789767000
H	-0.776275000	-3.882447000	-0.354685000
H	-2.918739000	3.475296000	-2.090972000
H	-1.365222000	3.826637000	-0.485322000

Sum of electronic and thermal Free Energies= -3039.973245

*Optimized structure and free energy for **1**-Ce^{IV}-**$TS_{IV\text{-}V}$***

O	-1.374448000	2.776180000	2.679216000
C	-1.715869000	4.157753000	2.288072000
H	-2.561344000	4.537172000	2.862399000
H	-0.814174000	4.724903000	2.510057000
H	-1.938512000	4.195106000	1.220199000
O	-1.769407000	0.600803000	3.052055000
C	-2.279202000	1.745858000	2.625341000
O	-2.451363000	1.418900000	0.862909000
C	-3.731663000	2.000693000	2.996503000
H	-4.269700000	1.051544000	2.943528000
H	-3.795547000	2.393369000	4.012655000
C	-3.776063000	1.546991000	0.264021000
H	-3.658129000	1.666148000	-0.814720000
H	-4.370379000	0.642707000	0.454020000
C	-4.506888000	2.766336000	0.791524000
O	-4.381699000	3.007900000	2.156543000
O	-5.173674000	3.523536000	0.100237000
Ce	-1.203488000	-0.636818000	1.163103000
Fe	1.993785000	-1.001620000	3.239451000

P	-2.028013000	-3.522499000	3.133139000
P	1.144824000	1.018967000	-0.905951000
N	-0.762542000	-2.493202000	2.533859000
N	0.829145000	0.468015000	0.697517000
O	-3.133626000	-1.705426000	1.115923000
O	-0.882652000	-1.021045000	-0.987380000
C	0.404710000	-2.405771000	3.347439000
C	0.530738000	-1.689012000	4.602585000
H	-0.224410000	-1.048414000	5.032771000
C	1.836517000	-1.946900000	5.122376000
H	2.246992000	-1.540266000	6.033831000
C	2.529771000	-2.803606000	4.199541000
H	3.545034000	-3.153297000	4.306638000
C	1.656768000	-3.086506000	3.103106000
H	1.873835000	-3.700704000	2.242589000
C	1.859430000	0.415895000	1.661675000
C	1.828427000	1.100070000	2.933853000
H	1.012101000	1.717455000	3.276898000
C	3.043961000	0.793812000	3.619672000
H	3.317898000	1.139488000	4.604635000
C	3.832782000	-0.072297000	2.787918000
H	4.797203000	-0.484917000	3.041339000
C	3.100067000	-0.327567000	1.585239000
H	3.408949000	-0.959104000	0.765257000
C	-3.263783000	-3.969591000	1.861849000
C	-3.771087000	-5.274452000	1.770581000
H	-3.423763000	-6.056640000	2.438355000
C	-4.736230000	-5.550831000	0.803249000
H	-5.146100000	-6.550090000	0.715226000
C	-5.170939000	-4.531681000	-0.058182000
H	-5.922437000	-4.758377000	-0.808056000
C	-4.665369000	-3.227243000	0.007691000
C	-3.687978000	-2.942207000	0.992025000
C	1.041705000	-0.285097000	-2.191441000
C	1.966790000	-0.402884000	-3.236900000
H	2.793878000	0.293837000	-3.333905000
C	1.800818000	-1.436225000	-4.159885000
H	2.498180000	-1.547096000	-4.982012000
C	0.730653000	-2.333515000	-4.018682000
H	0.614474000	-3.134408000	-4.742216000
C	-0.196474000	-2.238948000	-2.972049000
C	-0.033442000	-1.187076000	-2.040122000
C	-1.336933000	-3.211559000	-2.821990000
H	-1.291327000	-3.735556000	-1.859549000
H	-2.304230000	-2.696724000	-2.854422000
H	-1.320280000	-3.959425000	-3.619082000
C	-5.135170000	-2.142409000	-0.926290000
H	-5.670964000	-1.354046000	-0.382317000
H	-4.291305000	-1.663967000	-1.436142000
H	-5.813511000	-2.544096000	-1.683589000
H	-2.688299000	-2.926403000	4.259584000

H	-1.519519000	-4.750835000	3.652922000
H	2.421148000	1.641865000	-1.028331000
H	0.183751000	2.030333000	-1.210800000

Sum of electronic and thermal Free Energies= -3039.972509

*Optimized structure and free energy for **1**-Ce^{IV}-**V***

O	6.085993000	3.564120000	1.253246000
C	5.128390000	4.571586000	0.739783000
H	5.525674000	5.021681000	-0.171006000
H	4.219494000	4.009123000	0.541422000
H	4.966578000	5.343172000	1.494129000
O	7.723516000	5.169322000	1.430979000
C	7.351477000	4.001251000	1.522289000
O	5.482300000	-0.098393000	3.546350000
C	8.257619000	2.889753000	2.017573000
H	9.275487000	3.102360000	1.695742000
H	8.231799000	2.843027000	3.111335000
C	6.334340000	1.002523000	3.278615000
H	5.774694000	1.944847000	3.208541000
H	7.093631000	1.117544000	4.068281000
C	7.025191000	0.741015000	1.943383000
O	7.937955000	1.587308000	1.422498000
O	6.769000000	-0.308130000	1.312511000
Ce	5.115023000	-1.925789000	2.437584000
Fe	3.605840000	-2.301107000	-1.211874000
P	6.850935000	-4.847311000	1.143055000
P	2.012838000	-0.432121000	2.766998000
N	5.764186000	-3.534081000	0.809782000
N	3.208276000	-0.719629000	1.548003000
O	6.718695000	-3.049451000	3.433322000
O	3.454815000	-2.796785000	3.588522000
C	5.181352000	-3.518995000	-0.488311000
C	5.645159000	-2.723081000	-1.604540000
H	6.445556000	-2.000176000	-1.556359000
C	4.849803000	-3.058186000	-2.743490000
H	4.933798000	-2.620278000	-3.726468000
C	3.890980000	-4.053570000	-2.349461000
H	3.137835000	-4.490393000	-2.987463000
C	4.083761000	-4.337601000	-0.960640000
H	3.511980000	-5.028688000	-0.358989000
C	2.785573000	-0.936836000	0.216412000
C	3.319306000	-0.223133000	-0.919845000
H	4.104442000	0.515155000	-0.871242000
C	2.617186000	-0.661352000	-2.086586000
H	2.791987000	-0.321473000	-3.095957000
C	1.658690000	-1.654391000	-1.690335000
H	0.989305000	-2.185384000	-2.349816000
C	1.770720000	-1.845113000	-0.275294000
H	1.198793000	-2.536632000	0.325662000
C	8.249612000	-4.440356000	2.254228000
C	9.526001000	-4.989151000	2.062764000

H	9.733589000	-5.643376000	1.221603000
C	10.529760000	-4.679358000	2.980001000
H	11.523984000	-5.092093000	2.855535000
C	10.248916000	-3.831764000	4.063567000
H	11.037121000	-3.604224000	4.774511000
C	8.985161000	-3.263250000	4.261974000
C	7.966232000	-3.572197000	3.328496000
C	1.241035000	-1.900407000	3.558682000
C	-0.134043000	-2.000980000	3.811338000
H	-0.812255000	-1.198837000	3.535834000
C	-0.616894000	-3.151508000	4.435030000
H	-1.674666000	-3.250952000	4.649296000
C	0.272612000	-4.179825000	4.787428000
H	-0.114762000	-5.068201000	5.276876000
C	1.647191000	-4.105303000	4.528619000
C	2.137996000	-2.939797000	3.892350000
C	2.598532000	-5.211579000	4.903182000
H	3.071341000	-5.648141000	4.014159000
H	3.409922000	-4.836498000	5.537221000
H	2.079816000	-6.010498000	5.439724000
C	8.683648000	-2.355574000	5.425932000
H	8.358798000	-1.364024000	5.087402000
H	7.866205000	-2.755222000	6.037330000
H	9.562770000	-2.230657000	6.063569000
H	7.419474000	-5.375929000	-0.054445000
H	6.144792000	-5.964933000	1.703452000
H	0.939664000	0.400467000	2.323996000
H	2.727348000	0.293419000	3.759593000

Sum of electronic and thermal Free Energies= -3040.000937

*Optimized structure and free energy for **1**-Ce^{IV}-**VI***

O	4.445103000	1.633063000	0.684168000
C	5.673842000	2.333780000	0.405874000
H	6.152009000	2.644660000	1.342414000
H	6.364718000	1.683248000	-0.141634000
H	5.466191000	3.223621000	-0.199911000
Ce	3.197664000	0.023435000	1.116329000
Fe	-0.542457000	-0.641725000	2.380774000
P	2.960798000	-3.599047000	1.156861000
P	2.421883000	2.689059000	3.185333000
N	2.063829000	-2.112905000	1.248871000
N	1.625871000	1.726137000	1.984438000
O	4.664141000	-1.425175000	0.288567000
O	3.743506000	0.055962000	3.256544000
C	0.792084000	-2.210017000	1.888032000
C	-0.474650000	-2.402984000	1.214743000
H	-0.610571000	-2.444948000	0.144898000
C	-1.493124000	-2.523407000	2.210133000
H	-2.548516000	-2.653334000	2.025430000
C	-0.876628000	-2.402656000	3.502000000
H	-1.390945000	-2.429410000	4.450502000

C	0.528252000	-2.209347000	3.312401000
H	1.268517000	-2.066378000	4.085403000
C	0.288162000	1.347211000	2.235068000
C	-0.676012000	1.107433000	1.188016000
H	-0.472300000	1.181873000	0.132082000
C	-1.938751000	0.819064000	1.799918000
H	-2.858950000	0.601579000	1.280009000
C	-1.764002000	0.848198000	3.222428000
H	-2.527713000	0.654865000	3.959808000
C	-0.387684000	1.143191000	3.496682000
H	0.064831000	1.202353000	4.475516000
C	4.122742000	-3.678825000	-0.253306000
C	4.268191000	-4.832065000	-1.038490000
H	3.671375000	-5.718189000	-0.845515000
C	5.202748000	-4.821409000	-2.073299000
H	5.338701000	-5.700965000	-2.691724000
C	5.968008000	-3.667512000	-2.310632000
H	6.695395000	-3.672865000	-3.116768000
C	5.827070000	-2.503552000	-1.545755000
C	4.878535000	-2.511023000	-0.492631000
C	3.079361000	1.855408000	4.691648000
C	2.966149000	2.433772000	5.964639000
H	2.474651000	3.393460000	6.097146000
C	3.504441000	1.761566000	7.061273000
H	3.436249000	2.194293000	8.052615000
C	4.137405000	0.521945000	6.874109000
H	4.557146000	0.007869000	7.733454000
C	4.245132000	-0.081448000	5.615844000
C	3.696681000	0.597838000	4.498675000
C	4.922022000	-1.413363000	5.420633000
H	4.221898000	-2.162894000	5.029626000
H	5.739749000	-1.338645000	4.694370000
H	5.329994000	-1.788487000	6.363066000
C	6.646778000	-1.266797000	-1.806399000
H	6.007737000	-0.408468000	-2.048971000
H	7.228045000	-0.985329000	-0.920253000
H	7.340100000	-1.423203000	-2.637112000
H	2.100420000	-4.732301000	1.034916000
H	3.690729000	-3.859699000	2.367417000
H	1.608655000	3.760492000	3.670114000
H	3.498355000	3.266057000	2.465033000
O	2.107896000	0.416935000	-1.091214000
C	2.052309000	1.789701000	-1.698787000
C	1.486545000	-0.577196000	-2.021664000
C	1.110982000	1.641064000	-2.895959000
H	1.700397000	2.463086000	-0.916637000
H	3.071985000	2.053842000	-1.988814000
C	1.330232000	0.177639000	-3.343637000
H	2.153532000	-1.438484000	-2.070947000
H	0.528550000	-0.872876000	-1.584700000
H	1.341838000	2.358527000	-3.687979000

H	0.068979000	1.798009000	-2.593535000
H	2.243266000	0.094298000	-3.943546000
H	0.498082000	-0.207324000	-3.939319000

Sum of electronic and thermal Free Energies= -2816.79348

*Optimized structures and free energies for ligand set **2***

*Optimized structure and free energy for **2**-Ce^{III}-**I***

C	-0.121091000	0.201184000	0.132950000
H	0.446611000	0.865438000	-0.530865000
H	-1.191221000	0.429650000	0.011056000
C	0.141246000	-1.260142000	-0.253543000
H	-0.494866000	-1.903262000	0.370658000
H	-0.140383000	-1.427665000	-1.303798000
N	0.334041000	0.428009000	1.517494000
N	1.562015000	-1.623389000	-0.011412000
Ce	2.847447000	-0.092455000	1.693837000
C	-0.521937000	0.809473000	2.423916000
C	2.031720000	-2.648120000	-0.674509000
H	1.374396000	-3.117553000	-1.420160000
H	-1.560208000	0.988102000	2.109572000
C	-0.282975000	1.028991000	3.831947000
C	-1.379105000	1.486238000	4.607766000
C	0.976405000	0.792128000	4.471993000
C	-1.251402000	1.712287000	5.967632000
H	-2.331260000	1.660190000	4.112320000
C	1.098619000	1.023542000	5.874234000
C	-0.008170000	1.477514000	6.588118000
H	-2.094691000	2.064846000	6.551150000
H	0.095524000	1.653231000	7.655677000
C	3.316339000	-3.296240000	-0.554084000
C	3.582878000	-4.363346000	-1.451980000
C	4.294311000	-2.958186000	0.435183000
C	4.768486000	-5.074465000	-1.390655000
H	2.832304000	-4.617096000	-2.196766000
C	5.509352000	-3.703146000	0.500085000
C	5.722651000	-4.735238000	-0.409902000
H	4.963217000	-5.885521000	-2.083648000
H	6.653330000	-5.294171000	-0.357225000
C	6.528287000	-3.340741000	1.549751000
H	7.401300000	-3.998469000	1.494321000
H	6.868262000	-2.304220000	1.431677000
H	6.102042000	-3.412761000	2.557834000
C	2.427732000	0.771157000	6.538861000
H	3.214722000	1.399836000	6.103767000
H	2.376214000	0.976429000	7.612674000
H	2.750523000	-0.267718000	6.398568000
O	2.036977000	0.354215000	3.785055000
O	4.087167000	-1.964060000	1.301978000
O	3.590342000	1.538941000	0.547098000
C	4.118337000	2.630526000	-0.210296000

H	3.491669000	3.526638000	-0.098906000
H	5.133961000	2.884133000	0.123991000
H	4.167459000	2.378828000	-1.279057000

Sum of electronic and thermal Free Energies= -1546.643687

*Optimized structure and free energy for **2**-Ce^{III}-**II***

C	-0.508413000	-0.221937000	0.065608000
H	-0.074382000	0.382675000	-0.736116000
H	-1.605529000	-0.137262000	0.016632000
C	-0.104067000	-1.692073000	-0.124675000
H	-0.611901000	-2.290648000	0.644865000
H	-0.445413000	-2.050370000	-1.107966000
N	0.018287000	0.255044000	1.359994000
N	1.361813000	-1.867973000	0.036310000
Ce	2.633520000	0.077888000	1.410688000
C	-0.819302000	0.511809000	2.326537000
C	1.895041000	-2.919079000	-0.523797000
H	1.245813000	-3.564647000	-1.133479000
H	-1.895542000	0.478568000	2.101350000
C	-0.508925000	0.813809000	3.705277000
C	-1.579770000	1.217142000	4.543137000
C	0.797509000	0.650309000	4.268113000
C	-1.379210000	1.474042000	5.888826000
H	-2.570453000	1.324768000	4.107772000
C	0.992834000	0.901806000	5.659130000
C	-0.089157000	1.312797000	6.433806000
H	-2.202540000	1.789283000	6.520460000
H	0.069975000	1.508074000	7.491197000
C	3.258687000	-3.394203000	-0.438485000
C	3.576925000	-4.565353000	-1.173054000
C	4.270624000	-2.780439000	0.364068000
C	4.843988000	-5.122104000	-1.125321000
H	2.800670000	-5.026518000	-1.779077000
C	5.570558000	-3.364446000	0.418427000
C	5.830912000	-4.513657000	-0.324784000
H	5.076335000	-6.016873000	-1.692473000
H	6.825712000	-4.949540000	-0.282082000
C	6.624613000	-2.710645000	1.274483000
H	7.568212000	-3.263405000	1.228021000
H	6.810596000	-1.677759000	0.955060000
H	6.304988000	-2.654691000	2.322183000
C	2.369926000	0.716901000	6.242626000
H	3.099863000	1.373549000	5.752960000
H	2.375333000	0.931826000	7.315838000
H	2.729385000	-0.308000000	6.090425000
O	1.831286000	0.247851000	3.524075000
O	4.026036000	-1.667464000	1.063313000
O	3.979527000	1.840063000	1.492020000
C	4.924780000	2.613761000	2.248980000
H	4.562756000	2.793330000	3.271124000
H	5.895941000	2.103564000	2.313126000

H	5.097469000	3.596041000	1.779291000
O	2.235919000	1.178819000	-1.006915000
C	2.724809000	2.109751000	-1.685324000
O	2.562924000	2.095804000	-3.038876000
C	3.494124000	3.254785000	-1.085181000
H	2.817528000	4.080111000	-0.828755000
H	3.967029000	2.879702000	-0.162366000
C	2.973157000	3.290806000	-3.806245000
H	3.077278000	2.951042000	-4.833750000
H	2.169866000	4.034441000	-3.748512000
C	4.285497000	3.885806000	-3.328777000
O	4.549677000	3.753402000	-1.984213000
O	5.066581000	4.464588000	-4.085361000

Sum of electronic and thermal Free Energies= -2002.140524

*Optimized structure and free energy for **2**-Ce^{III}-**TS_{II-III}***

C	-0.614237000	-0.236690000	0.069881000
H	-0.174946000	0.426237000	-0.682086000
H	-1.710732000	-0.150525000	0.017684000
C	-0.203566000	-1.689070000	-0.213862000
H	-0.737308000	-2.343952000	0.489231000
H	-0.507135000	-1.971842000	-1.232891000
N	-0.097895000	0.158480000	1.395065000
N	1.257524000	-1.880440000	-0.014417000
Ce	2.483045000	0.004128000	1.395095000
C	-0.933951000	0.409038000	2.362819000
C	1.795737000	-2.931617000	-0.570611000
H	1.159385000	-3.558085000	-1.212101000
H	-2.009853000	0.394418000	2.136573000
C	-0.617606000	0.692503000	3.744703000
C	-1.693550000	1.026004000	4.605762000
C	0.705445000	0.603757000	4.281863000
C	-1.483028000	1.276127000	5.951531000
H	-2.696288000	1.083943000	4.189256000
C	0.914070000	0.851464000	5.670148000
C	-0.176262000	1.185316000	6.470880000
H	-2.311435000	1.534899000	6.601835000
H	-0.008854000	1.376316000	7.527688000
C	3.146779000	-3.429809000	-0.439021000
C	3.485927000	-4.578048000	-1.199852000
C	4.122521000	-2.865636000	0.440769000
C	4.740114000	-5.157364000	-1.105747000
H	2.736900000	-5.002346000	-1.864105000
C	5.407049000	-3.474819000	0.545331000
C	5.690255000	-4.598380000	-0.228324000
H	4.989752000	-6.033395000	-1.694316000
H	6.673606000	-5.054253000	-0.147333000
C	6.421660000	-2.876532000	1.485542000
H	7.350002000	-3.456333000	1.483545000
H	6.659205000	-1.841919000	1.207824000
H	6.036530000	-2.839248000	2.511656000

C	2.310785000	0.744506000	6.226227000
H	2.990031000	1.450541000	5.732526000
H	2.322976000	0.947506000	7.301629000
H	2.728727000	-0.255166000	6.056162000
O	1.749641000	0.279538000	3.509746000
O	3.851418000	-1.777644000	1.170798000
O	3.783942000	1.888291000	1.128898000
C	4.882700000	2.540202000	1.795088000
H	5.048557000	2.102350000	2.790727000
H	5.818558000	2.430490000	1.226528000
H	4.685664000	3.611613000	1.926214000
O	2.112036000	1.325255000	-0.778376000
C	3.027760000	2.178946000	-0.916048000
O	4.128718000	1.827678000	-1.645039000
C	2.750628000	3.649510000	-0.736002000
H	2.181045000	4.015568000	-1.600750000
H	2.175984000	3.797542000	0.172671000
C	5.126402000	2.839067000	-2.023900000
H	6.097788000	2.359394000	-1.916615000
H	4.966119000	3.079865000	-3.081323000
C	5.121523000	4.119715000	-1.212488000
O	3.951534000	4.479174000	-0.590586000
O	6.112291000	4.838992000	-1.143664000

Sum of electronic and thermal Free Energies= -2002.136747

*Optimized structure and free energy for **2**-Ce^{III}-**III***

C	-0.654728000	-0.345282000	0.034371000
H	-0.195234000	0.342637000	-0.686162000
H	-1.748309000	-0.258618000	-0.053755000
C	-0.222940000	-1.786455000	-0.271548000
H	-0.769472000	-2.464325000	0.398723000
H	-0.489492000	-2.047364000	-1.306084000
N	-0.181128000	0.019959000	1.382602000
N	1.235521000	-1.958856000	-0.031814000
Ce	2.370601000	-0.077876000	1.395399000
C	-1.034398000	0.298587000	2.326294000
C	1.808858000	-2.993167000	-0.589621000
H	1.198038000	-3.621814000	-1.252436000
H	-2.104581000	0.297960000	2.076045000
C	-0.741997000	0.607222000	3.707908000
C	-1.840473000	0.915146000	4.550045000
C	0.578690000	0.590569000	4.259336000
C	-1.655853000	1.202515000	5.892037000
H	-2.839801000	0.922758000	4.121781000
C	0.760983000	0.880382000	5.642437000
C	-0.352110000	1.181492000	6.425324000
H	-2.501608000	1.439450000	6.527993000
H	-0.204377000	1.403957000	7.478811000
C	3.164723000	-3.465429000	-0.437489000
C	3.537160000	-4.607313000	-1.193994000
C	4.118086000	-2.880550000	0.453864000

C	4.801088000	-5.160116000	-1.082598000
H	2.806054000	-5.046904000	-1.868022000
C	5.413844000	-3.461869000	0.574454000
C	5.728834000	-4.580105000	-0.194083000
H	5.076849000	-6.031085000	-1.666776000
H	6.720399000	-5.015237000	-0.101275000
C	6.405130000	-2.841279000	1.524860000
H	7.340518000	-3.409111000	1.543801000
H	6.635088000	-1.807241000	1.238711000
H	6.002582000	-2.798842000	2.544041000
C	2.154846000	0.853380000	6.215115000
H	2.806039000	1.577333000	5.709686000
H	2.145128000	1.085469000	7.284537000
H	2.620886000	-0.129870000	6.077197000
O	1.647234000	0.300502000	3.504070000
O	3.812353000	-1.801333000	1.182850000
O	4.056206000	1.857168000	1.144573000
C	5.407423000	2.294393000	1.504986000
H	5.648819000	1.772688000	2.431990000
H	6.107803000	2.016178000	0.716052000
H	5.426314000	3.375224000	1.666078000
O	2.309781000	1.595351000	-0.263135000
C	3.442431000	2.320988000	-0.147349000
O	4.463743000	2.014399000	-1.147494000
C	3.158772000	3.826861000	-0.116191000
H	2.382955000	4.046236000	-0.854922000
H	2.820425000	4.131606000	0.871715000
C	4.653059000	3.023515000	-2.185622000
H	5.468330000	2.668248000	-2.812914000
H	3.748636000	3.126474000	-2.801266000
C	5.037096000	4.354449000	-1.566453000
O	4.348922000	4.654053000	-0.399522000
O	5.889931000	5.118151000	-2.004714000

Sum of electronic and thermal Free Energies= -2002.145223

*Optimized structure and free energy for **2**-Ce^{III}-**IV***

C	-0.373838000	-0.214713000	-0.167658000
H	0.202742000	0.403127000	-0.866749000
H	-1.444226000	-0.010785000	-0.322046000
C	-0.086770000	-1.700151000	-0.425732000
H	-0.752188000	-2.301726000	0.208953000
H	-0.304432000	-1.948528000	-1.474245000
N	0.059372000	0.121238000	1.200844000
N	1.323464000	-2.030975000	-0.078565000
Ce	2.577333000	-0.223142000	1.336005000
C	-0.803716000	0.521711000	2.088427000
C	1.792138000	-3.161040000	-0.536985000
H	1.146387000	-3.753492000	-1.199964000
H	-1.851254000	0.644499000	1.779395000
C	-0.546705000	0.819735000	3.480304000
C	-1.635775000	1.283012000	4.259951000

C	0.729080000	0.637076000	4.101073000
C	-1.483371000	1.563483000	5.608081000
H	-2.601971000	1.416727000	3.779698000
C	0.877429000	0.916480000	5.489889000
C	-0.224417000	1.374964000	6.210655000
H	-2.321520000	1.920583000	6.196262000
H	-0.103150000	1.589569000	7.269150000
C	3.066777000	-3.785596000	-0.267113000
C	3.334604000	-5.015240000	-0.921945000
C	4.030308000	-3.261309000	0.648782000
C	4.508058000	-5.711573000	-0.686407000
H	2.595937000	-5.408088000	-1.616208000
C	5.228911000	-3.988817000	0.900315000
C	5.444587000	-5.190480000	0.228158000
H	4.705132000	-6.649599000	-1.193511000
H	6.363117000	-5.738773000	0.419837000
C	6.227904000	-3.433365000	1.882660000
H	7.082592000	-4.107073000	1.997974000
H	6.602335000	-2.453642000	1.560171000
H	5.770714000	-3.279252000	2.867385000
C	2.222909000	0.707475000	6.136557000
H	2.991532000	1.336448000	5.670362000
H	2.186615000	0.942279000	7.204836000
H	2.561334000	-0.329052000	6.019398000
O	1.786974000	0.197011000	3.403983000
O	3.822664000	-2.097851000	1.278054000
O	2.777258000	2.577449000	1.033520000
C	3.328202000	3.623497000	1.904274000
H	2.563245000	3.790756000	2.661815000
H	4.258932000	3.288499000	2.366651000
H	3.503203000	4.542250000	1.337547000
O	2.871284000	1.110000000	-0.675202000
C	3.586734000	2.060946000	-0.069069000
O	4.738324000	1.404195000	0.735469000
C	4.181199000	3.112078000	-1.003119000
H	4.383131000	2.632957000	-1.964314000
H	3.486018000	3.937728000	-1.148225000
C	6.033861000	1.431498000	0.072225000
H	6.749118000	0.936618000	0.727323000
H	5.994594000	0.895839000	-0.886840000
C	6.452632000	2.877414000	-0.127895000
O	5.421066000	3.730509000	-0.496635000
O	7.586649000	3.310230000	0.040424000

Sum of electronic and thermal Free Energies= -2002.139323

*Optimized structure and free energy for **2**-Ce^{III}-**$TS_{IV\text{-}V}$***

C	0.028649000	0.474588000	-0.158635000
H	0.005655000	0.500762000	0.936734000
H	1.058346000	0.673349000	-0.492655000
C	-0.415712000	-0.908386000	-0.655063000
H	-0.293105000	-0.946096000	-1.746417000

H	0.225636000	-1.686420000	-0.216514000
N	-0.916255000	1.490906000	-0.657137000
N	-1.849439000	-1.154577000	-0.334517000
Ce	-3.231457000	0.986625000	0.310205000
C	-0.506500000	2.438619000	-1.449087000
C	-2.257403000	-2.393909000	-0.377760000
H	-1.510944000	-3.175293000	-0.578339000
H	0.562769000	2.484629000	-1.699162000
C	-1.314097000	3.467427000	-2.068383000
C	-0.645812000	4.447883000	-2.843461000
C	-2.738059000	3.519671000	-1.953883000
C	-1.349441000	5.456241000	-3.482934000
H	0.437256000	4.398921000	-2.926974000
C	-3.457622000	4.551922000	-2.619743000
C	-2.752484000	5.497208000	-3.363809000
H	-0.829838000	6.205714000	-4.070010000
H	-3.306882000	6.286050000	-3.865567000
C	-3.601620000	-2.906359000	-0.230791000
C	-3.768189000	-4.312333000	-0.319625000
C	-4.753791000	-2.079301000	-0.057217000
C	-5.024186000	-4.891543000	-0.246660000
H	-2.886137000	-4.934292000	-0.451476000
C	-6.044656000	-2.677948000	0.000774000
C	-6.153358000	-4.064457000	-0.090461000
H	-5.140736000	-5.967541000	-0.313646000
H	-7.140756000	-4.515356000	-0.040135000
C	-7.253626000	-1.793009000	0.164722000
H	-7.326206000	-1.065296000	-0.652459000
H	-8.174091000	-2.384375000	0.184526000
H	-7.198564000	-1.210583000	1.092831000
C	-4.959116000	4.592718000	-2.494437000
H	-5.267780000	4.690977000	-1.446393000
H	-5.378379000	5.431953000	-3.058053000
H	-5.412953000	3.665108000	-2.863734000
O	-3.409772000	2.606283000	-1.236970000
O	-4.638724000	-0.748490000	0.051151000
O	-2.117886000	3.076574000	2.802327000
C	-2.675798000	4.321764000	3.348419000
H	-2.646191000	4.326904000	4.439257000
H	-2.035165000	5.103224000	2.942842000
H	-3.701560000	4.448948000	2.998515000
O	-2.066898000	0.859638000	2.472528000
C	-2.638729000	1.830085000	3.121272000
O	-4.298294000	1.968543000	2.316639000
C	-3.073041000	1.532645000	4.546353000
H	-3.409816000	0.493953000	4.577074000
H	-2.229973000	1.654134000	5.228948000
C	-5.449666000	1.677216000	3.136807000
H	-6.356523000	2.011266000	2.626824000
H	-5.547055000	0.596207000	3.329774000
C	-5.365287000	2.417475000	4.459537000

O	-4.114407000	2.420866000	5.069640000
O	-6.296160000	3.009801000	4.994196000

Sum of electronic and thermal Free Energies= -2002.135918

*Optimized structure and free energy for **2**-Ce^{III}-**V***

C	3.637443000	-0.361689000	-2.433828000
H	4.408220000	0.414494000	-2.399361000
H	2.812273000	-0.012176000	-3.073930000
C	4.228451000	-1.650259000	-3.023524000
H	3.419533000	-2.387156000	-3.128149000
H	4.633637000	-1.451264000	-4.026926000
N	3.182001000	-0.630377000	-1.055619000
N	5.267688000	-2.222084000	-2.126541000
Ce	5.183290000	-1.406907000	0.401305000
C	1.911336000	-0.560725000	-0.773813000
C	6.128862000	-3.039405000	-2.669931000
H	6.078632000	-3.188681000	-3.758146000
H	1.224047000	-0.221754000	-1.562626000
C	1.264950000	-0.897608000	0.474666000
C	-0.123678000	-0.629551000	0.580758000
C	1.942688000	-1.523989000	1.569568000
C	-0.830070000	-0.948337000	1.728227000
H	-0.629899000	-0.162809000	-0.261009000
C	1.205965000	-1.858082000	2.744914000
C	-0.153723000	-1.561269000	2.802273000
H	-1.890759000	-0.734528000	1.802131000
H	-0.705980000	-1.815544000	3.703330000
C	7.156282000	-3.829879000	-2.029780000
C	7.977071000	-4.621448000	-2.874048000
C	7.350424000	-3.891495000	-0.614053000
C	8.957061000	-5.449318000	-2.353071000
H	7.820878000	-4.569976000	-3.948941000
C	8.351811000	-4.757005000	-0.082217000
C	9.132580000	-5.510185000	-0.955990000
H	9.579901000	-6.048788000	-3.008024000
H	9.897019000	-6.163391000	-0.543031000
C	8.534806000	-4.821071000	1.412392000
H	9.331261000	-5.521840000	1.682044000
H	8.783371000	-3.835481000	1.824859000
H	7.610182000	-5.136737000	1.910969000
C	1.929155000	-2.520273000	3.889376000
H	2.758517000	-1.897826000	4.246844000
H	1.250473000	-2.710586000	4.726804000
H	2.373551000	-3.473703000	3.578268000
O	3.245729000	-1.813590000	1.510936000
O	6.613616000	-3.154382000	0.221492000
O	5.883235000	4.302735000	0.711976000
C	4.881754000	5.289308000	1.165177000
H	4.798057000	6.090907000	0.429240000
H	3.956702000	4.723583000	1.242419000
H	5.179402000	5.702932000	2.130235000

O	7.547604000	5.884032000	0.813731000
C	7.165285000	4.739082000	0.563162000
O	6.267361000	0.069455000	1.704395000
C	8.108503000	3.642380000	0.105918000
H	8.846552000	4.083293000	-0.563260000
H	8.629242000	3.223472000	0.973844000
C	6.963173000	1.247750000	1.407331000
H	6.566680000	2.124162000	1.944479000
H	8.039062000	1.178112000	1.659058000
C	6.851283000	1.521918000	-0.092502000
O	7.451530000	2.602642000	-0.676903000
O	6.230938000	0.741119000	-0.838126000

Sum of electronic and thermal Free Energies= -2002.156650

*Optimized structure and free energy for **2**-Ce^{III}-**VI***

C	-0.775389000	-0.359447000	0.340784000
H	-0.404622000	0.257776000	-0.483810000
H	-1.876405000	-0.321365000	0.346188000
C	-0.316103000	-1.813482000	0.142649000
H	-0.738623000	-2.420593000	0.955497000
H	-0.707879000	-2.207671000	-0.808120000
N	-0.201198000	0.142992000	1.602299000
N	1.165915000	-1.908411000	0.198026000
Ce	2.404201000	0.174951000	1.459839000
C	-0.985529000	0.327363000	2.628598000
C	1.710894000	-2.968465000	-0.331639000
H	1.051566000	-3.698952000	-0.824708000
H	-2.071651000	0.244381000	2.472921000
C	-0.593864000	0.595184000	3.992043000
C	-1.613674000	0.955133000	4.910240000
C	0.748688000	0.419509000	4.464432000
C	-1.331591000	1.163163000	6.249206000
H	-2.630196000	1.070099000	4.540884000
C	1.025050000	0.617156000	5.852608000
C	-0.008401000	0.990886000	6.706585000
H	-2.115550000	1.448411000	6.942342000
H	0.214598000	1.147731000	7.758957000
C	3.106921000	-3.349175000	-0.358940000
C	3.423586000	-4.565861000	-1.017503000
C	4.158733000	-2.593460000	0.252219000
C	4.724494000	-5.036097000	-1.077407000
H	2.617163000	-5.134076000	-1.475522000
C	5.497019000	-3.089556000	0.192917000
C	5.751892000	-4.289408000	-0.466174000
H	4.953022000	-5.968566000	-1.582053000
H	6.773977000	-4.657439000	-0.506163000
C	6.593266000	-2.291402000	0.850621000
H	7.565468000	-2.778309000	0.724129000
H	6.653183000	-1.278541000	0.433595000
H	6.402980000	-2.168051000	1.923824000
C	2.436338000	0.420119000	6.342509000

H	3.131613000	1.095530000	5.828873000
H	2.508676000	0.599998000	7.419941000
H	2.788300000	-0.597644000	6.134223000
O	1.734219000	0.051677000	3.646269000
O	3.921231000	-1.435593000	0.870335000
O	3.360526000	2.120697000	1.587011000
C	4.074784000	3.303658000	1.942612000
H	3.736562000	3.698459000	2.911763000
H	5.155599000	3.111773000	2.015764000
H	3.930607000	4.099756000	1.192590000
O	2.032146000	0.998734000	-1.019157000
C	2.190624000	2.450826000	-1.317679000
C	2.468074000	0.198982000	-2.203085000
C	3.248372000	2.487942000	-2.418919000
H	1.223209000	2.839532000	-1.657410000
H	2.490642000	2.909772000	-0.376415000
C	2.920336000	1.227760000	-3.254090000
H	3.279503000	-0.451789000	-1.870157000
H	1.623366000	-0.413415000	-2.525267000
H	4.248685000	2.408931000	-1.978694000
H	3.204396000	3.406866000	-3.010961000
H	3.778984000	0.870493000	-3.829725000
H	2.108508000	1.443097000	-3.958645000

Sum of electronic and thermal Free Energies= -1778.93616

*Optimized structure and free energy for **2**-Ce^{IV}-**I***

C	-0.142998000	0.239451000	0.070772000
H	0.421029000	0.920704000	-0.578399000
H	-1.209756000	0.475198000	-0.039292000
C	0.116686000	-1.213796000	-0.339639000
H	-0.540980000	-1.871700000	0.242860000
H	-0.118703000	-1.353002000	-1.402499000
N	0.316915000	0.435099000	1.464039000
N	1.532641000	-1.591549000	-0.053648000
Ce	2.748066000	-0.109160000	1.621392000
C	-0.524813000	0.819910000	2.385509000
C	2.007573000	-2.637829000	-0.683043000
H	1.363132000	-3.120783000	-1.426269000
H	-1.559792000	1.021542000	2.087237000
C	-0.252687000	1.005899000	3.792108000
C	-1.310361000	1.447462000	4.621655000
C	1.018154000	0.746820000	4.380925000
C	-1.110882000	1.625459000	5.984458000
H	-2.282243000	1.646403000	4.180179000
C	1.229509000	0.919051000	5.765937000
C	0.150224000	1.359914000	6.543045000
H	-1.922723000	1.965416000	6.616417000
H	0.299915000	1.497685000	7.609175000
C	3.288489000	-3.283072000	-0.513720000
C	3.583242000	-4.392524000	-1.342332000
C	4.243920000	-2.888838000	0.464994000

C	4.782082000	-5.079302000	-1.202954000
H	2.858857000	-4.702497000	-2.089490000
C	5.461216000	-3.585453000	0.622087000
C	5.705987000	-4.673879000	-0.225537000
H	5.004677000	-5.926406000	-1.840849000
H	6.639188000	-5.217384000	-0.117038000
C	6.452447000	-3.152810000	1.671390000
H	7.324113000	-3.811936000	1.680639000
H	6.803184000	-2.129196000	1.491474000
H	6.004547000	-3.165103000	2.671942000
C	2.581388000	0.634423000	6.368129000
H	3.355083000	1.280178000	5.935258000
H	2.569428000	0.798130000	7.448546000
H	2.890671000	-0.401095000	6.183192000
O	2.043386000	0.324014000	3.590581000
O	3.970087000	-1.819836000	1.260132000
O	3.424130000	1.483506000	0.537322000
C	3.961503000	2.606677000	-0.201699000
H	3.292841000	3.465993000	-0.095912000
H	4.948576000	2.863173000	0.193678000
H	4.051636000	2.338607000	-1.258391000

Sum of electronic and thermal Free Energies= -1546.411773

*Optimized structure and free energy for **1**-Ce^{IV}-**II***

C	-0.214121000	0.308762000	0.057772000
H	0.245617000	0.953317000	-0.702155000
H	-1.300314000	0.479230000	0.021007000
C	0.071017000	-1.172613000	-0.225059000
H	-0.528791000	-1.775332000	0.470432000
H	-0.243422000	-1.436045000	-1.243964000
N	0.326071000	0.644484000	1.390270000
N	1.503328000	-1.510689000	-0.007110000
Ce	2.808801000	0.042118000	1.652706000
C	-0.511328000	0.999625000	2.332255000
C	1.966446000	-2.549603000	-0.654387000
H	1.298272000	-3.055722000	-1.363392000
H	-1.550161000	1.198820000	2.048913000
C	-0.243781000	1.109478000	3.746262000
C	-1.221382000	1.704917000	4.571300000
C	0.913442000	0.533501000	4.350515000
C	-1.052693000	1.756714000	5.949021000
H	-2.109075000	2.125935000	4.112231000
C	1.081211000	0.557609000	5.756486000
C	0.093631000	1.181801000	6.527283000
H	-1.799398000	2.225281000	6.579744000
H	0.218210000	1.213682000	7.605799000
C	3.269505000	-3.166950000	-0.538767000
C	3.542372000	-4.294930000	-1.345411000
C	4.271142000	-2.722056000	0.371852000
C	4.758260000	-4.959768000	-1.251844000
H	2.782156000	-4.643019000	-2.039127000

C	5.510783000	-3.392003000	0.478172000
C	5.729750000	-4.505577000	-0.342672000
H	4.961638000	-5.822659000	-1.876657000
H	6.677591000	-5.027593000	-0.268061000
C	6.546512000	-2.901541000	1.456672000
H	7.454624000	-3.506820000	1.399298000
H	6.814777000	-1.856294000	1.264396000
H	6.168983000	-2.944281000	2.485740000
C	2.299891000	-0.074593000	6.379108000
H	3.223078000	0.364502000	5.988708000
H	2.292248000	0.049075000	7.464572000
H	2.341888000	-1.145092000	6.155378000
O	1.840501000	-0.069398000	3.570073000
O	4.034269000	-1.631558000	1.138979000
O	4.045925000	1.575490000	2.219759000
C	5.001924000	2.565129000	2.649780000
H	4.548250000	3.219908000	3.399590000
H	5.877545000	2.068280000	3.082763000
H	5.321633000	3.163986000	1.791616000
O	2.995200000	1.290715000	-0.513643000
C	2.994308000	1.989995000	-1.540007000
O	4.036840000	1.943349000	-2.387799000
C	1.833930000	2.898473000	-1.882708000
H	1.089258000	2.328384000	-2.454612000
H	1.366162000	3.255468000	-0.964821000
C	3.980337000	2.679078000	-3.681521000
H	5.018986000	2.887715000	-3.932559000
H	3.553068000	2.008487000	-4.431754000
C	3.209365000	3.983453000	-3.616048000
O	2.245056000	4.087869000	-2.618714000
O	3.410360000	4.904379000	-4.385526000

Sum of electronic and thermal Free Energies= -2001.912932

*Optimized structure and free energy for **2**-Ce^{IV}-**$TS_{II\text{-}III}$***

C	-0.659680000	-0.228406000	-0.034554000
H	-0.224919000	0.496559000	-0.730219000
H	-1.753501000	-0.157277000	-0.097098000
C	-0.208724000	-1.647895000	-0.395216000
H	-0.771028000	-2.368856000	0.211852000
H	-0.420463000	-1.852493000	-1.452160000
N	-0.171721000	0.093523000	1.325034000
N	1.246671000	-1.827796000	-0.103167000
Ce	2.330035000	0.004098000	1.317115000
C	-1.012582000	0.352325000	2.287293000
C	1.818686000	-2.894732000	-0.598366000
H	1.220402000	-3.540614000	-1.250951000
H	-2.083295000	0.361326000	2.054078000
C	-0.685766000	0.624334000	3.668971000
C	-1.740747000	0.906712000	4.566661000
C	0.648391000	0.597131000	4.165131000
C	-1.477132000	1.154050000	5.908111000

H	-2.761012000	0.928519000	4.195757000
C	0.926929000	0.841838000	5.527803000
C	-0.152963000	1.119171000	6.375866000
H	-2.287779000	1.371791000	6.593401000
H	0.046282000	1.311124000	7.425388000
C	3.162162000	-3.375529000	-0.370619000
C	3.570590000	-4.551012000	-1.043169000
C	4.069123000	-2.755220000	0.532472000
C	4.833982000	-5.085910000	-0.825620000
H	2.883429000	-5.033226000	-1.731790000
C	5.351441000	-3.296014000	0.770378000
C	5.709383000	-4.459043000	0.076619000
H	5.143773000	-5.985355000	-1.344453000
H	6.693129000	-4.884722000	0.247319000
C	6.288442000	-2.626529000	1.742417000
H	7.231824000	-3.173420000	1.814971000
H	6.514183000	-1.598307000	1.434796000
H	5.848391000	-2.570289000	2.745147000
C	2.347091000	0.801194000	6.030037000
H	2.973130000	1.540221000	5.515613000
H	2.387923000	1.008332000	7.102302000
H	2.803701000	-0.180107000	5.854139000
O	1.670807000	0.326272000	3.308626000
O	3.685050000	-1.621612000	1.177653000
O	3.876750000	1.652523000	1.060159000
C	5.287748000	1.888551000	1.333492000
H	5.621137000	1.184574000	2.102462000
H	5.875848000	1.720886000	0.424737000
H	5.428775000	2.912194000	1.686641000
O	1.970210000	1.539695000	-0.433076000
C	3.030781000	2.290681000	-0.532427000
O	3.937640000	1.954113000	-1.506277000
C	2.916642000	3.764766000	-0.222850000
H	2.288510000	4.240592000	-0.987409000
H	2.472545000	3.916995000	0.756182000
C	4.727434000	3.035562000	-2.147465000
H	5.614733000	2.550132000	-2.546394000
H	4.134960000	3.443628000	-2.974403000
C	5.134536000	4.136304000	-1.187048000
O	4.225674000	4.419126000	-0.178499000
O	6.186124000	4.750781000	-1.272953000

Sum of electronic and thermal Free Energies= -2001.898044

*Optimized structure and free energy for **2**-Ce^{IV}-**III***

C	-0.647258000	-0.218782000	-0.026147000
H	-0.187009000	0.516657000	-0.696268000
H	-1.737876000	-0.124891000	-0.108393000
C	-0.212101000	-1.636338000	-0.413530000
H	-0.790388000	-2.362804000	0.171539000
H	-0.414563000	-1.814791000	-1.476916000
N	-0.179078000	0.062402000	1.349281000

N	1.237639000	-1.836653000	-0.109824000
Ce	2.305098000	-0.054663000	1.357452000
C	-1.028431000	0.322279000	2.303928000
C	1.813326000	-2.888064000	-0.633962000
H	1.219922000	-3.511946000	-1.311700000
H	-2.095536000	0.351243000	2.057030000
C	-0.713545000	0.575181000	3.691713000
C	-1.777776000	0.843449000	4.582875000
C	0.616776000	0.551418000	4.198705000
C	-1.527404000	1.078681000	5.929032000
H	-2.794800000	0.863780000	4.203217000
C	0.881683000	0.784795000	5.565582000
C	-0.207213000	1.047035000	6.407314000
H	-2.345098000	1.284829000	6.609437000
H	-0.017916000	1.229571000	7.460314000
C	3.156068000	-3.374503000	-0.414338000
C	3.568575000	-4.527387000	-1.122708000
C	4.060761000	-2.780195000	0.508613000
C	4.833536000	-5.065004000	-0.920617000
H	2.883833000	-4.989668000	-1.827224000
C	5.344253000	-3.323513000	0.730454000
C	5.706062000	-4.463740000	0.001161000
H	5.146608000	-5.946738000	-1.467049000
H	6.690894000	-4.891542000	0.159475000
C	6.280177000	-2.680430000	1.721024000
H	7.214137000	-3.242719000	1.797074000
H	6.526106000	-1.652671000	1.427117000
H	5.829807000	-2.628959000	2.719175000
C	2.297367000	0.749369000	6.080993000
H	2.920946000	1.503737000	5.586179000
H	2.325647000	0.938957000	7.156852000
H	2.765514000	-0.224244000	5.893657000
O	1.649138000	0.297103000	3.347426000
O	3.670733000	-1.668953000	1.189883000
O	3.993227000	1.768578000	1.110660000
C	5.375131000	2.156580000	1.455708000
H	5.599652000	1.637263000	2.386935000
H	6.048917000	1.834781000	0.661044000
H	5.427447000	3.237016000	1.597204000
O	2.203812000	1.522829000	-0.199992000
C	3.377434000	2.260095000	-0.163565000
O	4.295061000	1.906327000	-1.197069000
C	3.104032000	3.760162000	-0.131759000
H	2.344686000	3.995562000	-0.883792000
H	2.751400000	4.071175000	0.849137000
C	4.582043000	2.934119000	-2.213597000
H	5.396877000	2.533481000	-2.812337000
H	3.705574000	3.088767000	-2.854757000
C	5.018274000	4.230865000	-1.557883000
O	4.324491000	4.535626000	-0.385659000
O	5.907003000	4.960741000	-1.965658000

Sum of electronic and thermal Free Energies= -2001.904546

*Optimized structure and free energy for **2**-Ce^{IV}-**IV***

C	-0.461524000	-0.206809000	-0.233602000
H	0.054281000	0.434617000	-0.957138000
H	-1.541734000	-0.037072000	-0.328501000
C	-0.133567000	-1.679827000	-0.501513000
H	-0.776416000	-2.312064000	0.124067000
H	-0.329866000	-1.925185000	-1.552448000
N	0.028281000	0.142102000	1.118620000
N	1.290853000	-1.965394000	-0.148642000
Ce	2.488659000	-0.137758000	1.141784000
C	-0.795364000	0.539243000	2.047111000
C	1.786911000	-3.101476000	-0.565372000
H	1.155174000	-3.734474000	-1.198369000
H	-1.855941000	0.641604000	1.792284000
C	-0.461222000	0.851744000	3.419071000
C	-1.496717000	1.274025000	4.283371000
C	0.856942000	0.721391000	3.941303000
C	-1.229873000	1.555311000	5.618040000
H	-2.505018000	1.375144000	3.893531000
C	1.137276000	0.993836000	5.298022000
C	0.076689000	1.411965000	6.112771000
H	-2.025895000	1.879965000	6.277654000
H	0.277269000	1.627343000	7.157437000
C	3.081319000	-3.672702000	-0.271051000
C	3.406357000	-4.918505000	-0.856413000
C	4.016001000	-3.070354000	0.615341000
C	4.615690000	-5.539382000	-0.569188000
H	2.697959000	-5.387050000	-1.532800000
C	5.240534000	-3.698432000	0.927687000
C	5.516854000	-4.930031000	0.318852000
H	4.862254000	-6.492270000	-1.022227000
H	6.456437000	-5.423353000	0.546470000
C	6.205271000	-3.048845000	1.886139000
H	7.089396000	-3.674015000	2.033176000
H	6.539002000	-2.071035000	1.517788000
H	5.740517000	-2.878147000	2.864270000
C	2.537595000	0.831906000	5.830909000
H	3.243485000	1.488913000	5.308652000
H	2.579252000	1.068335000	6.897013000
H	2.898565000	-0.194236000	5.693943000
O	1.862732000	0.320513000	3.115504000
O	3.713325000	-1.865118000	1.170787000
O	2.477866000	2.612078000	0.691361000
C	2.878405000	3.813779000	1.454086000
H	2.052857000	3.992996000	2.140281000
H	3.804157000	3.626035000	2.000615000
H	3.001786000	4.661391000	0.777737000
O	2.721604000	0.978135000	-0.814807000
C	3.378681000	2.067418000	-0.297990000

O	4.501587000	1.533708000	0.579178000
C	3.940974000	3.022852000	-1.336524000
H	4.275253000	2.443313000	-2.201038000
H	3.185805000	3.739681000	-1.655110000
C	5.862874000	1.667770000	0.042758000
H	6.541941000	1.327170000	0.822065000
H	5.986814000	1.043743000	-0.851227000
C	6.134736000	3.131921000	-0.260221000
O	5.051941000	3.821761000	-0.802487000
O	7.189286000	3.702591000	-0.034914000

Sum of electronic and thermal Free Energies= -2001.898869

*Optimized structure and free energy for **2**-Ce^{IV}-**$TS_{IV\text{-}V}$***

C	0.089670000	0.483226000	-0.067336000
H	0.071186000	0.550653000	1.025374000
H	1.108546000	0.700006000	-0.413296000
C	-0.329409000	-0.918900000	-0.522020000
H	-0.161308000	-1.013723000	-1.602263000
H	0.279138000	-1.676546000	-0.013164000
N	-0.884289000	1.463001000	-0.599103000
N	-1.783898000	-1.144053000	-0.256042000
Ce	-3.124974000	0.937626000	0.345494000
C	-0.499886000	2.415532000	-1.401375000
C	-2.214636000	-2.375938000	-0.334990000
H	-1.478294000	-3.165618000	-0.521517000
H	0.565087000	2.490623000	-1.646919000
C	-1.345243000	3.404819000	-2.031857000
C	-0.740113000	4.379290000	-2.857577000
C	-2.759926000	3.423335000	-1.873295000
C	-1.514937000	5.337428000	-3.500491000
H	0.338287000	4.372193000	-2.983598000
C	-3.557616000	4.387037000	-2.527659000
C	-2.909501000	5.333139000	-3.332850000
H	-1.047790000	6.084627000	-4.131155000
H	-3.509269000	6.081885000	-3.840417000
C	-3.575869000	-2.854520000	-0.242962000
C	-3.799671000	-4.246029000	-0.361425000
C	-4.697618000	-1.994166000	-0.091225000
C	-5.091051000	-4.758691000	-0.334204000
H	-2.949595000	-4.911392000	-0.478132000
C	-6.014720000	-2.500411000	-0.077074000
C	-6.183104000	-3.886609000	-0.197701000
H	-5.257532000	-5.825637000	-0.424119000
H	-7.190206000	-4.291082000	-0.186478000
C	-7.188164000	-1.565125000	0.064270000
H	-7.177397000	-0.792575000	-0.713128000
H	-8.132502000	-2.110111000	-0.009009000
H	-7.173189000	-1.045940000	1.030754000
C	-5.053809000	4.382145000	-2.348409000
H	-5.330444000	4.554172000	-1.301014000
H	-5.521849000	5.161372000	-2.955009000

H	-5.486551000	3.417258000	-2.637253000
O	-3.351876000	2.490399000	-1.077219000
O	-4.487617000	-0.654578000	0.041825000
O	-2.138844000	3.098393000	2.745651000
C	-2.619736000	4.346402000	3.379886000
H	-2.539885000	4.288643000	4.465489000
H	-1.959083000	5.113531000	2.982890000
H	-3.652310000	4.534785000	3.082284000
O	-2.045937000	0.896208000	2.371731000
C	-2.662387000	1.865984000	3.052889000
O	-4.236193000	1.916617000	2.242276000
C	-3.057871000	1.532195000	4.478714000
H	-3.360043000	0.483054000	4.519127000
H	-2.210721000	1.683650000	5.149487000
C	-5.424409000	1.641957000	3.041917000
H	-6.296395000	2.000272000	2.492788000
H	-5.536697000	0.562779000	3.218512000
C	-5.365069000	2.378749000	4.368865000
O	-4.118760000	2.397370000	4.993770000
O	-6.315551000	2.942522000	4.887082000

Sum of electronic and thermal Free Energies= -2001.896186

*Optimized structure and free energy for **2**-Ce^{IV}-**V***

C	3.641510000	-0.280681000	-2.502265000
H	4.379447000	0.524609000	-2.445217000
H	2.804644000	0.054937000	-3.129185000
C	4.275964000	-1.533748000	-3.115340000
H	3.491334000	-2.279962000	-3.296444000
H	4.739086000	-1.286132000	-4.079087000
N	3.191376000	-0.602231000	-1.128188000
N	5.279133000	-2.131992000	-2.183390000
Ce	5.166220000	-1.319689000	0.267118000
C	1.920730000	-0.560917000	-0.833628000
C	6.109893000	-3.000963000	-2.697140000
H	6.065808000	-3.175979000	-3.778398000
H	1.221396000	-0.217751000	-1.604838000
C	1.305897000	-0.943818000	0.417095000
C	-0.087944000	-0.756844000	0.566569000
C	2.037615000	-1.538980000	1.483398000
C	-0.728523000	-1.139500000	1.737965000
H	-0.652545000	-0.309321000	-0.245999000
C	1.393843000	-1.938891000	2.675703000
C	0.013712000	-1.725136000	2.777592000
H	-1.796096000	-0.991973000	1.851250000
H	-0.492851000	-2.025812000	3.689313000
C	7.088539000	-3.815896000	-2.012718000
C	7.890195000	-4.686137000	-2.788035000
C	7.246987000	-3.819028000	-0.599695000
C	8.812868000	-5.526656000	-2.178471000
H	7.773799000	-4.692287000	-3.867654000
C	8.174096000	-4.676644000	0.032303000

C	8.945183000	-5.517543000	-0.779781000
H	9.425921000	-6.190874000	-2.776203000
H	9.663828000	-6.180361000	-0.308183000
C	8.310930000	-4.667948000	1.533015000
H	9.069463000	-5.383639000	1.860132000
H	8.594303000	-3.675327000	1.903015000
H	7.363443000	-4.927462000	2.020085000
C	2.189310000	-2.573860000	3.786897000
H	2.992479000	-1.911507000	4.131058000
H	1.549025000	-2.807723000	4.641245000
H	2.666965000	-3.502949000	3.453412000
O	3.374919000	-1.732003000	1.344742000
O	6.490663000	-2.976282000	0.150031000
O	5.950233000	4.280883000	0.869501000
C	4.968420000	5.279785000	1.360583000
H	4.784721000	6.020837000	0.581544000
H	4.074439000	4.701198000	1.578310000
H	5.358678000	5.767826000	2.254684000
O	7.557064000	5.913429000	0.648322000
C	7.186313000	4.748374000	0.528225000
O	6.191271000	0.035801000	1.567074000
C	8.104998000	3.644793000	0.036609000
H	8.809817000	4.065528000	-0.677654000
H	8.657622000	3.208347000	0.875167000
C	6.904163000	1.244989000	1.351654000
H	6.474295000	2.074709000	1.925428000
H	7.960502000	1.138559000	1.640401000
C	6.796504000	1.548267000	-0.138501000
O	7.386265000	2.603960000	-0.716763000
O	6.147084000	0.757827000	-0.867891000

Sum of electronic and thermal Free Energies= -2001.929376

*Optimized structure and free energy for **2**-Ce^{IV}-**VI***

C	-0.284243000	0.390096000	0.103043000
H	0.255167000	1.031892000	-0.600234000
H	-1.357457000	0.610285000	0.021324000
C	-0.030367000	-1.087787000	-0.226762000
H	-0.664732000	-1.706392000	0.421476000
H	-0.306075000	-1.296371000	-1.269119000
N	0.225779000	0.642783000	1.467107000
N	1.398245000	-1.439657000	0.028341000
Ce	2.725926000	0.262438000	1.538234000
C	-0.616811000	0.844822000	2.444970000
C	1.822343000	-2.576143000	-0.456933000
H	1.121736000	-3.178744000	-1.048283000
H	-1.676821000	0.979532000	2.197802000
C	-0.311716000	0.860502000	3.855527000
C	-1.327739000	1.245758000	4.762998000
C	0.937993000	0.404226000	4.368958000
C	-1.105144000	1.197706000	6.131455000
H	-2.284409000	1.582015000	4.373934000

C	1.162429000	0.332287000	5.764113000
C	0.132844000	0.740942000	6.618405000
H	-1.881124000	1.501379000	6.824250000
H	0.298087000	0.695897000	7.690462000
C	3.129497000	-3.178745000	-0.312830000
C	3.349399000	-4.431202000	-0.935847000
C	4.188966000	-2.589700000	0.433198000
C	4.573901000	-5.074152000	-0.820299000
H	2.543606000	-4.887439000	-1.503483000
C	5.438110000	-3.240029000	0.559343000
C	5.604334000	-4.475991000	-0.075267000
H	4.736045000	-6.033537000	-1.297302000
H	6.559187000	-4.984001000	0.016179000
C	6.541253000	-2.601119000	1.363338000
H	7.439798000	-3.223428000	1.357693000
H	6.805544000	-1.613841000	0.965872000
H	6.236557000	-2.449765000	2.405847000
C	2.481421000	-0.175063000	6.287795000
H	3.315387000	0.446106000	5.939235000
H	2.492754000	-0.179152000	7.380810000
H	2.681157000	-1.194828000	5.938395000
O	1.910195000	0.011096000	3.510319000
O	3.999435000	-1.385057000	1.027612000
O	3.838623000	1.903437000	2.111057000
C	4.641573000	2.875518000	2.813058000
H	4.443781000	2.816159000	3.888252000
H	5.703785000	2.682466000	2.629863000
H	4.392184000	3.882050000	2.459989000
O	2.887423000	1.358185000	-0.715507000
C	3.120649000	2.834324000	-0.902199000
C	3.197451000	0.638991000	-1.997040000
C	3.331936000	3.008929000	-2.407488000
H	2.244707000	3.351756000	-0.507556000
H	4.001020000	3.091200000	-0.311166000
C	3.958149000	1.663617000	-2.838738000
H	3.772037000	-0.250075000	-1.736219000
H	2.244121000	0.349486000	-2.448413000
H	3.979754000	3.860542000	-2.630929000
H	2.376291000	3.169026000	-2.918930000
H	5.026912000	1.642057000	-2.598486000
H	3.848220000	1.475007000	-3.909831000

Sum of electronic and thermal Free Energies= -1778.72097

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