Supporting Information

A Ce(III) complex potently inhibits the activity and expression of tyrosine phosphatase SHP-2

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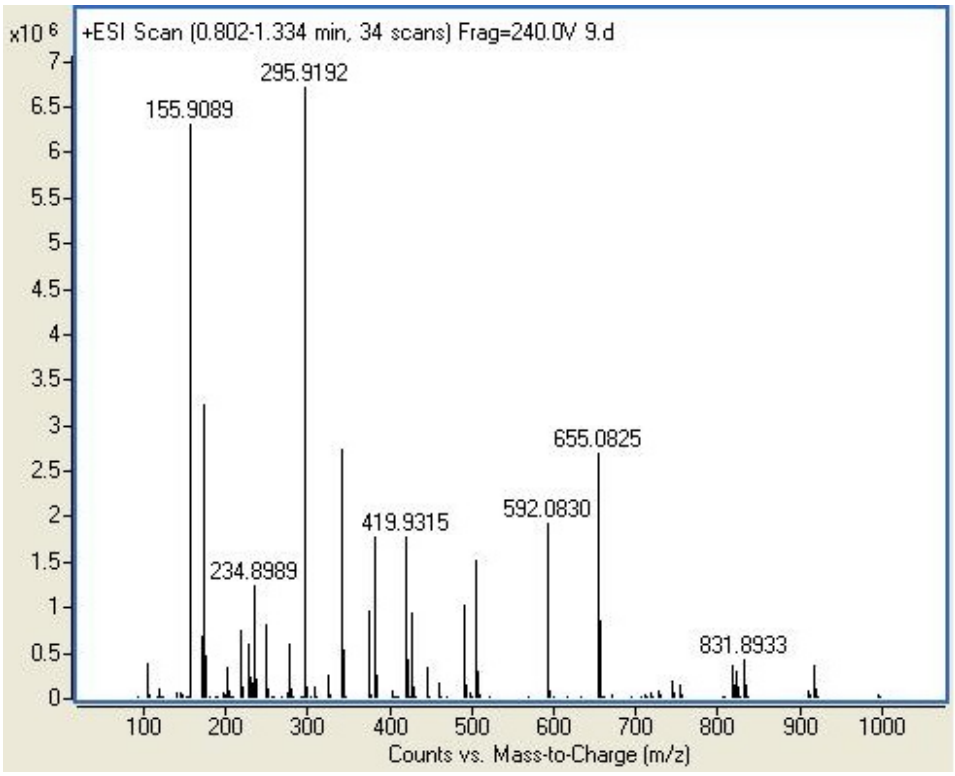
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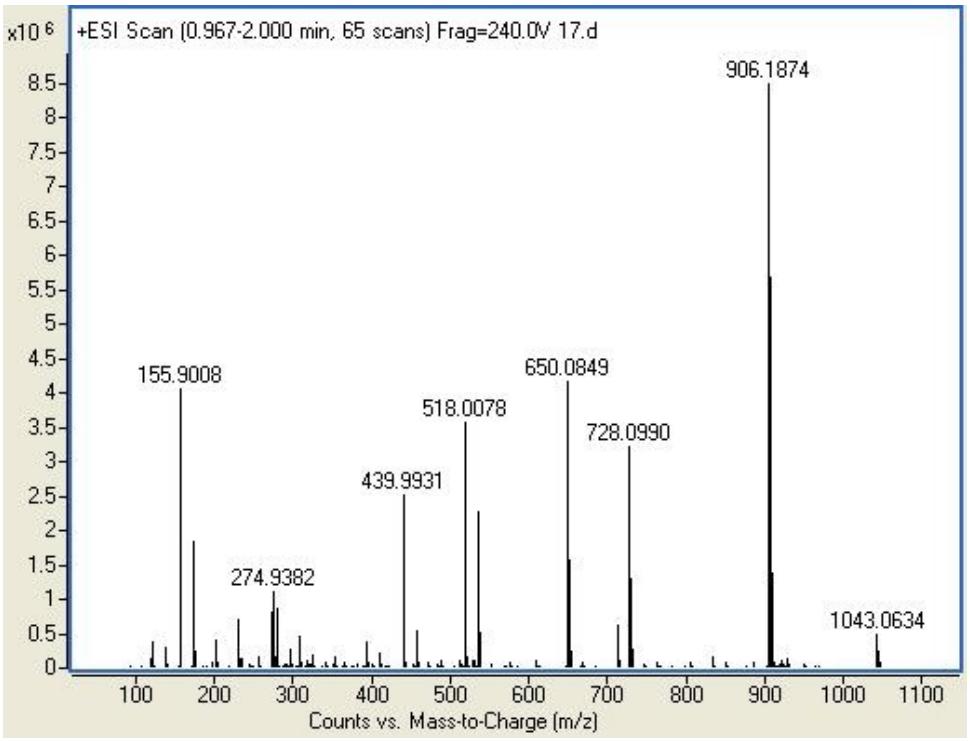
295.9192
155.9089
655.0825
592.0830
419.9315
234.8989
831.8933
Counts vs. Mass-to-Charge (m/z)

(a)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155.9008
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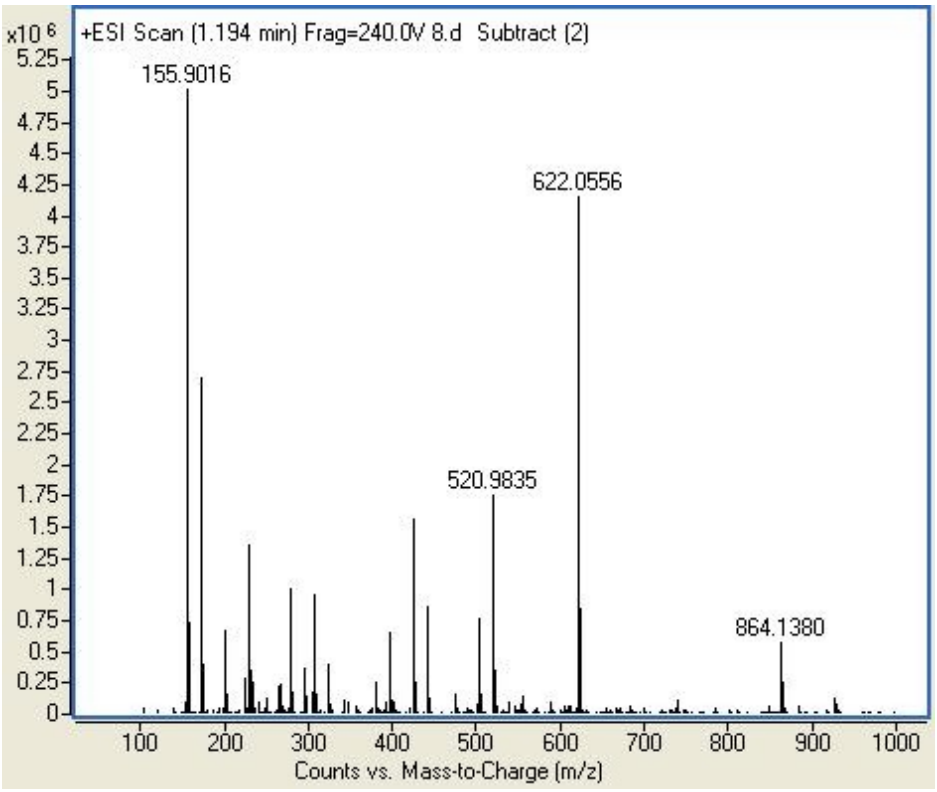
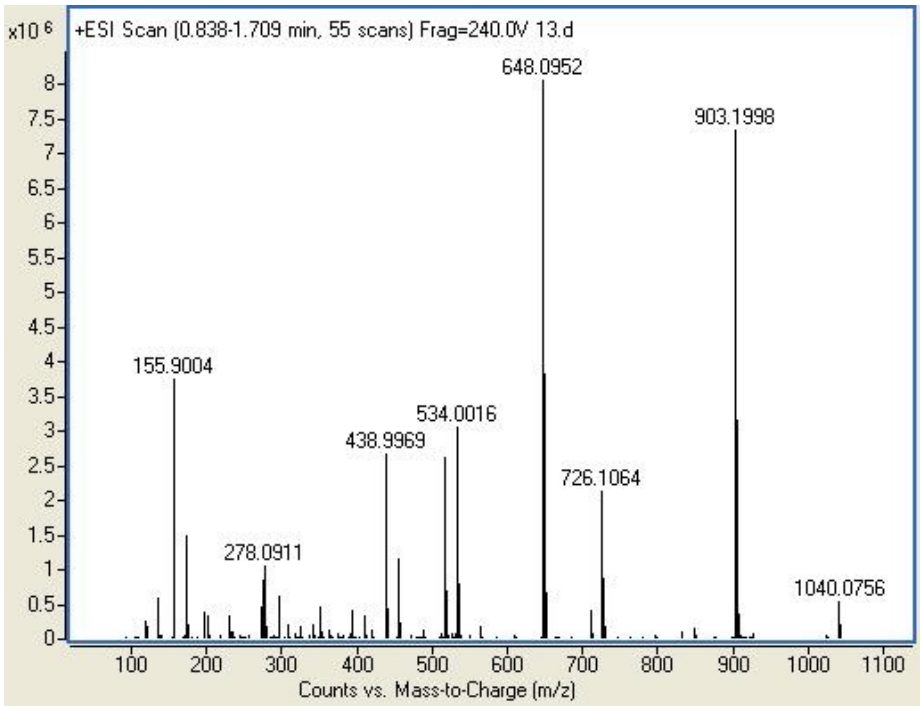
518.0078
728.0990
439.9931
274.9382
1043.0634
Counts vs. Mass-to-Charge (m/z)

(b)

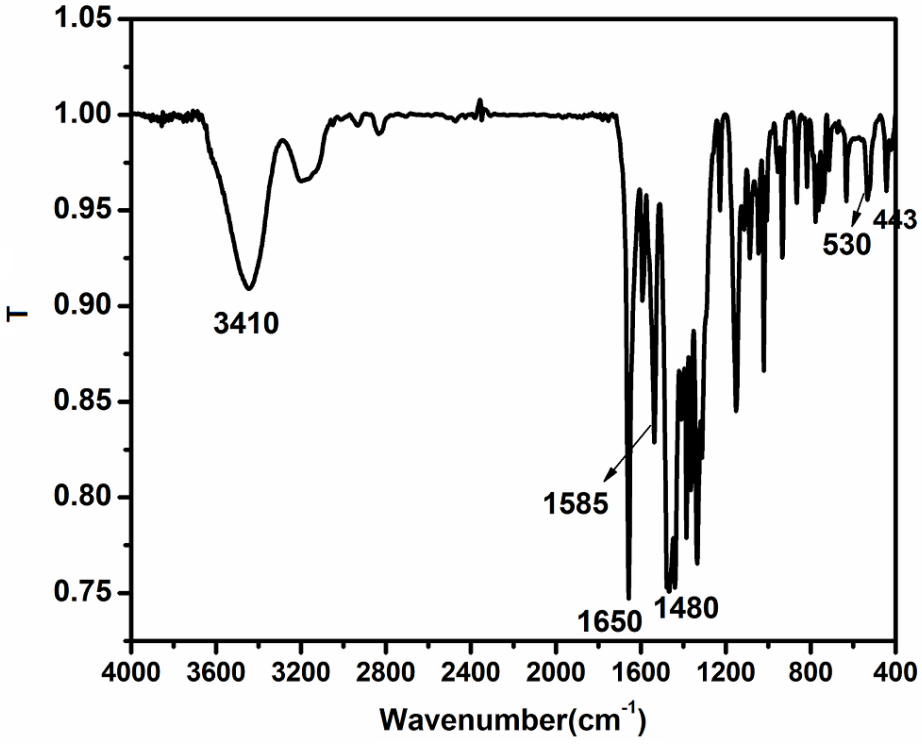


(c)

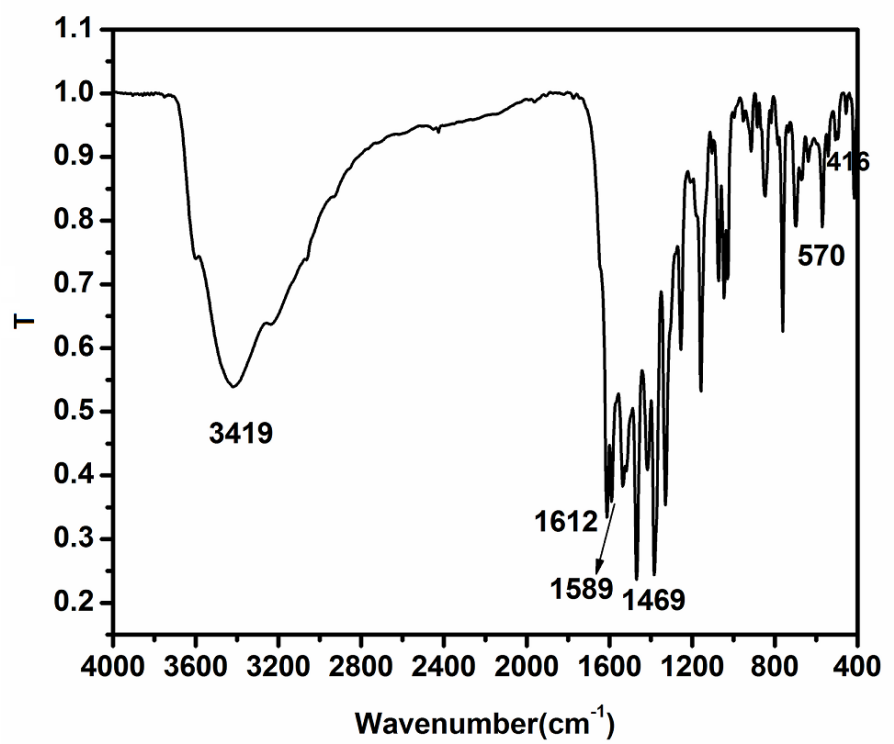


(d)

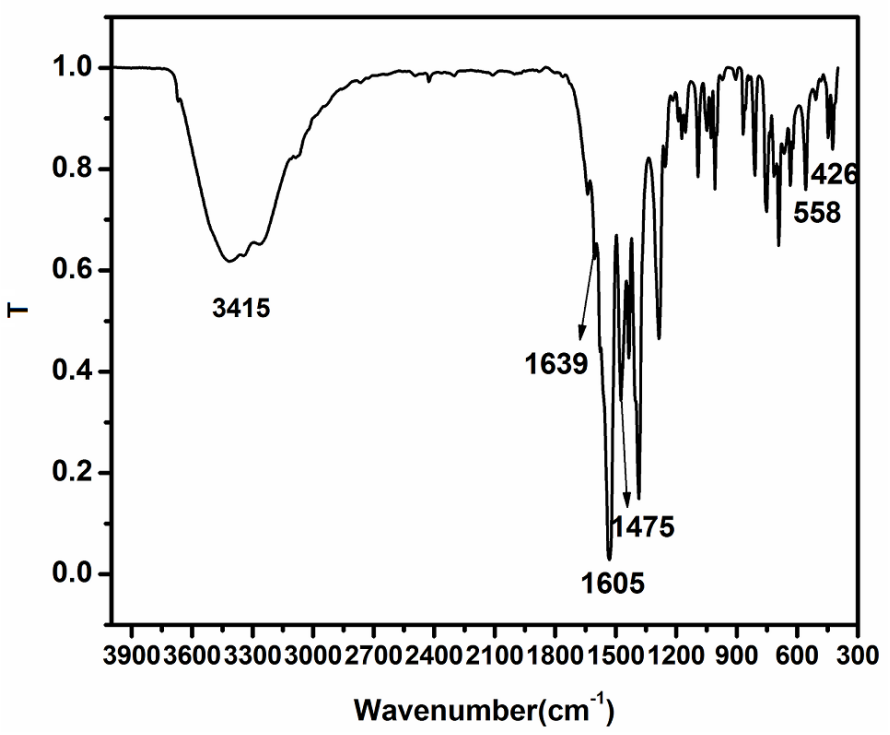
Fig. S1 The ESI-MS characterization data of Ce(III) complexes **1-4**. (a) ESI-MS: m/z, [**1**-2NO_3-H-2CH_3OH]$^+$ calculated for $C_{22}H_{17}CeN_{11}O_5^+$: 655.05; measured: 655.08. (b) ESI-MS: m/z, [**2**-NO_3-2H-3H_2O]$^{2+}$ calculated for $C_{26}H_{22}CeN_8O_4^{2+}$: 650.08; measured: 650.08. (c) ESI-MS: m/z, [**3**-Br-NO_3-H-H_2O+CH_3OH]$^+$ calculated for $C_{25}H_{22}CeN_8O_3^+$: 622.09; measured: 622.06. (d) ESI-MS: m/z, [**4**-NO_3-2H-3H_2O]$^{2+}$ calculated for $C_{28}H_{24}CeN_6O_4^{2+}$: 648.09; measured: 648.10.


1.05
1.00
0.95
0.90
0.85
0.80
0.75
T
3410
1585
1650
1480
530
443
4000 3600 3200 2800 2400 2000 1600 1200 800 400
Wavenumber(cm-1)

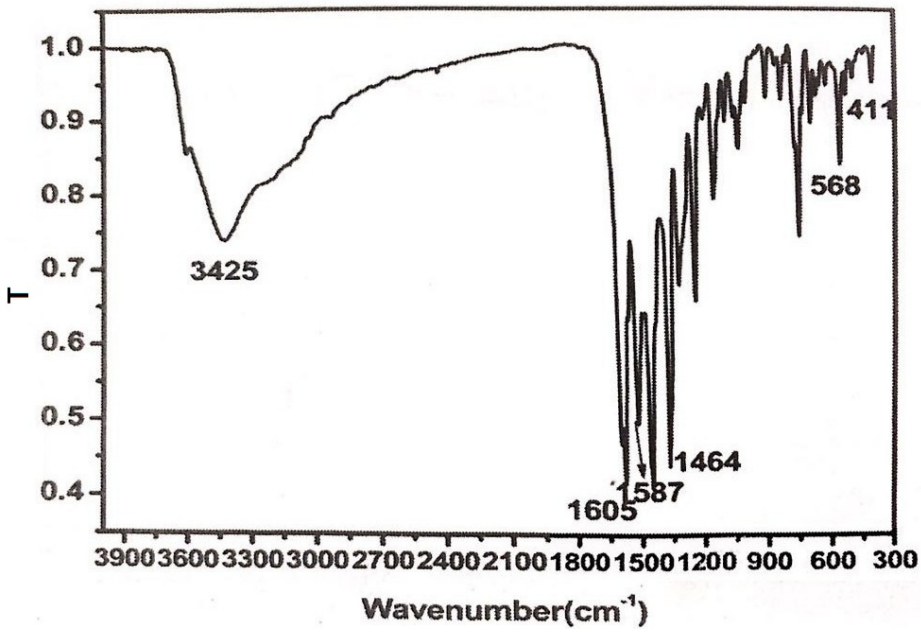
(a)


1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
T
3419
1612
1589
1469
570
416
4000 3600 3200 2800 2400 2000 1600 1200 800 400
Wavenumber(cm-1)

(b)

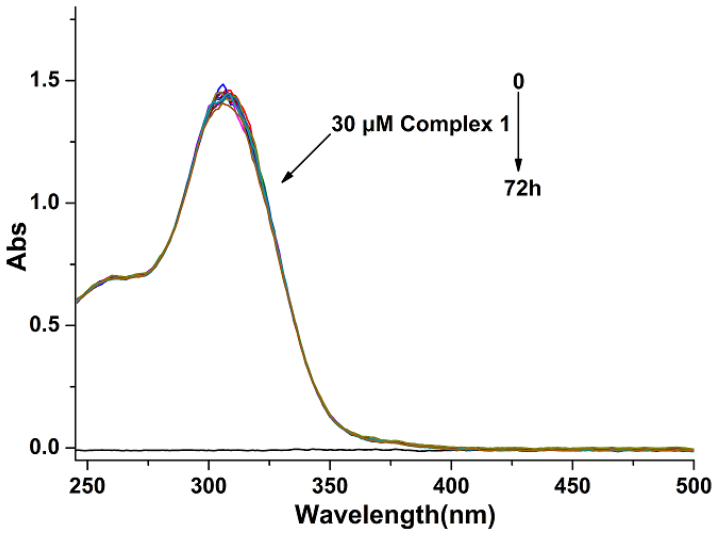


(c)

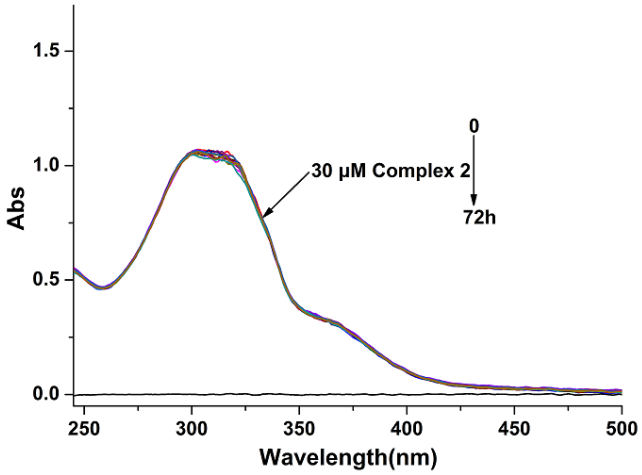


(d)

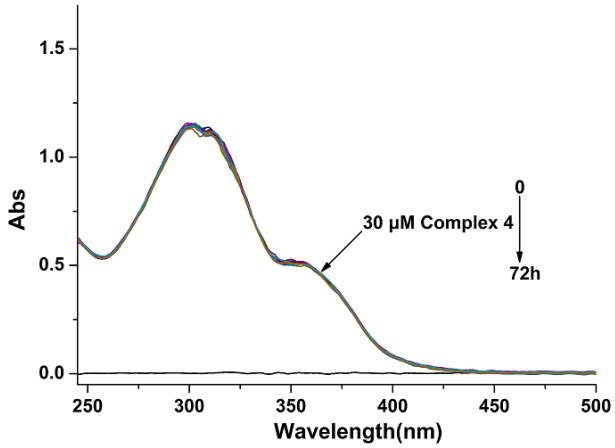
Fig. S2 The IR characterization data of Ce(III) complexes **1-4**. IR (ν/cm^{-1}, "s" stands for strong, "m" stands for medium, "w" stands for weak). (a) Infrared spectra of complex **1**, $\nu_{(O-H,\ N-H)}$ 3410s, $\nu_{(C=O)}$ 1650s, $\nu_{(C=N)}$ 1585s, $\nu_{(NO3^-)}$ 1480s, $\nu_{(Ce-N)}$ 443s, $\nu_{(Ce-O)}$ 530s. (b) Infrared spectra of complex **2**, $\nu_{(O-H,\ N-H)}$ 3419s, $\nu_{(C=O)}$ 1612s, $\nu_{(C=N)}$ 1589s, $\nu_{(NO3^-)}$ 1469s, $\nu_{(Ce-N)}$ 416s, $\nu_{(Ce-O)}$ 570s. (c) Infrared spectra of complex **3**, $\nu_{(O-H,\ N-H)}$ 3415s, $\nu_{(C=O)}$ 1639s, $\nu_{(C=N)}$ 1605s, $\nu_{(NO3^-)}$ 1475s, $\nu_{(Ce-N)}$ 426s, $\nu_{(Ce-O)}$ 558s. (d) Infrared spectra of complex **4**, $\nu_{(O-H,\ N-H)}$ 3425s, $\nu_{(C=O)}$ 1605s, $\nu_{(C=N)}$ 1587s, $\nu_{(NO3^-)}$ 1464s, $\nu_{(Ce-N)}$ 411s, $\nu_{(Ce-O)}$ 568s.



(a)



(b)



(c)

Fig. S3 The UV-vis absorption spectra of complex **1**(a), complex **2**(b), and complex **4**(c) recorded at 310 K in 2 mL MOPS/DMSO = 9/1 (v/v) solution, time scale: 0–72 h.

Table S1 Crystal data and structure refinement parameters for complex **1**.

CCDC No	1944188
Formula	$C_{24}H_{26}CeN_{13}O_{13}$
Formula weight	844.70
Radiation type	Mo-$K\alpha$, λ = 0.71073 Å
Crystal system	monoclinic
Space group	$C2/c$
Temperature (K)	298 (2)
a/Å	23.8474(12)
b/Å	9.3378(5)
c/Å	18.2600(16)
α/°	90
β/°	126.4470(10)
γ/°	90
V/Å^3	3270.9(4)
Z	4
D_{calc}/g cm^{-3}	1.715
μ/mm^{-1}	1.407
F_{000}	1692
ϑ range/°	3.09 to 28.28
GOF	1.036
Limiting indices	-29 ≤ h ≤ 29, -11 ≤ k ≤9, -22≤ l ≤ 22
Reflection collected	12617
R_{int}	0.06
R_1/wR_2 [I > 2σ(I)]	0.039/ 0.058
Largest diff. peak (e/Å^3) and hole	0.65 and -0.59

Table S2 Selected bond lengths (Å) and bond angles (°) for complex **1**.

Bond lengths, Å					
Ce1—O2	2.626 (2)	Ce1—O1	2.630 (2)	Ce1—N2	2.732(3)
Ce1—O3	2.733 (2)	Ce1—O5	2.646 (2)	Ce1—N1	2.768 (2)
Bond angles, °					
O2—Ce1—O2^{i}	167.97(11)	O2—Ce1—O1	128.76 (7)	O2—Ce1—O5	66.32 (8)
O2—Ce1—O1^{i}	62.68(7)	O1^{i}—Ce1—O1	74.11 (10)	O2^{i}—Ce1—O5	102.15 (7)
O5^{i}—Ce1—N2	129.55 (8)	O1—Ce1—N2^{i}	62.03 (8)	O1^{i}—Ce1—O5	119.52 (7)
O2—Ce1—N2^{i}	72.18 (8)	O5—Ce1—O3^{i}	69.03 (7)	O2—Ce1—O3^{i}	126.20 (7)
O2—Ce1—O3	47.29 (7)	N2—Ce1—O3^{i}	64.97 (8)	O3^{i}—Ce1—O3	130.58 (11)
O1—Ce1—O3^{i}	98.69 (7)	N2—Ce1—O3	160.61 (7)	O2—Ce1—N1	71.83 (8)
O1—Ce1—O3	121.07 (7)	O5—Ce1—O3	66.06 (7)	O3—Ce1—N1	113.66 (8)
O1—Ce1—N1^{i}	67.48 (7)	O5—Ce1—N1	67.48 (8)	O2—Ce1—N1^{i}	107.69 (7)
O1—Ce1—N1	116.24 (8)	O5—Ce1—N1^{i}	108.31 (8)	O3—Ce1—N1^{i}	64.36 (7)
N2—Ce1—N1^{i}	124.17 (8)	N2—Ce1—N1	59.01 (8)	N2—Ce1—N2^{i}	103.05 (11)
N1—Ce1—N1^{i}	175.68 (12)	O5^{i}—Ce1—O5	48.06 (9)	O1—Ce1—N2	58.40 (7)
O5—Ce1—N2	119.98 (8)				

Symmetry code: (i) -*x*, *y*, -*z*+1/2.

Table S3 Selected hydrogen-bond geometry (Å, °) for complex **1**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O7	0.84(3)	2.06(4)	2.843(5)	154(3)
O7—H7···O3^{i}	0.89(10)	2.23(10)	3.038(5)	150(10)

Symmetry code: (i) x, -y, z-1/2