

Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>	Zhong, Zeng, Liu & Luo (2006a)	10.1107/S1600536806041122	KERQEE
<i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
<i>Tris(quinolin-8-olato-κ²N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2006b)	10.1107/S1600536806050240	MEQHEW
<i>(8-Quinololinol-κ²N,O)bis(8-quinolinolato-κ²N,O)nickel(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
<i>(8-Quinololinol-κ²N,O)-bis(8-quinolinolato-κ²N,O)zinc(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')nickel(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007a)	10.1107/S1600536807004102	YEYGOZ
<i>(Dimethylglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')zinc(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007b)	10.1107/S1600536807004096	YEYGUF
<i>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITCPCO1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>	Zhong, Zeng, Yang & Luo (2007b)	10.1107/S160053680701879X	AVUJEG02
<i>Tetrakis(nitrato-κ²O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007c)	10.1107/S1600536807018831	CICDOI
<i>Bis(4,4'-bipyridine-κ²N,N')tetrakis(nitrato-κ²O,O')cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007d)	10.1107/S1600536807021502	YIDNEF
<i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
<i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>	Zhong, Yang, Luo & Xu (2007a)	10.1107/S1600536807028061	EDUTUT
<i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>	Zhong, Yang, Luo & Xu (2007b)	10.1107/S1600536807028693	RIGQEE
<i>(1,10-Phenanthroline-κ²N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007c)	10.1107/S1600536807030371	UDUMEM
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)nickel(II)</i>	Zhong, Yang, Luo & Xu (2007d)	10.1107/S1600536807031613	YEJGOJ01
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(isothiocyanato-κN)copper(II)</i>	Zhong, Yang, Luo & Xu (2007e)	10.1107/S1600536807033181	UFAPOH
<i>Bis(2,2'-bipyridyl-κ²N,N')bis(thiocyanato-κN)zinc(II)</i>	Zhong, Yang, Luo & Xu (2007f)	10.1107/S1600536807035337	TIGFAR
<i>(1,10-Phenanthroline-κ²N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007g)	10.1107/S1600536807035350	TIGFEV
<i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007j)	10.1107/S1600536807038676	VIKGAY
<i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007k)	10.1107/S1600536807039724	KILKIA
<i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007l)	10.1107/S1600536807040779	AFETAH
<i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007m)	10.1107/S160053680704086X	AFINAF
<i>catena-Poly[[bis(μ-anilinoacetato-κ²O:O')bis(μ-anilinoacetato-κ²O:O')bis(1,10-phenanthroline-κ²N,N')samarium(III)]-μ-anilinoacetato-κ²O:O']</i>	Zhong, Yang, Xie & Luo (2007a)	10.1107/S1600536807043528	PILDAQ
<i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>	Zhong, Yang, Xie & Luo (2007n)	10.1107/S1600536807045199	XILWIZ
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaaquacopper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007d)	10.1107/S1600536807051240	GIMZEI
<i>Hexaaquachromium(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007e)	10.1107/S1600536807051227	GIMZIM
<i>Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007f)	10.1107/S1600536807052051	QUKQES01
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007g)	10.1107/S1600536807053494	NIQLAB
<i>Hexaaquanickel(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007a)	10.1107/S1600536807054372	HIPZOW
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007h)	10.1107/S160053680705622X	XIRGOV
<i>Hexaaquazinc(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007b)	10.1107/S1600536807056498	XIRJEO
<i>catena-Poly[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-κ^2O:O']</i>	Zhong, Yang, Xie & Luo (2007i)	10.1107/S1600536807058540	HIQJOH
<i>Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
<i>(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dintrate dihydrate</i>	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
<i>catena-Poly[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-κ^4O:O'-[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-κ^4O:O'-di-μ-phenoxyacetato-κ^3O,O':κ^3O:O,O']</i>	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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Bis(4,4'-bipyridine- κ^2N,N')tetrakis-(nitrate- κ^2O,O')cerium(IV)

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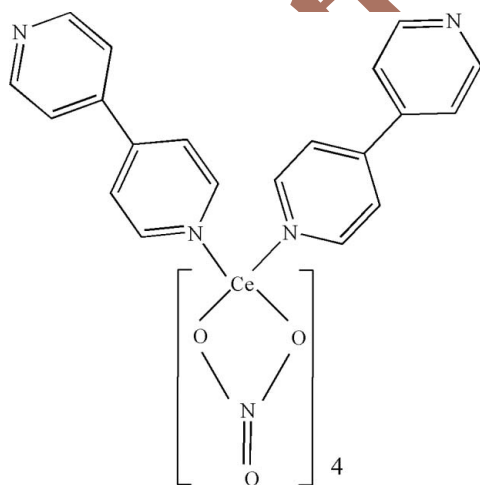
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.024; wR factor = 0.074; data-to-parameter ratio = 13.9.

The asymmetric unit of the title compound, $[Ce(NO_3)_4(C_{10}H_8N_2)_2]$, contains one half-molecule. The Ce^{IV} atom, lying on a crystallographic twofold rotation axis, is ten-coordinated by two N atoms of 4,4'-bipyridine and eight O atoms of four NO₃⁻ ligands. In the crystal structure, intra- and intermolecular C—H...O hydrogen bonds link the molecules into a supramolecular network.

Related literature

For general background, see: Allen *et al.* (1987); Benelli *et al.* (1992); Deborah *et al.* (2000); Farrugia *et al.* (2000); Miller & Drillon (2001*a,b*, 2002); Modolo & Odoj (1998).



Experimental

Crystal data

$[Ce(NO_3)_4(C_{10}H_8N_2)_2]$
 $M_r = 700.53$
Monoclinic, $C2/c$
 $a = 19.106$ (2) Å
 $b = 7.8107$ (8) Å
 $c = 19.000$ (7) Å
 $\beta = 116.004$ (2)°

$V = 2548.4$ (10) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.87$ mm⁻¹
 $T = 273$ (2) K
 $0.40 \times 0.33 \times 0.21$ mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.491$, $T_{max} = 0.675$

8401 measured reflections
2593 independent reflections
2537 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.074$
 $S = 1.07$
2593 reflections

186 parameters
H atom parameters constrained
 $\Delta\rho_{max} = 0.42$ e Å⁻³
 $\Delta\rho_{min} = -0.54$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ce1—O1	2.591 (3)	Ce1—O6	2.385 (2)
Ce1—O3	2.604 (3)	Ce1—N3	2.585 (3)
Ce1—O4	2.596 (3)		
O1—Ce1—O3	46.95 (8)	O4—Ce1—O6	49.94 (8)
O1—Ce1—O4	143.55 (9)	O1—Ce1—N3	72.52 (9)
O1—Ce1—O6	118.27 (8)	O3—Ce1—N3	69.32 (9)
O3—Ce1—O4	105.94 (9)	O4—Ce1—N3	126.48 (9)
O3—Ce1—O6	71.80 (9)	O6—Ce1—N3	80.59 (9)

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C3—H3...O6	0.93	2.391	3.030 (4)	125.71
C8—H8...O1 ⁱ	0.93	2.451	3.009 (3)	118.54
C9—H9...O2 ⁱⁱ	0.93	2.415	3.292 (4)	157.25
C10—H10...O3 ⁱⁱⁱ	0.93	2.252	3.149 (3)	161.36

Symmetry codes: (i) $x - \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $-x + 2, -y + 2, -z + 2$; (iii) $x, y + 1, z$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2243).

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Article retracted

supplementary materials

Article retracted

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Bis(4,4'-bipyridine- κ^2N,N')tetrakis(nitrato- κ^2O,O')cerium(IV)

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Comment

Molecular magnetic compounds, such as molecular ferro- and ferrimagnets, organic magnets, single-molecule magnets and high-spin molecules, have recently attracted attention (Miller & Drillon, 2001*a,b*, 2002). Owing to lanthanide metals unique physical and chemical properties, lanthanide complexes play an important role in special materials having optical, electronic, magnetic and biological importance (Benelli *et al.*, 1992; Deborah *et al.*, 2000; Farrugia *et al.*, 2000). More importantly, since the removal of lanthanides from radioactive high level liquid waste (HLLW) has been shown to improve the transmutation of long-lived transuranic elements to shortlived or even stable nuclides (Modolo & Odoj, 1998), the coordination chemistry of the 4f metals continues to attract interest. We herein report the crystal structure of the title compound, (I).

The asymmetric unit of the title compound, (I), contains one-half molecule (Fig. 1). The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The irregular ten-coordinate environment of the Ce^{IV} atom, lying on a crystallographic twofold rotation axis, is completed by the two N atoms of 4,4'-bipyridine and eight O atoms of four NO₃⁻ ligands (Table 1). The Ce—O bonds are between 2.385 (2)–2.604 (3) Å, while the Ce—N bond length is 2.585 (3) Å.

Rings A (N3/C1—C5) and B (N4/C6—C10) are, of course, planar and the dihedral angle between them is A/B = 37.56 (2)°.

As can be seen from the packing diagram (Fig. 2), the intra- and intermolecular C—H...O hydrogen bonds (Table 2) link the molecules into a supramolecular network structure, in which they may be effective in the stabilization of the crystal structure. Dipole-dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

For the preparation of the title compound, ammonium cerium(IV) nitrate (109.6 mg, 0.2 mmol), 4,4'-bipyridine (62.4 mg, 0.4 mmol), and distilled water (4000.0 mg) were placed into a Teflon-lined Parr bomb (23 ml) and sealed. The bomb was then heated under autogenous pressure for 7 d at 413 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals, which were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature (yield; 58.6 mg, 34%).

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

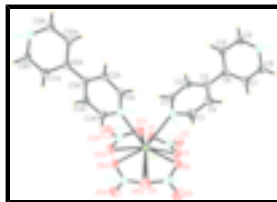


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $2 - x, y, 1 - z$].

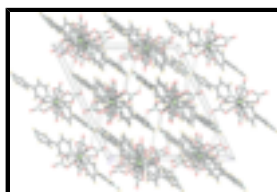


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Bis(4,4'-bipyridine- κ^2N,N')tetrakis(nitrato- κ^2O,O')cerium(IV)

Crystal data

[Ce(NO₃)₄(C₁₀H₈N₂)₂]

$M_r = 700.53$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 19.106\ (2)\ \text{\AA}$

$b = 7.8107\ (8)\ \text{\AA}$

$c = 19.000\ (7)\ \text{\AA}$

$\beta = 116.004\ (2)^\circ$

$V = 2548.4\ (10)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1384$

$D_x = 1.826\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 8351 reflections

$\theta = 2.5\text{--}29.5^\circ$

$\mu = 1.87\ \text{mm}^{-1}$

$T = 273\ (2)\ \text{K}$

Plane, colorless

$0.40 \times 0.33 \times 0.21\ \text{mm}$

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273\ (2)\ \text{K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.491, T_{\max} = 0.675$

8401 measured reflections

2593 independent reflections

2537 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.015$

$\theta_{\text{max}} = 26.7^\circ$

$\theta_{\text{min}} = 2.4^\circ$

$h = -23 \rightarrow 24$

$k = -9 \rightarrow 9$

$l = -24 \rightarrow 24$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.024$$

$$wR(F^2) = 0.074$$

$$S = 1.07$$

2593 reflections

186 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 3.3178P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ce1	1.0000	0.33854 (2)	0.7500	0.03153 (9)
O1	1.09207 (13)	0.4419 (3)	0.88993 (15)	0.0569 (6)
O2	1.0829 (2)	0.4126 (4)	1.00244 (16)	0.0779 (8)
O3	0.99750 (16)	0.3044 (3)	0.88522 (16)	0.0573 (6)
O4	0.92877 (16)	0.0719 (3)	0.66851 (18)	0.0669 (7)
O5	0.81807 (17)	-0.0040 (4)	0.65285 (18)	0.0730 (8)
O6	0.87813 (15)	0.2149 (3)	0.72864 (16)	0.0571 (6)
N1	1.05818 (17)	0.3858 (4)	0.92901 (17)	0.0504 (6)
N2	0.87324 (16)	0.0902 (3)	0.68201 (17)	0.0485 (6)
N3	0.93573 (16)	0.6018 (4)	0.78013 (17)	0.0477 (6)
C1	0.9748 (2)	0.7369 (4)	0.8261 (2)	0.0500 (7)
H1	1.0263	0.7512	0.8348	0.060*
C2	0.9466 (2)	0.8530 (4)	0.8604 (2)	0.0475 (7)
H2	0.9768	0.9434	0.8901	0.057*
C3	0.8644 (2)	0.5861 (5)	0.7672 (2)	0.0526 (7)
H3	0.8344	0.4991	0.7344	0.063*
C4	0.8317 (2)	0.6939 (4)	0.8003 (2)	0.0496 (7)
H4	0.7800	0.6774	0.7904	0.060*
C5	0.8740 (2)	0.8308 (3)	0.8494 (2)	0.0419 (7)
C6	0.84260 (17)	0.9442 (4)	0.89068 (17)	0.0421 (6)
C7	0.7947 (2)	0.8785 (4)	0.9185 (2)	0.0478 (7)
H7	0.7817	0.7629	0.9126	0.057*

supplementary materials

C8	0.7657 (2)	0.9864 (4)	0.9555 (2)	0.0531 (7)
H8	0.7325	0.9414	0.9749	0.064*
N4	0.7822 (2)	1.1529 (3)	0.9655 (2)	0.0545 (7)
C9	0.8276 (3)	1.2173 (5)	0.9398 (3)	0.0669 (10)
H9	0.8389	1.3337	0.9463	0.080*
C10	0.8600 (2)	1.1175 (5)	0.9028 (3)	0.0609 (10)
H10	0.8942	1.1661	0.8855	0.073*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.03102 (14)	0.02770 (13)	0.04625 (14)	0.000	0.02651 (10)	0.000
O1	0.0442 (12)	0.0573 (14)	0.0749 (15)	-0.0090 (10)	0.0314 (11)	0.0003 (12)
O2	0.097 (2)	0.078 (2)	0.0546 (14)	-0.0085 (18)	0.0294 (14)	-0.0023 (14)
O3	0.0553 (15)	0.0614 (13)	0.0687 (15)	-0.0134 (12)	0.0397 (13)	-0.0034 (12)
O4	0.0621 (16)	0.0520 (14)	0.105 (2)	-0.0035 (12)	0.0533 (15)	-0.0174 (14)
O5	0.0616 (16)	0.0654 (16)	0.0906 (19)	-0.0287 (13)	0.0321 (14)	-0.0171 (14)
O6	0.0552 (14)	0.0488 (12)	0.0831 (16)	-0.0098 (11)	0.0449 (13)	-0.0164 (12)
N1	0.0530 (16)	0.0455 (13)	0.0567 (15)	0.0008 (13)	0.0277 (13)	0.0032 (12)
N2	0.0481 (15)	0.0409 (13)	0.0605 (15)	-0.0058 (12)	0.0277 (12)	-0.0031 (12)
N3	0.0499 (15)	0.0440 (14)	0.0641 (15)	0.0027 (12)	0.0386 (13)	-0.0034 (12)
C1	0.0507 (18)	0.0407 (16)	0.077 (2)	-0.0029 (13)	0.0447 (16)	-0.0034 (15)
C2	0.0475 (18)	0.0409 (16)	0.069 (2)	-0.0060 (12)	0.0389 (17)	-0.0078 (13)
C3	0.0469 (17)	0.0502 (18)	0.0668 (19)	-0.0022 (14)	0.0306 (15)	-0.0151 (15)
C4	0.0412 (17)	0.0516 (16)	0.0623 (18)	0.0015 (13)	0.0284 (15)	-0.0098 (15)
C5	0.0434 (17)	0.0405 (16)	0.0520 (16)	0.0037 (11)	0.0302 (14)	0.0013 (11)
C6	0.0404 (14)	0.0412 (14)	0.0527 (15)	0.0023 (12)	0.0278 (12)	-0.0028 (12)
C7	0.0444 (17)	0.0458 (15)	0.0639 (18)	-0.0028 (13)	0.0336 (15)	-0.0062 (14)
C8	0.0475 (17)	0.0573 (19)	0.0694 (19)	-0.0006 (14)	0.0393 (15)	-0.0059 (16)
N4	0.0531 (18)	0.0536 (18)	0.0732 (19)	0.0049 (11)	0.0428 (16)	-0.0106 (12)
C9	0.079 (3)	0.0452 (18)	0.105 (3)	-0.0039 (18)	0.068 (2)	-0.015 (2)
C10	0.072 (2)	0.0422 (16)	0.099 (3)	-0.0057 (16)	0.065 (2)	-0.0103 (18)

Geometric parameters (\AA , $^\circ$)

Ce1—O1	2.591 (3)	C1—C2	1.359 (4)
Ce1—O3	2.604 (3)	C1—H1	0.9300
Ce1—O4	2.596 (3)	C2—C5	1.319 (5)
Ce1—O6	2.385 (2)	C2—H2	0.9300
Ce1—N3	2.585 (3)	C3—C4	1.356 (4)
Ce1—O6 ⁱ	2.386 (2)	C3—H3	0.9300
Ce1—N3 ⁱ	2.585 (3)	C4—C5	1.417 (5)
Ce1—O1 ⁱ	2.591 (3)	C4—H4	0.9300
Ce1—O4 ⁱ	2.596 (3)	C5—C6	1.474 (4)
Ce1—O3 ⁱ	2.604 (3)	C6—C7	1.344 (4)
Ce1—N2 ⁱ	2.925 (3)	C6—C10	1.388 (5)
O1—N1	1.258 (4)	C7—C8	1.362 (4)

O2—N1	1.279 (4)	C7—H7	0.9300
O3—N1	1.263 (4)	C8—N4	1.332 (4)
O4—N2	1.204 (4)	C8—H8	0.9300
O5—N2	1.203 (4)	N4—C9	1.272 (5)
O6—N2	1.292 (4)	C9—C10	1.368 (5)
N3—C3	1.280 (4)	C9—H9	0.9300
N3—C1	1.365 (5)	C10—H10	0.9300
O1—Ce1—O3	46.95 (8)	O1—Ce1—N2 ⁱ	72.25 (8)
O1—Ce1—O4	143.55 (9)	O4—Ce1—N2 ⁱ	81.22 (8)
O1—Ce1—O6	118.27 (8)	O4 ⁱ —Ce1—N2 ⁱ	24.28 (8)
O3—Ce1—O4	105.94 (9)	O3—Ce1—N2 ⁱ	82.31 (9)
O3—Ce1—O6	71.80 (9)	O3 ⁱ —Ce1—N2 ⁱ	89.89 (8)
O4—Ce1—O6	49.94 (8)	N1—O1—Ce1	101.74 (19)
O1—Ce1—N3	72.52 (9)	N1—O3—Ce1	100.94 (18)
O3—Ce1—N3	69.32 (9)	N2—O4—Ce1	93.31 (19)
O4—Ce1—N3	126.48 (9)	N2—O6—Ce1	101.16 (18)
O6—Ce1—N3	80.59 (9)	O1—N1—O3	110.4 (3)
O6—Ce1—O6 ⁱ	132.25 (13)	O1—N1—O2	123.1 (3)
O6—Ce1—N3 ⁱ	143.85 (9)	O3—N1—O2	126.5 (3)
O6 ⁱ —Ce1—N3 ⁱ	80.59 (9)	O5—N2—O4	120.3 (3)
O6 ⁱ —Ce1—N3	143.85 (10)	O5—N2—O6	124.2 (3)
N3 ⁱ —Ce1—N3	74.59 (12)	O4—N2—O6	115.5 (3)
O6—Ce1—O1 ⁱ	77.21 (9)	C3—N3—C1	115.8 (3)
O6 ⁱ —Ce1—O1 ⁱ	118.27 (8)	C3—N3—Ce1	116.8 (2)
N3 ⁱ —Ce1—O1 ⁱ	72.52 (9)	C1—N3—Ce1	125.2 (2)
N3—Ce1—O1 ⁱ	78.74 (9)	C2—C1—N3	127.0 (3)
O6 ⁱ —Ce1—O1	77.21 (9)	C2—C1—H1	116.5
N3 ⁱ —Ce1—O1	78.74 (9)	N3—C1—H1	116.5
O1 ⁱ —Ce1—O1	143.71 (12)	C5—C2—C1	116.6 (3)
O6 ⁱ —Ce1—O4	89.66 (9)	C5—C2—H2	121.7
N3 ⁱ —Ce1—O4	133.00 (9)	C1—C2—H2	121.7
O1 ⁱ —Ce1—O4	72.27 (9)	N3—C3—C4	121.3 (3)
O6—Ce1—O4 ⁱ	89.66 (9)	N3—C3—H3	119.3
O6 ⁱ —Ce1—O4 ⁱ	49.94 (8)	C4—C3—H3	119.3
N3 ⁱ —Ce1—O4 ⁱ	126.48 (9)	C3—C4—C5	121.9 (3)
N3—Ce1—O4 ⁱ	133.00 (9)	C3—C4—H4	119.1
O1 ⁱ —Ce1—O4 ⁱ	143.55 (9)	C5—C4—H4	119.1
O1—Ce1—O4 ⁱ	72.27 (9)	C2—C5—C4	117.4 (3)
O4—Ce1—O4 ⁱ	73.30 (14)	C2—C5—C6	118.8 (3)
O6 ⁱ —Ce1—O3	103.27 (9)	C4—C5—C6	123.8 (3)
N3 ⁱ —Ce1—O3	121.06 (8)	C7—C6—C10	117.6 (3)
O1 ⁱ —Ce1—O3	138.28 (8)	C7—C6—C5	119.1 (3)

supplementary materials

O4 ⁱ —Ce1—O3	63.97 (9)	C10—C6—C5	123.3 (3)
O6—Ce1—O3 ⁱ	103.27 (9)	C6—C7—C8	117.9 (3)
O6 ⁱ —Ce1—O3 ⁱ	71.80 (9)	C6—C7—H7	121.1
N3 ⁱ —Ce1—O3 ⁱ	69.32 (9)	C8—C7—H7	121.1
N3—Ce1—O3 ⁱ	121.06 (8)	N4—C8—C7	123.7 (3)
O1 ⁱ —Ce1—O3 ⁱ	46.95 (8)	N4—C8—H8	118.2
O1—Ce1—O3 ⁱ	138.27 (8)	C7—C8—H8	118.2
O4—Ce1—O3 ⁱ	63.97 (9)	C9—N4—C8	119.3 (3)
O4 ⁱ —Ce1—O3 ⁱ	105.94 (9)	N4—C9—C10	120.8 (4)
O3—Ce1—O3 ⁱ	168.25 (12)	N4—C9—H9	119.6
O6—Ce1—N2 ⁱ	111.37 (9)	C10—C9—H9	119.6
O6 ⁱ —Ce1—N2 ⁱ	25.69 (8)	C9—C10—C6	120.7 (3)
N3 ⁱ —Ce1—N2 ⁱ	104.09 (8)	C9—C10—H10	119.6
N3—Ce1—N2 ⁱ	144.26 (9)	C6—C10—H10	119.6
O1 ⁱ —Ce1—N2 ⁱ	135.89 (7)		

Symmetry codes: (i) $-x+2, y, -z+3/2$.

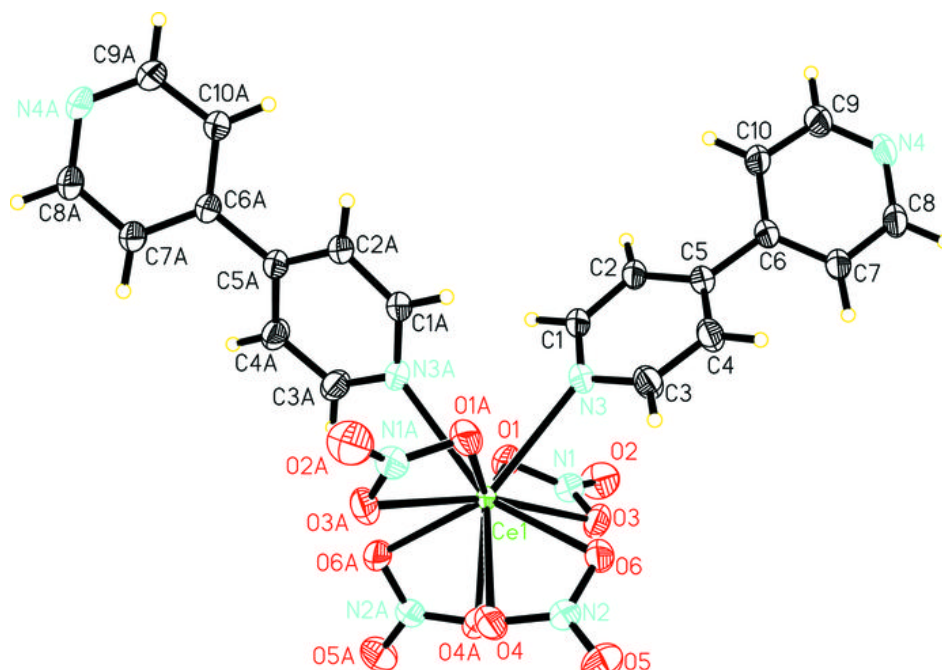
Table 2

Table 1. Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C3—H3...O6	0.93	2.391	3.030 (4)	125.71
C8—H8...O1 ⁱ	0.93	2.451	3.009 (3)	118.54
C9—H9...O2 ⁱⁱ	0.93	2.415	3.292 (4)	157.25
C10—H10...O3 ⁱⁱⁱ	0.93	2.252	3.149 (3)	161.36

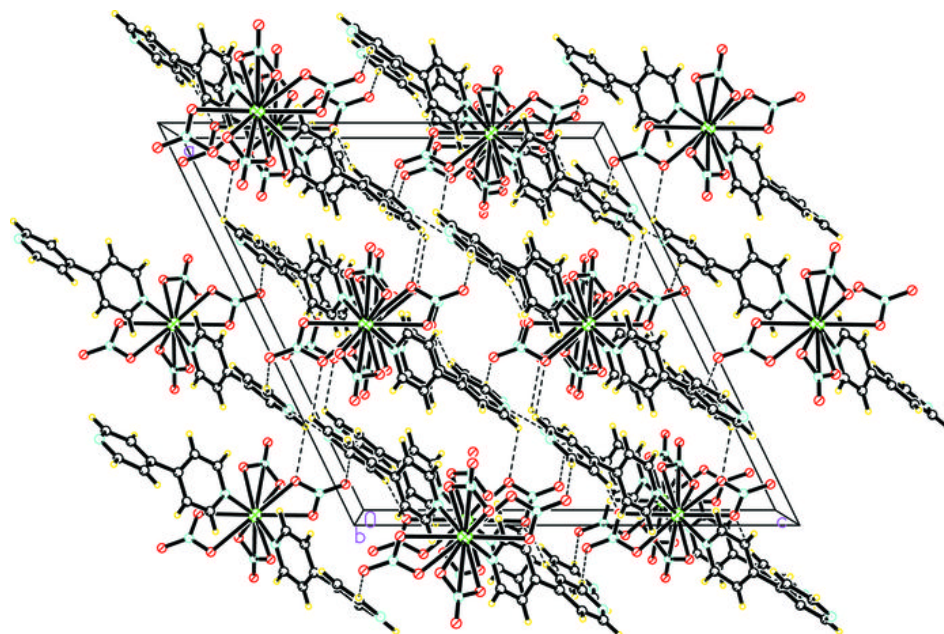
Symmetry codes: (i) $x - 1/2, y + 1/2, z$; (ii) $-x + 2, -y + 2, -z + 2$; (iii) $x, y + 1, z$.

Fig. 1



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Fig. 2



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