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Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. 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	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^2N^2:$N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

 doi:10.1107/S1600536809054300

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O′-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diyl-bis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)

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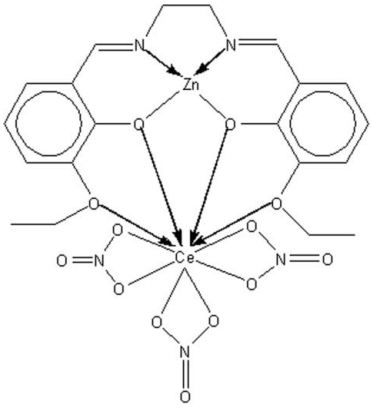
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.020; wR factor = 0.048; data-to-parameter ratio = 17.1.

In the title heteronuclear Zn^{II}–Ce^{III} complex (systematic name: {6,6′-diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}trinitrato-1$\kappa^6O,O'$-cerium(III)zinc(II)), $[CeZn(C_{20}H_{22}N_2O_4)(NO_3)_3]$, with the hexadentate Schiff base compartmental ligand *N*,*N*′-bis(3-ethoxysalicylidene)ethylenediamine, the Zn and Ce atoms are doubly bridged by two phenolate O atoms provided by the Schiff base ligand. The coordination of the Zn atom is square planar with the donor centers of two imine N atoms and two phenolate O atoms. The cerium(III) center has a decacoordination environment of O atoms, involving the phenolate O atoms, two ethoxy O atoms and two O atoms each from the three nitrate ligands. Some weak C—H···O and O···Zn [O···Zn = 3.156 (4) Å] interactions generate a two-dimensional zigzag sheet.

Related literature

For related literature, see: Baggio *et al.* (2000); Caravan *et al.* (1999); Edder *et al.* (2000); Knoer *et al.* (2005); Sui *et al.* (2006).



Experimental

Crystal data

$[CeZn(C_{20}H_{22}N_2O_4)(NO_3)_3]$
M_r = 745.92
Orthorhombic, $P2_12_12_1$
a = 8.6418 (14) Å
b = 13.904 (2) Å
c = 21.157 (3) Å
V = 2542.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.79 mm^{-1}
T = 293 (2) K
0.31 × 0.22 × 0.20 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.494, T_{max} = 0.572
19190 measured reflections
6211 independent reflections
5407 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.048
S = 1.01
6211 reflections
363 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 2625 Friedel pairs
Flack parameter: 0.017 (9)

Table 1
Selected bond lengths (Å).

Ce1—O1	2.4293 (16)	Ce1—O11	2.539 (2)
Ce1—O2	2.4712 (17)	Ce1—O12	2.576 (2)
Ce1—O4	2.6917 (18)	O3—Ce1	2.6572 (18)
Ce1—O5	2.607 (2)	Zn1—O1	1.9078 (18)
Ce1—O6	2.575 (2)	Zn1—O2	1.9039 (18)
Ce1—O8	2.571 (2)	Zn1—N1	1.922 (2)
Ce1—O9	2.610 (2)	Zn1—N2	1.913 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O7^{i}	0.93	2.36	3.275 (4)	168
C9—H9A···O7^{ii}	0.97	2.43	3.286 (4)	147
C17—H17B···O9	0.97	2.87	3.337 (4)	111
C20—H20A···O8	0.96	2.45	3.166 (4)	131

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2253).

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supplementary materials

Acta Cryst. (2007). E**63**, m2089-m2090 [**doi:10.1107/S1600536807032564**]

{μ-6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}trinitratocerium(III)zinc(II)

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Comment

The potential applications of trivalent lanthanide complexes as contrast agent for magnetic resonance imaging and stains for fluorescence imaging have prompted considerable interest in the preparation, magnetic and optical properties of 3 d-4f hetorometallic dinuclear complexes (Baggio *et al.*, 2000; Caravan *et al.*, 1999; Edder *et al.*, 2000; Knoer *et al.*, 2005). As part of our investigations into the structure and applications of 3 d-4f hetorometallic Schiff base complexes (Sui *et al.*, 2006), we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new Zn^{II}—Ce^{III} complex with salen-type Schiff base *N*,*N*'-bis(3-ethoxysalicylidene) ethylenediamine(H_2L).

Complex (I) crystallizes in the space group $P2_12_12_1$, with zinc and cerium doubly bridged by two phenolate O atoms provided by a salen-type Schiff base ligand. The inner salen-type cavity is occupied by zinc(II), while cerium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand. The dihedral angles between the mean planes of Zn1/O1/O2 and Ce1/O1/O2 is 3.62 (11)° suggesting that the bridging moiety is almost planar; the deviation of atoms from the least squares Zn1/O1/O2/Ce1 plane being 0.0310 (3)Å for Zn, 0.0208 (3)Å for Ce, −0.0262 (2)Å for O1 and −0.0256 (2)Å for O2.

The cerium(III) center in (I) has a decacoordination environment of O atoms. In addition to the phenolate ligands, two ethoxy O atoms coordinate to this metal center, two O atoms from each of the three nitrates chelate to cerium to complete the decacoordination. The three kinds of Ce—O bond distances are significantly different, the shortest being the Ce—O(phenolate) and longest being the Ce—*O*(ethoxy) separations.

The coordination of zinc(II) is approximately square planar. The donor centers are alternatively above and below the mean N_2O_2 plane with an average deviation from the plane of 0.0879 (2) Å, while Zn1 is 0.0453 (2)Å below this square plane.

Adjacent molecules are held together by weak interactions (O10···Zn1=3.156 (4) Å, C7—H7···$O7^{i}$=3.275 (4) and C9—H9A···$O7^{ii}$=3.286 (4); symmetry codes:(i)-*x*, *y* − 1/2, 1/2 − *z*; (ii)*x* − 1, *y*, *z*). these link the molecules into a two-dimensional zigzag sheet(Fig 2).

Experimental

H_2L was prepared by the 2:1 condensation of 3-ethoxysalicylaldehyde and ethylenediamine in methanol. Complex (I) was obtained by the treatment of zinc(II) acetate dihydrate (0.188 g, 1 mmol) with H_2L(0.356 g, 1 mmol) in methanol solution (80 ml) under reflux for 3 h and then for another 3 h after the addition of cerium(III) nitrate hexahydrate (0.434 g, 1 mmol). The reaction mixture was cooled and the resulting precipitate was filtered off, washed with diethyl ether and dried *in vacuo*. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation at room temperature of a methanol

solution. Analysis calculated for $C_{20}H_{22}CeN_5O_{13}Zn$: C 32.20, H 2.97, Ce 18.78, N 9.39,Zn 8.77%; found: C 32.00, H 2.85, Ce 18.10, N 9.40, Zn 8.68%. IR(KBr, cm^{-1}): 1642(C=N), 1386,1490(nitrate).

Refinement

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.97 (methylene) and 0.96 Å (methyl), and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms.

Figures

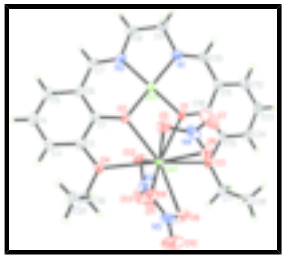

Fig.1. The molecular structure of (I), showing 30% probability displacement ellipsoids. All the H atoms on carbon have been omitted for clarity.

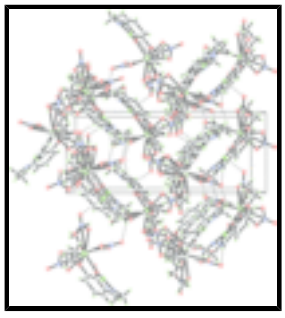

Fig.2. The packing diagram of (I), viewed along the *b* axis; hydrogen bonds are shown as dashed lines.

Table 1. Selected geometric parameters (Å).

{6,6'-diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-\ 1κ^4*O*^{1},*O*$^{1'}$,*O*^{6},*O*$^{6'}$:2κ^4*O*^{1},\ *N*,*N*',*O*$^{1'}$}trinitrato-1κ^6*O*,*O*'-\ cerium(III)zinc(II))

Crystal data

$[CeZn(C_{20}H_{22}N_2O_4)(NO_3)_3]$	F_{000} = 1476
M_r = 745.92	D_x = 1.949 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 19190 reflections
a = 8.6418 (14) Å	θ = 1.8–28.4°
b = 13.904 (2) Å	μ = 2.79 mm^{-1}
c = 21.157 (3) Å	*T* = 293 (2) K
V = 2542.2 (7) $Å^3$	Block, yellow
Z = 4	0.31 × 0.22 × 0.20 mm

Data collection

Bruker APEX II area-detector	6211 independent reflections

diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 0 pixels mm^{-1}
T = 293(2) K
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.494, T_{max} = 0.572
19190 measured reflections

5407 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 28.4°
θ_{min} = 1.8°
h = −11→11
k = −17→18
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.048
S = 1.01
6211 reflections
363 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.36 e $Å^{-3}$
Extinction correction: none
Absolute structure: Flack (1983), 2611 Friedel pairs
Flack parameter: 0.017 (9)

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 ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}
O3	0.1524 (2)	1.17630 (12)	0.07489 (8)	0.0360 (4)
Ce1	0.258940 (14)	0.999427 (11)	0.094132 (6)	0.03050 (4)
Zn1	−0.06773 (4)	0.94379 (2)	0.182756 (15)	0.03842 (8)
O1	0.03669 (19)	1.05629 (13)	0.15369 (8)	0.0333 (4)
O2	0.0841 (2)	0.87424 (12)	0.13626 (8)	0.0365 (4)
N1	−0.2006 (2)	1.01384 (18)	0.23926 (10)	0.0378 (5)
C2	0.2071 (3)	0.74270 (18)	0.09013 (12)	0.0330 (5)

N3	0.1260 (3)	0.9950 (2)	−0.03637 (11)	0.0477 (5)
O11	0.2673 (2)	1.01379 (16)	−0.02545 (9)	0.0552 (6)
N2	−0.1791 (3)	0.83178 (18)	0.20894 (11)	0.0369 (6)
O12	0.0487 (2)	0.96785 (17)	0.01035 (9)	0.0582 (6)
C1	0.0857 (3)	0.77948 (18)	0.12660 (12)	0.0308 (6)
O13	0.0704 (3)	1.00237 (19)	−0.08932 (9)	0.0772 (7)
C10	−0.2207 (3)	1.1039 (2)	0.23934 (12)	0.0386 (6)
H10	−0.2889	1.1292	0.2691	0.046*
C8	−0.3148 (3)	0.8559 (2)	0.24897 (14)	0.0460 (7)
H8A	−0.3351	0.8045	0.2788	0.055*
H8B	−0.4061	0.8649	0.2229	0.055*
C7	−0.1515 (3)	0.7458 (2)	0.19162 (14)	0.0390 (7)
H7	−0.2175	0.6979	0.2064	0.047*
C6	−0.0260 (3)	0.71665 (19)	0.15084 (12)	0.0342 (6)
C9	−0.2763 (3)	0.9481 (2)	0.28377 (12)	0.0442 (7)
H9A	−0.3701	0.9772	0.3002	0.053*
H9B	−0.2078	0.9345	0.3190	0.053*
O4	0.3101 (2)	0.81227 (13)	0.06922 (9)	0.0375 (4)
O6	0.3652 (2)	1.11280 (15)	0.17999 (11)	0.0512 (5)
O5	0.3227 (3)	0.96826 (17)	0.21283 (10)	0.0547 (6)
N4	0.3655 (3)	1.0532 (2)	0.22490 (12)	0.0499 (7)
C3	0.2149 (4)	0.6458 (2)	0.07543 (13)	0.0423 (7)
H3	0.2962	0.6222	0.0512	0.051*
O8	0.5474 (2)	0.96187 (15)	0.11091 (10)	0.0549 (5)
O7	0.4055 (3)	1.0771 (2)	0.27813 (10)	0.0801 (9)
C19	0.4453 (3)	0.7805 (2)	0.03486 (13)	0.0432 (7)
H19A	0.4880	0.8343	0.0115	0.052*
H19B	0.4150	0.7315	0.0046	0.052*
C17	0.2251 (3)	1.2415 (2)	0.02918 (12)	0.0421 (7)
H17A	0.1457	1.2807	0.0095	0.051*
H17B	0.2742	1.2037	−0.0038	0.051*
C4	0.1003 (4)	0.5844 (2)	0.09727 (14)	0.0494 (7)
H4	0.1033	0.5195	0.0867	0.059*
O9	0.5073 (3)	1.08024 (19)	0.04820 (11)	0.0674 (7)
C16	−0.0230 (3)	1.14433 (18)	0.15577 (11)	0.0313 (6)
N5	0.6032 (3)	1.0273 (2)	0.07704 (12)	0.0531 (8)
C5	−0.0159 (4)	0.6184 (2)	0.13382 (14)	0.0452 (7)
H5	−0.0912	0.5760	0.1482	0.054*
C14	−0.0200 (3)	1.3047 (2)	0.11232 (14)	0.0424 (7)
H14	0.0197	1.3489	0.0836	0.051*
C20	0.5678 (4)	0.7401 (2)	0.07790 (16)	0.0581 (9)
H20A	0.5984	0.7884	0.1079	0.087*
H20B	0.6559	0.7210	0.0533	0.087*
H20C	0.5273	0.6854	0.1000	0.087*
C11	−0.1455 (3)	1.1711 (2)	0.19646 (13)	0.0372 (7)
C12	−0.1973 (4)	1.2667 (2)	0.19550 (15)	0.0455 (8)
H12	−0.2734	1.2863	0.2238	0.055*
C15	0.0375 (3)	1.21237 (18)	0.11412 (12)	0.0319 (6)
O10	0.7407 (3)	1.0400 (3)	0.07259 (14)	0.0962 (9)

C13	−0.1373 (4)	1.3313 (2)	0.15352 (15)	0.0516 (8)
H13	−0.1755	1.3938	0.1525	0.062*
C18	0.3432 (4)	1.3058 (2)	0.05866 (16)	0.0563 (9)
H18A	0.2930	1.3498	0.0870	0.084*
H18B	0.3959	1.3413	0.0262	0.084*
H18C	0.4166	1.2677	0.0817	0.084*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0427 (10)	0.0243 (10)	0.0411 (10)	−0.0017 (8)	0.0064 (8)	0.0068 (8)
Ce1	0.03051 (6)	0.02503 (7)	0.03596 (7)	−0.00109 (8)	0.00364 (5)	0.00254 (7)
Zn1	0.03818 (16)	0.03034 (16)	0.04675 (16)	−0.00153 (14)	0.00994 (14)	0.00350 (15)
O1	0.0324 (9)	0.0221 (9)	0.0455 (10)	0.0025 (8)	0.0094 (7)	0.0046 (8)
O2	0.0391 (10)	0.0214 (9)	0.0489 (11)	−0.0013 (8)	0.0137 (9)	0.0013 (8)
N1	0.0370 (10)	0.0386 (15)	0.0377 (11)	0.0013 (10)	0.0053 (8)	0.0027 (10)
C2	0.0382 (13)	0.0242 (13)	0.0366 (14)	−0.0008 (10)	−0.0052 (11)	0.0029 (11)
N3	0.0623 (15)	0.0346 (13)	0.0461 (13)	0.0027 (14)	−0.0048 (11)	−0.0069 (14)
O11	0.0560 (13)	0.0659 (16)	0.0437 (10)	−0.0115 (13)	0.0044 (9)	−0.0018 (9)
N2	0.0352 (13)	0.0366 (14)	0.0389 (13)	−0.0050 (10)	0.0038 (10)	0.0097 (10)
O12	0.0476 (12)	0.0795 (18)	0.0475 (12)	−0.0123 (11)	−0.0001 (10)	−0.0032 (10)
C1	0.0335 (14)	0.0242 (13)	0.0346 (13)	−0.0009 (11)	−0.0038 (11)	0.0027 (10)
O13	0.1096 (19)	0.0728 (17)	0.0491 (12)	−0.0055 (18)	−0.0273 (12)	−0.0007 (15)
C10	0.0377 (15)	0.0407 (17)	0.0375 (14)	0.0074 (13)	0.0058 (11)	−0.0004 (12)
C8	0.0364 (15)	0.055 (2)	0.0471 (17)	−0.0042 (14)	0.0103 (13)	0.0123 (14)
C7	0.0364 (15)	0.0335 (16)	0.0471 (17)	−0.0108 (12)	−0.0027 (13)	0.0137 (13)
C6	0.0385 (15)	0.0267 (14)	0.0375 (14)	−0.0044 (11)	−0.0045 (11)	0.0048 (11)
C9	0.0444 (16)	0.0456 (17)	0.0426 (14)	0.0042 (14)	0.0121 (12)	0.0091 (13)
O4	0.0355 (10)	0.0300 (11)	0.0469 (11)	0.0012 (8)	0.0088 (8)	−0.0020 (8)
O6	0.0581 (13)	0.0451 (13)	0.0503 (12)	0.0004 (10)	−0.0065 (11)	−0.0019 (11)
O5	0.0580 (14)	0.0570 (16)	0.0490 (12)	0.0053 (11)	0.0024 (10)	0.0148 (10)
N4	0.0385 (13)	0.065 (2)	0.0465 (16)	0.0180 (14)	−0.0025 (11)	−0.0092 (15)
C3	0.0536 (18)	0.0287 (15)	0.0448 (15)	0.0051 (13)	−0.0058 (13)	−0.0029 (12)
O8	0.0402 (11)	0.0460 (13)	0.0787 (15)	0.0012 (10)	0.0019 (10)	0.0088 (11)
O7	0.0849 (18)	0.111 (2)	0.0440 (12)	0.0480 (17)	−0.0205 (12)	−0.0234 (14)
C19	0.0379 (15)	0.0417 (17)	0.0500 (17)	0.0051 (13)	0.0093 (13)	−0.0039 (13)
C17	0.0559 (18)	0.0301 (15)	0.0404 (14)	−0.0031 (13)	0.0087 (13)	0.0099 (11)
C4	0.064 (2)	0.0234 (15)	0.0608 (19)	−0.0002 (13)	−0.0094 (16)	−0.0015 (13)
O9	0.0461 (13)	0.087 (2)	0.0695 (15)	−0.0173 (12)	0.0004 (11)	0.0304 (14)
C16	0.0346 (14)	0.0236 (14)	0.0358 (13)	0.0012 (10)	−0.0050 (10)	0.0010 (10)
N5	0.0366 (13)	0.069 (2)	0.0537 (15)	−0.0074 (13)	0.0065 (11)	−0.0126 (13)
C5	0.0583 (19)	0.0249 (15)	0.0525 (17)	−0.0106 (13)	−0.0065 (14)	0.0050 (12)
C14	0.0429 (16)	0.0293 (16)	0.0550 (18)	0.0002 (12)	−0.0027 (13)	0.0076 (13)
C20	0.0496 (18)	0.052 (2)	0.073 (2)	0.0172 (17)	−0.0047 (17)	−0.0103 (16)
C11	0.0381 (15)	0.0324 (15)	0.0412 (17)	0.0037 (12)	0.0019 (12)	0.0015 (12)
C12	0.0413 (17)	0.0392 (18)	0.0559 (19)	0.0105 (13)	0.0077 (13)	−0.0042 (14)
C15	0.0316 (14)	0.0264 (14)	0.0376 (14)	−0.0017 (11)	−0.0039 (10)	−0.0021 (11)
O10	0.0352 (12)	0.146 (3)	0.107 (2)	−0.0259 (16)	0.0072 (13)	0.000 (2)

C13	0.0542 (19)	0.0285 (16)	0.072 (2)	0.0148 (14)	−0.0005 (16)	−0.0035 (15)
C18	0.062 (2)	0.043 (2)	0.064 (2)	−0.0126 (16)	0.0158 (16)	−0.0037 (16)

Geometric parameters (Å, °)

O3—C15	1.388 (3)	C6—C5	1.416 (4)
O3—C17	1.467 (3)	C9—H9A	0.9700
Ce1—O1	2.4293 (16)	C9—H9B	0.9700
Ce1—O2	2.4712 (17)	O4—C19	1.445 (3)
Ce1—O4	2.6917 (18)	O6—N4	1.261 (3)
Ce1—O5	2.607 (2)	O5—N4	1.264 (4)
Ce1—O6	2.575 (2)	N4—O7	1.224 (3)
Ce1—O8	2.571 (2)	C3—C4	1.387 (4)
Ce1—O9	2.610 (2)	C3—H3	0.9300
Ce1—O11	2.539 (2)	O8—N5	1.255 (3)
Ce1—O12	2.576 (2)	C19—C20	1.505 (4)
O3—Ce1	2.6572 (18)	C19—H19A	0.9700
Zn1—O1	1.9078 (18)	C19—H19B	0.9700
Zn1—O2	1.9039 (18)	C17—C18	1.493 (4)
Zn1—N1	1.922 (2)	C17—H17A	0.9700
Zn1—N2	1.913 (2)	C17—H17B	0.9700
O1—C16	1.329 (3)	C4—C5	1.352 (4)
O2—C1	1.333 (3)	C4—H4	0.9300
N1—C10	1.264 (3)	O9—N5	1.265 (3)
N1—C9	1.466 (3)	C16—C15	1.395 (3)
C2—C3	1.384 (4)	C16—C11	1.414 (4)
C2—O4	1.387 (3)	N5—O10	1.205 (3)
C2—C1	1.399 (4)	C5—H5	0.9300
N3—O13	1.223 (3)	C14—C15	1.376 (4)
N3—O12	1.251 (3)	C14—C13	1.388 (4)
N3—O11	1.269 (3)	C14—H14	0.9300
N2—C7	1.273 (4)	C20—H20A	0.9600
N2—C8	1.485 (4)	C20—H20B	0.9600
C1—C6	1.399 (4)	C20—H20C	0.9600
C10—C11	1.456 (4)	C11—C12	1.403 (4)
C10—H10	0.9300	C12—C13	1.365 (4)
C8—C9	1.515 (4)	C12—H12	0.9300
C8—H8A	0.9700	C13—H13	0.9300
C8—H8B	0.9700	C18—H18A	0.9600
C7—C6	1.444 (4)	C18—H18B	0.9600
C7—H7	0.9300	C18—H18C	0.9600
C15—O3—C17	118.5 (2)	N2—C8—H8A	110.3
C15—O3—Ce1	119.39 (14)	C9—C8—H8A	110.3
C17—O3—Ce1	121.63 (15)	N2—C8—H8B	110.3
O1—Ce1—O2	63.82 (6)	C9—C8—H8B	110.3
O1—Ce1—O11	120.91 (6)	H8A—C8—H8B	108.5
O2—Ce1—O11	115.61 (7)	N2—C7—C6	125.1 (3)
O1—Ce1—O8	139.54 (6)	N2—C7—H7	117.4
O2—Ce1—O8	113.57 (7)	C6—C7—H7	117.4

O11—Ce1—O8	97.24 (7)	C1—C6—C5	117.8 (3)
O1—Ce1—O6	73.55 (7)	C1—C6—C7	124.2 (2)
O2—Ce1—O6	113.26 (6)	C5—C6—C7	118.0 (2)
O11—Ce1—O6	130.15 (7)	N1—C9—C8	108.3 (2)
O8—Ce1—O6	71.40 (7)	N1—C9—H9A	110.0
O1—Ce1—O12	81.65 (7)	C8—C9—H9A	110.0
O2—Ce1—O12	72.36 (7)	N1—C9—H9B	110.0
O11—Ce1—O12	49.29 (7)	C8—C9—H9B	110.0
O8—Ce1—O12	138.08 (7)	H9A—C9—H9B	108.4
O6—Ce1—O12	147.30 (7)	C2—O4—C19	117.8 (2)
O1—Ce1—O5	73.83 (7)	C2—O4—Ce1	120.42 (14)
O2—Ce1—O5	70.41 (7)	C19—O4—Ce1	121.82 (15)
O11—Ce1—O5	165.21 (7)	N4—O6—Ce1	97.47 (18)
O8—Ce1—O5	68.19 (7)	N4—O5—Ce1	95.80 (17)
O6—Ce1—O5	49.22 (7)	O7—N4—O6	121.0 (3)
O12—Ce1—O5	141.58 (7)	O7—N4—O5	121.5 (3)
O1—Ce1—O9	134.68 (8)	O6—N4—O5	117.5 (3)
O2—Ce1—O9	160.08 (7)	C2—C3—C4	119.3 (3)
O11—Ce1—O9	64.65 (7)	C2—C3—H3	120.3
O8—Ce1—O9	48.83 (7)	C4—C3—H3	120.3
O6—Ce1—O9	72.88 (8)	N5—O8—Ce1	98.45 (17)
O12—Ce1—O9	113.40 (7)	O4—C19—C20	112.2 (2)
O5—Ce1—O9	104.85 (8)	O4—C19—H19A	109.2
O1—Ce1—O3	60.29 (6)	C20—C19—H19A	109.2
O2—Ce1—O3	119.69 (6)	O4—C19—H19B	109.2
O11—Ce1—O3	77.55 (6)	C20—C19—H19B	109.2
O8—Ce1—O3	123.02 (6)	H19A—C19—H19B	107.9
O6—Ce1—O3	70.43 (6)	O3—C17—C18	112.8 (2)
O12—Ce1—O3	78.93 (7)	O3—C17—H17A	109.0
O5—Ce1—O3	112.00 (6)	C18—C17—H17A	109.0
O9—Ce1—O3	80.18 (7)	O3—C17—H17B	109.0
O1—Ce1—O4	123.10 (6)	C18—C17—H17B	109.0
O2—Ce1—O4	59.35 (5)	H17A—C17—H17B	107.8
O11—Ce1—O4	82.89 (6)	C5—C4—C3	120.3 (3)
O8—Ce1—O4	70.81 (6)	C5—C4—H4	119.8
O6—Ce1—O4	132.18 (6)	C3—C4—H4	119.8
O12—Ce1—O4	79.42 (7)	N5—O9—Ce1	96.24 (16)
O5—Ce1—O4	89.61 (7)	O1—C16—C15	117.3 (2)
O9—Ce1—O4	102.01 (7)	O1—C16—C11	123.6 (2)
O3—Ce1—O4	157.17 (6)	C15—C16—C11	119.1 (2)
O2—Zn1—O1	85.63 (7)	O10—N5—O8	122.0 (3)
O2—Zn1—N2	94.75 (9)	O10—N5—O9	121.5 (3)
O1—Zn1—N2	177.44 (9)	O8—N5—O9	116.4 (2)
O2—Zn1—N1	171.99 (9)	C4—C5—C6	121.9 (3)
O1—Zn1—N1	93.87 (9)	C4—C5—H5	119.0
N2—Zn1—N1	86.10 (11)	C6—C5—H5	119.0
C16—O1—Zn1	124.13 (15)	C15—C14—C13	119.7 (3)
C16—O1—Ce1	128.59 (15)	C15—C14—H14	120.2
Zn1—O1—Ce1	105.92 (8)	C13—C14—H14	120.2

C1—O2—Zn1	126.02 (16)	C19—C20—H20A	109.5
C1—O2—Ce1	129.39 (16)	C19—C20—H20B	109.5
Zn1—O2—Ce1	104.48 (7)	H20A—C20—H20B	109.5
C10—N1—C9	123.7 (2)	C19—C20—H20C	109.5
C10—N1—Zn1	125.8 (2)	H20A—C20—H20C	109.5
C9—N1—Zn1	110.48 (18)	H20B—C20—H20C	109.5
C3—C2—O4	125.2 (2)	C12—C11—C16	118.7 (3)
C3—C2—C1	121.1 (2)	C12—C11—C10	118.3 (3)
O4—C2—C1	113.7 (2)	C16—C11—C10	123.0 (2)
O13—N3—O12	122.6 (3)	C13—C12—C11	120.7 (3)
O13—N3—O11	121.8 (3)	C13—C12—H12	119.6
O12—N3—O11	115.6 (2)	C11—C12—H12	119.6
N3—O11—Ce1	97.92 (15)	C14—C15—O3	125.3 (2)
C7—N2—C8	121.6 (3)	C14—C15—C16	121.0 (2)
C7—N2—Zn1	126.0 (2)	O3—C15—C16	113.6 (2)
C8—N2—Zn1	112.23 (19)	C12—C13—C14	120.7 (3)
N3—O12—Ce1	96.64 (15)	C12—C13—H13	119.6
O2—C1—C6	123.6 (2)	C14—C13—H13	119.6
O2—C1—C2	116.9 (2)	C17—C18—H18A	109.5
C6—C1—C2	119.4 (2)	C17—C18—H18B	109.5
N1—C10—C11	125.0 (3)	H18A—C18—H18B	109.5
N1—C10—H10	117.5	C17—C18—H18C	109.5
C11—C10—H10	117.5	H18A—C18—H18C	109.5
N2—C8—C9	107.1 (2)	H18B—C18—H18C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O7^{i}	0.93	2.36	3.275 (4)	168
C9—H9A···O7^{ii}	0.97	2.43	3.286 (4)	147
C17—H17B···O9	0.97	2.87	3.337 (4)	111
C20—H20A···O8	0.96	2.45	3.166 (4)	131

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*−1, *y*, *z*.

Fig. 1

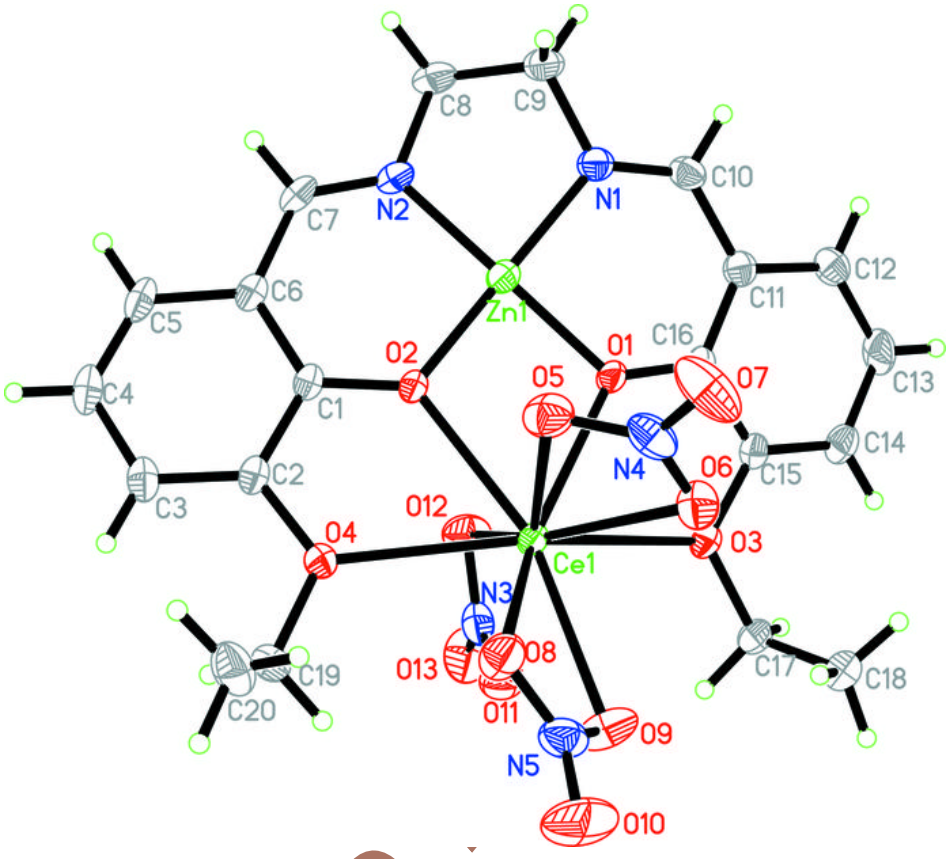

Fig. 2