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Retraction of articles by T. Liu *et al.*

T. Liu,[a]* Y.-X. Wang,[b] Z.-W. Wang,[a] Z.-P. Xie[a,c] and J. Y. Zhu[d]

[a]College of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, [b]College of Mathematics and Physics, Jinggangshan University, Jian 343009, People's Republic of China, [c]Department of Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, People's Republic of China, and [d]Department of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China
Correspondence e-mail: taoliu07@126.com

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *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
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*d*)	10.1107/S1600536807031224	WIHJED
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]	Liu, Wang, Wang & Xie (2007*e*)	10.1107/S1600536807032679	WIHQEK
Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-κ^2N,N')-[(2-pyridyloxy)acetato-κO]neodymium(III)}	Liu, Wang, Wang & Xie (2007*f*)	10.1107/S1600536807035349	TIGDAP
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*g*)	10.1107/S1600536807035076	TIGDET
2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)	Liu & Zhu (2007*j*)	10.1107/S1600536807040068	KIKQAX
2-Hydroxy-3,5-dinitrobenzamide monohydrate	Liu & Zhu (2007*k*)	10.1107/S1600536807039712	KIKQEB
2-(1-Hydroxy-2-pyridyl)acetamide monohydrate	Liu & Zhu (2007*l*)	10.1107/S1600536807040652	CIKQOD
Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)	Liu & Zhu (2007*a*)	10.1107/S1600536807043486	XIFXOA
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]	Liu & Zhu (2007*b*)	10.1107/S1600536807045485	XILNAI
3-Hydroxy-2,4,6-trinitropyridine monohydrate	Liu & Zhu (2007*m*)	10.1107/S1600536807045230	PILNOO
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]	Liu & Zhu (2007*c*)	10.1107/S1600536807047733	SILZET
catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]	Liu & Zhu (2007*d*)	10.1107/S1600536807050969	GIMZOS
Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)	Liu & Zhu (2007*e*)	10.1107/S1600536807051756	WINFAB
2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate	Liu & Zhu (2007*n*)	10.1107/S1600536807048477	GINFEP
2-(Benzoylhydrazinocarbonyl)benzoic acid	Liu & Zhu (2007*o*)	10.1107/S160053680705204X	TINZIA
Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)	Liu & Zhu (2007*f*)	10.1107/S1600536807054529	HIPZIQ
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*g*)	10.1107/S1600536807056504	XIRGIP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*h*)	10.1107/S1600536807059077	HIQROP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]	Liu & Zhu (2007*i*)	10.1107/S1600536807060631	YIQMER
N′-Benzoyl-4-nitronicotinohydrazide	Liu & Zhu (2007*p*)	10.1107/S1600536807053068	CIPVON
N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide	Liu & Zhu (2007*q*)	10.1107/S1600536807054876	RIRWEV

 doi:10.1107/S1600536809049976

Table 1 (continued)

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007*r*)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007*s*)	10.1107/S1600536807059909	HIRYEN
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')manganese(II)]-μ-nitrato-$\kappa^2O:O'$]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]

T. Liu[a]* and J. Y. Zhu[b]

[a]College of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, and [b]Department of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China
Correspondence e-mail: taoliu07@126.com

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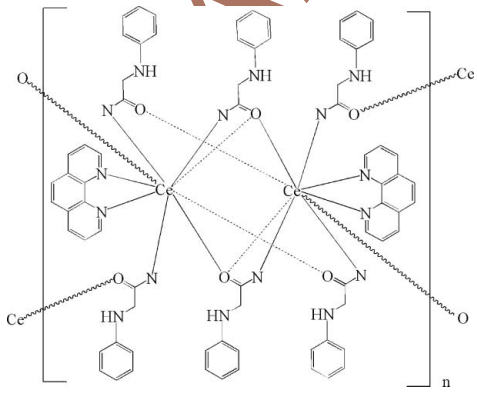
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.011 Å; R factor = 0.043; wR factor = 0.117; data-to-parameter ratio = 17.1.

The title compound, $[Ce_2(C_8H_8N_2O)_6(C_{12}H_8N_2)_2]_n$, is a polymeric complex based on a binuclear unit with an inversion centre midway between the two Ce^{III} ions, which are bridged by two tridentate, two bidentate and four monodentate (within the binuclear unit) acetamide groups. Each Ce atom is nine-coordinated by two 1,10-phenanthroline N atoms, four O and three N atoms of anilinoacetamide ligands. In the crystal structure, C—H···O, C—H···N, N—H···N and N—H···O hydrogen bonds result in the formation of a supramolecular network structure; an N—H···O hydrogen bond is also present within one ligand.

Related literature

For related structures, see: Liu & Zhu (2007*a*,*b*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Ce_2(C_8H_8N_2O)_6(C_{12}H_8N_2)_2]$
M_r = 1535.68
Monoclinic, $P2_1/n$
a = 20.1131 (12) Å
b = 8.5037 (11) Å
c = 20.6993 (15) Å
β = 107.011 (2)°
V = 3385.4 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.39 mm^{-1}
T = 273 (2) K
0.33 × 0.13 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.653, T_{max} = 0.904
25721 measured reflections
7024 independent reflections
4796 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.117
S = 1.07
7024 reflections
411 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ce1—O1	2.565 (3)	Ce1—N2^{i}	2.435 (3)
Ce1—O2^{i}	2.526 (3)	Ce1—N3	2.469 (3)
Ce1—O3^{ii}	2.541 (3)	Ce1—N4	2.743 (4)
Ce1—N1	2.415 (3)	Ce1—N5	2.703 (4)
Ce1—N2	2.828 (4)		
N1—Ce1—N2	140.11 (10)	N3—Ce1—N5	81.15 (11)
N1—Ce1—N3	145.53 (11)	N4—Ce1—N5	59.72 (13)
N1—Ce1—N4	77.43 (12)	O1—Ce1—N1	139.17 (11)
N1—Ce1—N5	96.53 (11)	O1—Ce1—N2	48.26 (9)
N2—Ce1—N3	64.79 (10)	O1—Ce1—N3	73.55 (10)
N2—Ce1—N4	102.47 (11)	O1—Ce1—N4	63.38 (11)
N2—Ce1—N5	118.19 (10)	O1—Ce1—N5	74.08 (10)
N3—Ce1—N4	127.42 (11)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O2^{i}	0.93	2.43	3.125 (7)	131
C10—H10···O1^{iii}	0.93	2.34	3.210 (6)	155
C12—H12···N6^{ii}	0.93	2.58	3.425 (7)	152
C12—H12···O3^{ii}	0.93	2.47	3.062 (7)	122
C22—H22*B*···N1^{iv}	0.97	2.38	3.319 (6)	164
N1—H1*A*···O2^{i}	0.80 (2)	2.32 (3)	3.048 (5)	152 (6)
N2—H2*A*···N2^{i}	0.86	2.63	3.144 (7)	120
N2—H2*A*···O2^{i}	0.86	2.15	2.900 (5)	145
N7—H7*A*···O2	0.86	2.28	2.627 (4)	104

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $-x+2, -y+1, -z+2$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, y-1, z$.

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: HK2343).

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supplementary materials

Acta Cryst. (2007). E**63**, m2775-m2776 [**doi:10.1107/S1600536807050969**]

catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]

T. Liu and J. Y. Zhu

Comment

The crystal structures of *catena*-Poly[hexakis(μ_2-anilinoacetamide-*O*,*N*)bis- (1,10-phenanthroline-N,*N*')disamarium(III)], (II), and *catena*-Poly[hexakis- (μ_2-anilinoacetamide-*O*,*N*)bis(1,10-phenanthroline-N,*N*')diprasеodymium(III)], (III), have previously been reported (Liu & Zhu, 2007*a*,b). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with those of (II) and (III). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). It has an inversion centre midway between the two Ce^{III} ions, which are bridged by two tridentate, two bidentate and four monodentate (within the binuclear unit) acetamide groups. Each Ce atom is nine-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand and four O and three N atoms of anilinoacetamide ligands. The Ce—O and Ce—N bonds are in the range of [2.526 (3)–2.565 (3) Å] and [2.415 (3)–2.828 (4) Å], respectively (Table 1), as in (II) and (III).

In the crystal structure, intermolecular C—H···O, C—H···N, N—H···N and N—H···O hydrogen bonds (Table 2, Fig. 2) result in the formation of a supramolecular network structure; an intramolecular N—H···O hydrogen bond (Table 2) is also present, as in (II) and (III).

The three compounds, (I), (II) and (III), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Cerium (III) nitrate hexahydrate (434.1 mg, 1 mmol), phen (198 mg, 1 mmol), anilinoacetamide (290.4 mg, 2 mmol) and distilled water (12 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H1A and H6A (for NH) were located in difference syntheses and refined isotropically [N—H = 0.80 (2) and 0.84 (5) Å, U_{iso}(H) = 0.073 (19) and 0.09 (2) Å^2]. The remaining H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93 and 0.97 Å, for aromatic and methylene H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

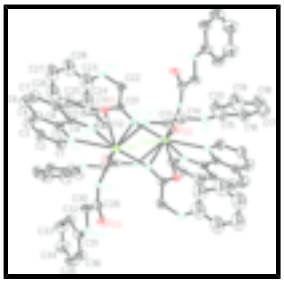

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): 2 − *x*, −*y*, 2 − *z*]. H atoms have been omitted for clarity.

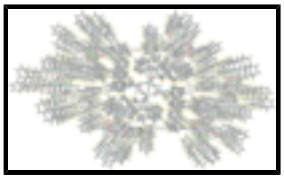

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10- phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]

Crystal data

$[Ce_2(C_8H_8N_2O)_6(C_{12}H_8N_2)_2]$	F_{000} = 1556
M_r = 1535.68	D_x = 1.506 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8802 reflections
a = 20.1131 (12) Å	θ = 2.4–26.6°
b = 8.5037 (11) Å	μ = 1.39 mm^{-1}
c = 20.6993 (15) Å	T = 273 (2) K
β = 107.011 (2)°	Plate, colorless
V = 3385.4 (5) Å^3	0.33 × 0.13 × 0.07 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	7024 independent reflections
Radiation source: fine-focus sealed tube	4796 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 273(2) K	θ_{max} = 26.7°
φ and ω scans	θ_{min} = 2.1°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→24
T_{min} = 0.653, T_{max} = 0.904	k = −10→10
25721 measured reflections	l = −26→26

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.117$

$S = 1.07$

7024 reflections

411 parameters

6 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 1.36$ e Å^{-3}

$\Delta\rho_{min} = -0.64$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.931202 (12)	0.19065 (3)	0.964279 (11)	0.03965 (10)
O1	0.84610 (15)	−0.0357 (4)	0.91874 (15)	0.0497 (7)
O2	1.06674 (17)	−0.0827 (4)	0.92144 (15)	0.0542 (8)
O3	1.00727 (19)	0.6128 (4)	1.09090 (15)	0.0618 (9)
N1	0.94022 (18)	0.4223 (4)	1.03386 (16)	0.0355 (7)
H1A	0.925 (3)	0.336 (3)	1.035 (3)	0.073 (19)*
N2	0.94701 (16)	−0.1394 (4)	0.97694 (15)	0.0373 (8)
H2A	0.9440	−0.0471	0.9928	0.045*
N3	0.97072 (17)	0.0611 (4)	0.87531 (15)	0.0350 (7)
H3A	0.9398	0.0552	0.8366	0.042*
N4	0.7968 (2)	0.2339 (5)	0.9667 (2)	0.0515 (9)
N5	0.8345 (2)	0.3062 (4)	0.85476 (19)	0.0520 (10)
N6	0.9878 (2)	0.5261 (5)	1.20638 (17)	0.0490 (10)
H6A	0.962 (3)	0.604 (4)	1.2059 (19)	0.09 (2)*
N7	1.11808 (19)	−0.0158 (5)	0.82168 (18)	0.0541 (10)
H7A	1.1397	−0.0730	0.8556	0.065*

N9	0.78536 (19)	−0.3271 (4)	0.8986 (2)	0.0504 (10)
H9A	0.7626	−0.3418	0.8569	0.060*
C1	0.7788 (3)	0.1913 (6)	1.0203 (3)	0.0682 (15)
H1	0.8136	0.1682	1.0599	0.082*
C2	0.7093 (3)	0.1792 (8)	1.0200 (4)	0.089 (2)
H2	0.6982	0.1509	1.0590	0.107*
C3	0.6579 (3)	0.2098 (9)	0.9611 (4)	0.094 (2)
H3	0.6115	0.1976	0.9594	0.113*
C4	0.6746 (3)	0.2577 (9)	0.9055 (4)	0.0814 (18)
C5	0.7462 (3)	0.2665 (6)	0.9092 (3)	0.0567 (13)
C6	0.6222 (4)	0.2944 (10)	0.8394 (5)	0.115 (3)
H6	0.5751	0.2828	0.8350	0.138*
C7	0.6417 (4)	0.3426 (10)	0.7877 (4)	0.107 (3)
H7	0.6080	0.3704	0.7480	0.128*
C8	0.7136 (3)	0.3534 (7)	0.7909 (3)	0.0742 (17)
C9	0.7659 (3)	0.3093 (5)	0.8506 (3)	0.0573 (13)
C10	0.7356 (4)	0.4047 (8)	0.7375 (3)	0.093 (2)
H10	0.7032	0.4408	0.6984	0.112*
C11	0.8044 (4)	0.4030 (8)	0.7413 (3)	0.088 (2)
H11	0.8192	0.4366	0.7050	0.105*
C12	0.8525 (3)	0.3499 (6)	0.8009 (3)	0.0687 (15)
H12	0.8992	0.3451	0.8026	0.082*
C13	1.0285 (3)	0.0024 (5)	0.8772 (2)	0.0483 (11)
C14	1.0524 (3)	0.0514 (6)	0.8173 (2)	0.0587 (12)
H14A	1.0186	0.0174	0.7758	0.070*
H14B	1.0556	0.1651	0.8162	0.070*
C15	1.1459 (3)	0.0139 (7)	0.7695 (3)	0.0664 (14)
C16	1.2075 (3)	−0.0554 (8)	0.7761 (3)	0.0832 (18)
H16	1.2281	−0.1165	0.8139	0.100*
C17	1.2400 (4)	−0.0360 (9)	0.7268 (4)	0.098 (2)
H17	1.2828	−0.0829	0.7313	0.118*
C18	1.2088 (5)	0.0529 (9)	0.6711 (5)	0.113 (3)
H18	1.2303	0.0642	0.6373	0.136*
C19	1.1478 (5)	0.1241 (10)	0.6646 (4)	0.113 (3)
H19	1.1271	0.1848	0.6267	0.136*
C20	1.1152 (4)	0.1057 (8)	0.7160 (3)	0.088 (2)
H20	1.0734	0.1561	0.7130	0.106*
C21	0.8841 (2)	−0.1526 (6)	0.9390 (2)	0.0490 (11)
C22	0.8580 (3)	−0.3151 (6)	0.9197 (3)	0.0603 (13)
H22A	0.8758	−0.3515	0.8836	0.072*
H22B	0.8762	−0.3840	0.9582	0.072*
C23	0.7536 (6)	−0.3148 (9)	0.9457 (7)	0.1322 (16)
C24	0.7844 (6)	−0.2804 (9)	1.0110 (6)	0.1322 (16)
H24	0.8321	−0.2630	1.0270	0.159*
C25	0.7417 (5)	−0.2714 (10)	1.0549 (6)	0.1322 (16)
H25	0.7615	−0.2502	1.1006	0.159*
C26	0.6741 (6)	−0.2932 (9)	1.0306 (6)	0.1322 (16)
H26	0.6473	−0.2810	1.0601	0.159*
C27	0.6392 (6)	−0.3342 (10)	0.9624 (6)	0.1322 (16)

H27	0.5918	−0.3557	0.9477	0.159*
C28	0.6799 (5)	−0.3398 (10)	0.9198 (6)	0.1322 (16)
H28	0.6598	−0.3599	0.8741	0.159*
C29	0.9694 (2)	0.4994 (5)	1.0863 (2)	0.0488 (11)
C30	0.9489 (3)	0.4458 (6)	1.1474 (2)	0.0604 (13)
H30A	0.8997	0.4653	1.1401	0.072*
H30B	0.9568	0.3335	1.1535	0.072*
C31	0.9744 (3)	0.4884 (6)	1.2657 (2)	0.0597 (13)
C32	0.9277 (3)	0.3792 (8)	1.2718 (3)	0.0761 (17)
H32	0.9014	0.3243	1.2342	0.091*
C33	0.9198 (4)	0.3506 (11)	1.3348 (4)	0.111 (3)
H33	0.8894	0.2725	1.3400	0.133*
C34	0.9565 (4)	0.4364 (10)	1.3898 (3)	0.107 (2)
H34	0.9484	0.4218	1.4314	0.129*
C35	1.0041 (4)	0.5418 (9)	1.3836 (3)	0.094 (2)
H35	1.0303	0.5962	1.4215	0.112*
C36	1.0145 (3)	0.5699 (8)	1.3222 (3)	0.0767 (16)
H36	1.0478	0.6422	1.3182	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.04649 (16)	0.03386 (16)	0.03378 (14)	−0.00159 (11)	0.00422 (10)	0.00055 (10)
O1	0.0509 (17)	0.0379 (18)	0.0521 (18)	0.0000 (15)	0.0024 (14)	−0.0035 (14)
O2	0.068 (2)	0.050 (2)	0.0463 (18)	0.0089 (16)	0.0186 (15)	0.0125 (15)
O3	0.090 (3)	0.054 (2)	0.0426 (18)	−0.026 (2)	0.0214 (17)	−0.0037 (15)
N1	0.057 (2)	0.0186 (17)	0.0296 (17)	−0.0075 (16)	0.0104 (14)	−0.0058 (14)
N2	0.0371 (18)	0.0324 (18)	0.0354 (18)	−0.0023 (14)	−0.0003 (14)	0.0033 (14)
N3	0.0417 (18)	0.0379 (19)	0.0238 (15)	0.0063 (16)	0.0071 (13)	0.0012 (14)
N4	0.051 (2)	0.046 (2)	0.051 (2)	0.0040 (18)	0.0046 (18)	−0.0080 (18)
N5	0.064 (3)	0.043 (2)	0.040 (2)	0.0017 (19)	0.0006 (17)	0.0005 (17)
N6	0.072 (3)	0.046 (2)	0.0306 (19)	−0.022 (2)	0.0181 (17)	−0.0057 (16)
N7	0.055 (2)	0.069 (3)	0.044 (2)	0.018 (2)	0.0241 (18)	0.0224 (19)
N9	0.047 (2)	0.035 (2)	0.057 (2)	−0.0140 (17)	−0.0025 (18)	−0.0067 (17)
C1	0.063 (3)	0.079 (4)	0.063 (3)	0.007 (3)	0.019 (3)	0.002 (3)
C2	0.062 (4)	0.120 (6)	0.092 (5)	0.008 (4)	0.032 (4)	−0.012 (4)
C3	0.054 (4)	0.112 (6)	0.113 (6)	−0.005 (4)	0.018 (4)	−0.013 (5)
C4	0.056 (3)	0.093 (5)	0.080 (4)	0.006 (3)	−0.004 (3)	−0.021 (4)
C5	0.055 (3)	0.042 (3)	0.064 (3)	0.006 (2)	0.003 (2)	−0.009 (2)
C6	0.058 (4)	0.154 (9)	0.106 (6)	0.016 (4)	−0.017 (4)	−0.026 (6)
C7	0.082 (5)	0.116 (6)	0.087 (5)	0.038 (4)	−0.030 (4)	−0.019 (5)
C8	0.079 (4)	0.067 (4)	0.053 (3)	0.018 (3)	−0.018 (3)	−0.011 (3)
C9	0.067 (3)	0.037 (3)	0.053 (3)	0.004 (2)	−0.007 (2)	−0.006 (2)
C10	0.121 (6)	0.074 (5)	0.052 (4)	0.018 (4)	−0.024 (4)	0.000 (3)
C11	0.129 (6)	0.080 (5)	0.038 (3)	−0.004 (4)	0.000 (3)	0.012 (3)
C12	0.087 (4)	0.057 (3)	0.053 (3)	−0.001 (3)	0.005 (3)	0.009 (2)
C13	0.066 (3)	0.038 (3)	0.038 (2)	−0.011 (2)	0.011 (2)	−0.0029 (19)
C14	0.069 (3)	0.058 (3)	0.051 (3)	0.004 (3)	0.020 (2)	0.009 (2)

C15	0.073 (4)	0.073 (4)	0.061 (3)	−0.008 (3)	0.032 (3)	0.001 (3)
C16	0.084 (4)	0.098 (5)	0.079 (4)	0.004 (4)	0.041 (3)	−0.005 (4)
C17	0.099 (5)	0.096 (6)	0.119 (6)	−0.003 (4)	0.063 (5)	−0.004 (5)
C18	0.155 (7)	0.088 (5)	0.139 (7)	−0.015 (5)	0.109 (6)	−0.003 (5)
C19	0.151 (7)	0.119 (6)	0.096 (5)	0.020 (6)	0.076 (5)	0.034 (5)
C20	0.107 (5)	0.097 (5)	0.080 (4)	0.004 (4)	0.056 (4)	0.023 (4)
C21	0.052 (3)	0.054 (3)	0.036 (2)	−0.003 (2)	0.0047 (19)	−0.005 (2)
C22	0.069 (3)	0.047 (3)	0.059 (3)	0.004 (3)	0.009 (3)	−0.005 (2)
C23	0.144 (4)	0.095 (3)	0.183 (4)	0.018 (3)	0.087 (4)	0.031 (3)
C24	0.144 (4)	0.095 (3)	0.183 (4)	0.018 (3)	0.087 (4)	0.031 (3)
C25	0.144 (4)	0.095 (3)	0.183 (4)	0.018 (3)	0.087 (4)	0.031 (3)
C26	0.144 (4)	0.095 (3)	0.183 (4)	0.018 (3)	0.087 (4)	0.031 (3)
C27	0.144 (4)	0.095 (3)	0.183 (4)	0.018 (3)	0.087 (4)	0.031 (3)
C28	0.144 (4)	0.095 (3)	0.183 (4)	0.018 (3)	0.087 (4)	0.031 (3)
C29	0.060 (3)	0.036 (3)	0.050 (3)	−0.002 (2)	0.016 (2)	0.006 (2)
C30	0.080 (3)	0.057 (3)	0.044 (3)	−0.022 (3)	0.019 (2)	−0.006 (2)
C31	0.080 (3)	0.058 (3)	0.040 (3)	−0.003 (3)	0.016 (2)	0.004 (2)
C32	0.081 (4)	0.094 (4)	0.056 (3)	−0.034 (4)	0.024 (3)	−0.004 (3)
C33	0.128 (6)	0.146 (7)	0.070 (4)	−0.050 (6)	0.047 (4)	0.000 (5)
C34	0.130 (6)	0.145 (7)	0.055 (4)	−0.032 (6)	0.040 (4)	0.008 (4)
C35	0.124 (6)	0.103 (5)	0.047 (3)	−0.018 (4)	0.014 (3)	−0.006 (3)
C36	0.092 (4)	0.082 (4)	0.052 (3)	−0.019 (3)	0.015 (3)	−0.012 (3)

Geometric parameters (Å, °)

Ce1—O1	2.565 (3)	C8—C9	1.418 (7)
Ce1—O2^{i}	2.526 (3)	C10—C11	1.363 (9)
Ce1—O3^{ii}	2.541 (3)	C10—H10	0.9300
Ce1—N1	2.415 (3)	C11—C12	1.401 (8)
Ce1—N2	2.828 (4)	C11—H11	0.9300
Ce1—N2^{i}	2.435 (3)	C12—H12	0.9300
Ce1—N3	2.469 (3)	C13—C14	1.513 (6)
Ce1—N4	2.743 (4)	C14—H14A	0.9700
Ce1—N5	2.703 (4)	C14—H14B	0.9700
O1—C21	1.249 (5)	C15—C16	1.342 (8)
O2—C13	1.242 (5)	C15—C20	1.348 (8)
O2—Ce1^{i}	2.526 (3)	C16—C17	1.373 (9)
O3—C29	1.215 (5)	C16—H16	0.9300
O3—Ce1^{ii}	2.541 (3)	C17—C18	1.368 (10)
N1—C29	1.257 (6)	C17—H17	0.9300
N1—H1A	0.80 (2)	C18—C19	1.339 (10)
N2—C21	1.285 (5)	C18—H18	0.9300
N2—Ce1^{i}	2.435 (3)	C19—C20	1.413 (8)
N2—H2A	0.8600	C19—H19	0.9300
N3—C13	1.254 (5)	C20—H20	0.9300
N3—H3A	0.8600	C21—C22	1.490 (7)
N4—C1	1.314 (6)	C22—H22A	0.9700
N4—C5	1.349 (6)	C22—H22B	0.9700

N5—C12	1.323 (6)	C23—C24	1.344 (15)
N5—C9	1.358 (7)	C23—C28	1.438 (14)
N6—C31	1.369 (6)	C24—C25	1.424 (12)
N6—C30	1.418 (6)	C24—H24	0.9300
N6—H6A	0.84 (5)	C25—C26	1.317 (13)
N7—C15	1.377 (6)	C25—H25	0.9300
N7—C14	1.419 (6)	C26—C27	1.425 (14)
N7—H7A	0.8600	C26—H26	0.9300
N9—C23	1.317 (11)	C27—C28	1.367 (11)
N9—C22	1.401 (6)	C27—H27	0.9300
N9—H9A	0.8600	C28—H28	0.9300
C1—C2	1.400 (8)	C29—C30	1.510 (6)
C1—H1	0.9300	C30—H30A	0.9700
C2—C3	1.373 (10)	C30—H30B	0.9700
C2—H2	0.9300	C31—C32	1.353 (7)
C3—C4	1.353 (9)	C31—C36	1.396 (7)
C3—H3	0.9300	C32—C33	1.380 (8)
C4—C5	1.421 (8)	C32—H32	0.9300
C4—C6	1.496 (10)	C33—C34	1.372 (10)
C5—C9	1.430 (8)	C33—H33	0.9300
C6—C7	1.308 (11)	C34—C35	1.345 (9)
C6—H6	0.9300	C34—H34	0.9300
C7—C8	1.433 (10)	C35—C36	1.368 (8)
C7—H7	0.9300	C35—H35	0.9300
C8—C10	1.376 (9)	C36—H36	0.9300
N1—Ce1—N2	140.11 (10)	N4—C5—C4	121.9 (5)
N1—Ce1—N3	145.53 (11)	N4—C5—C9	118.5 (5)
N1—Ce1—N4	77.43 (12)	C4—C5—C9	119.6 (5)
N1—Ce1—N5	96.53 (11)	C7—C6—C4	120.9 (7)
N2—Ce1—N3	64.79 (10)	C7—C6—H6	119.5
N2—Ce1—N4	102.47 (11)	C4—C6—H6	119.5
N2—Ce1—N5	118.19 (10)	C6—C7—C8	121.5 (6)
N3—Ce1—N4	127.42 (11)	C6—C7—H7	119.2
N3—Ce1—N5	81.15 (11)	C8—C7—H7	119.2
N4—Ce1—N5	59.72 (13)	C10—C8—C9	117.0 (6)
O1—Ce1—N1	139.17 (11)	C10—C8—C7	122.7 (6)
O1—Ce1—N2	48.26 (9)	C9—C8—C7	120.3 (6)
O1—Ce1—N3	73.55 (10)	N5—C9—C8	122.8 (5)
O1—Ce1—N4	63.38 (11)	N5—C9—C5	118.0 (4)
O1—Ce1—N5	74.08 (10)	C8—C9—C5	119.2 (5)
N1—Ce1—N2^{i}	87.65 (12)	C11—C10—C8	120.6 (5)
N2^{i}—Ce1—N3	78.25 (11)	C11—C10—H10	119.7
N1—Ce1—O2^{i}	76.13 (11)	C8—C10—H10	119.7
N2^{i}—Ce1—O2^{i}	74.24 (10)	C10—C11—C12	118.9 (6)
N3—Ce1—O2^{i}	128.00 (11)	C10—C11—H11	120.6
N1—Ce1—O2^{i}	76.13 (11)	C12—C11—H11	120.6
N2^{i}—Ce1—O2^{i}	74.24 (10)	N5—C12—C11	123.0 (6)

N3—Ce1—O2^{i}	128.00 (11)	N5—C12—H12	118.5
O2^{i}—Ce1—O2^{i}	0.0 (2)	C11—C12—H12	118.5
N1—Ce1—O2^{i}	76.13 (11)	O2—C13—N3	128.5 (4)
N2^{i}—Ce1—O2^{i}	74.24 (10)	O2—C13—C14	119.2 (4)
N3—Ce1—O2^{i}	128.00 (11)	N3—C13—C14	112.2 (4)
O2^{i}—Ce1—O2^{i}	0.0 (2)	N7—C14—C13	110.5 (4)
O2^{i}—Ce1—O2^{i}	0.0 (2)	N7—C14—H14A	109.6
N1—Ce1—O3^{ii}	76.71 (11)	C13—C14—H14A	109.6
N2^{i}—Ce1—O3^{ii}	77.95 (11)	N7—C14—H14B	109.6
N3—Ce1—O3^{ii}	69.69 (11)	C13—C14—H14B	109.6
O2^{i}—Ce1—O3^{ii}	141.55 (11)	H14A—C14—H14B	108.1
O2^{i}—Ce1—O3^{ii}	141.55 (11)	C16—C15—C20	121.7 (5)
O2^{i}—Ce1—O3^{ii}	141.55 (11)	C16—C15—N7	114.5 (5)
N2^{i}—Ce1—O1	121.00 (11)	C20—C15—N7	123.8 (5)
O2^{i}—Ce1—O1	84.14 (10)	C15—C16—C17	119.8 (7)
O2^{i}—Ce1—O1	84.14 (10)	C15—C16—H16	120.1
O2^{i}—Ce1—O1	84.14 (10)	C17—C16—H16	120.1
O3^{ii}—Ce1—O1	133.54 (10)	C18—C17—C16	119.5 (7)
N2^{i}—Ce1—N5	148.86 (12)	C18—C17—H17	120.3
O2^{i}—Ce1—N5	136.73 (12)	C16—C17—H17	120.3
O2^{i}—Ce1—N5	136.73 (12)	C19—C18—C17	121.0 (7)
O2^{i}—Ce1—N5	136.73 (12)	C19—C18—H18	119.5
O3^{ii}—Ce1—N5	73.10 (12)	C17—C18—H18	119.5
N2^{i}—Ce1—N4	150.19 (11)	C18—C19—C20	119.2 (7)
O2^{i}—Ce1—N4	77.16 (11)	C18—C19—H19	120.4
O2^{i}—Ce1—N4	77.16 (11)	C20—C19—H19	120.4
O2^{i}—Ce1—N4	77.16 (11)	C15—C20—C19	118.8 (7)
O3^{ii}—Ce1—N4	122.16 (12)	C15—C20—H20	120.6
N2^{i}—Ce1—N2	72.94 (12)	C19—C20—H20	120.6
O2^{i}—Ce1—N2	65.30 (10)	O1—C21—N2	122.1 (4)
O2^{i}—Ce1—N2	65.30 (10)	O1—C21—C22	121.0 (4)
O2^{i}—Ce1—N2	65.30 (10)	N2—C21—C22	116.8 (4)
O3^{ii}—Ce1—N2	129.65 (10)	N9—C22—C21	113.8 (4)
N1—Ce1—H1A	17.2 (9)	N9—C22—H22A	108.8
N2^{i}—Ce1—H1A	90.7 (17)	C21—C22—H22A	108.8
N3—Ce1—H1A	161.7 (11)	N9—C22—H22B	108.8
O2^{i}—Ce1—H1A	60.8 (11)	C21—C22—H22B	108.8
O2^{i}—Ce1—H1A	60.8 (11)	H22A—C22—H22B	107.7
O2^{i}—Ce1—H1A	60.8 (11)	N9—C23—C24	125.5 (11)
O3^{ii}—Ce1—H1A	93.9 (9)	N9—C23—C28	112.6 (11)
O1—Ce1—H1A	124.8 (11)	C24—C23—C28	121.9 (10)

N5—Ce1—H1A	102.3 (16)	C23—C24—C25	117.9 (11)
N4—Ce1—H1A	67.9 (15)	C23—C24—H24	121.1
N2—Ce1—H1A	126.1 (12)	C25—C24—H24	121.1
C21—O1—Ce1	101.4 (3)	C26—C25—C24	119.8 (12)
C13—O2—Ce1^{i}	137.7 (3)	C26—C25—H25	120.1
C29—O3—Ce1^{ii}	149.7 (3)	C24—C25—H25	120.1
C29—N1—Ce1	151.1 (3)	C25—C26—C27	124.5 (10)
C29—N1—H1A	122 (4)	C25—C26—H26	117.7
Ce1—N1—H1A	47 (4)	C27—C26—H26	117.7
C21—N2—Ce1^{i}	163.2 (3)	C28—C27—C26	115.7 (11)
C21—N2—Ce1	88.1 (3)	C28—C27—H27	122.2
Ce1^{i}—N2—Ce1	107.06 (12)	C26—C27—H27	122.2
C21—N2—H2A	98.4	C27—C28—C23	120.1 (11)
Ce1^{i}—N2—H2A	98.4	C27—C28—H28	119.9
C13—N3—Ce1	130.7 (3)	C23—C28—H28	119.9
C13—N3—H3A	114.6	O3—C29—N1	127.2 (4)
Ce1—N3—H3A	114.6	O3—C29—C30	119.5 (4)
C1—N4—C5	118.6 (5)	N1—C29—C30	113.1 (4)
C1—N4—Ce1	119.7 (3)	N6—C30—C29	111.0 (4)
C5—N4—Ce1	120.3 (3)	N6—C30—H30A	109.4
C12—N5—C9	117.7 (4)	C29—C30—H30A	109.4
C12—N5—Ce1	120.2 (3)	N6—C30—H30B	109.4
C9—N5—Ce1	121.9 (3)	C29—C30—H30B	109.4
C31—N6—C30	117.1 (4)	H30A—C30—H30B	108.0
C31—N6—H6A	84.8 (17)	C32—C31—N6	124.7 (5)
C30—N6—H6A	101 (4)	C32—C31—C36	120.5 (5)
C15—N7—C14	117.4 (4)	N6—C31—C36	114.7 (5)
C15—N7—H7A	121.3	C32—C31—H6A	124 (2)
C14—N7—H7A	121.3	C36—C31—H6A	106 (2)
C23—N9—C22	116.8 (7)	C31—C32—C33	119.1 (6)
C23—N9—H9A	121.6	C31—C32—H32	120.5
C22—N9—H9A	121.6	C33—C32—H32	120.5
N4—C1—C2	122.6 (6)	C34—C33—C32	120.5 (7)
N4—C1—H1	118.7	C34—C33—H33	119.8
C2—C1—H1	118.7	C32—C33—H33	119.8
C3—C2—C1	118.8 (6)	C35—C34—C33	120.0 (6)
C3—C2—H2	120.6	C35—C34—H34	120.0
C1—C2—H2	120.6	C33—C34—H34	120.0
C4—C3—C2	120.2 (6)	C34—C35—C36	120.8 (6)
C4—C3—H3	119.9	C34—C35—H35	119.6
C2—C3—H3	119.9	C36—C35—H35	119.6
C3—C4—C5	118.0 (6)	C35—C36—C31	119.0 (6)
C3—C4—C6	123.8 (7)	C35—C36—H36	120.5
C5—C4—C6	118.1 (7)	C31—C36—H36	120.5

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	0.93	2.43	3.125 (7)	131
C10—H10···O1^{iii}	0.93	2.34	3.210 (6)	155
C12—H12···N6^{ii}	0.93	2.58	3.425 (7)	152
C12—H12···O3^{ii}	0.93	2.47	3.062 (7)	122
C22—H22B···N1^{iv}	0.97	2.38	3.319 (6)	164
N1—H1A···O2^{i}	0.80 (2)	2.32 (3)	3.048 (5)	152 (6)
N2—H2A···N2^{i}	0.86	2.63	3.144 (7)	120
N2—H2A···O2^{i}	0.86	2.15	2.900 (5)	145
N7—H7A···O2	0.86	2.28	2.627 (4)	104

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (iii) −*x*+3/2, *y*+1/2, −*z*+3/2; (ii) −*x*+2, −*y*+1, −*z*+2; (iv) *x*, *y*−1, *z*.

Fig. 1

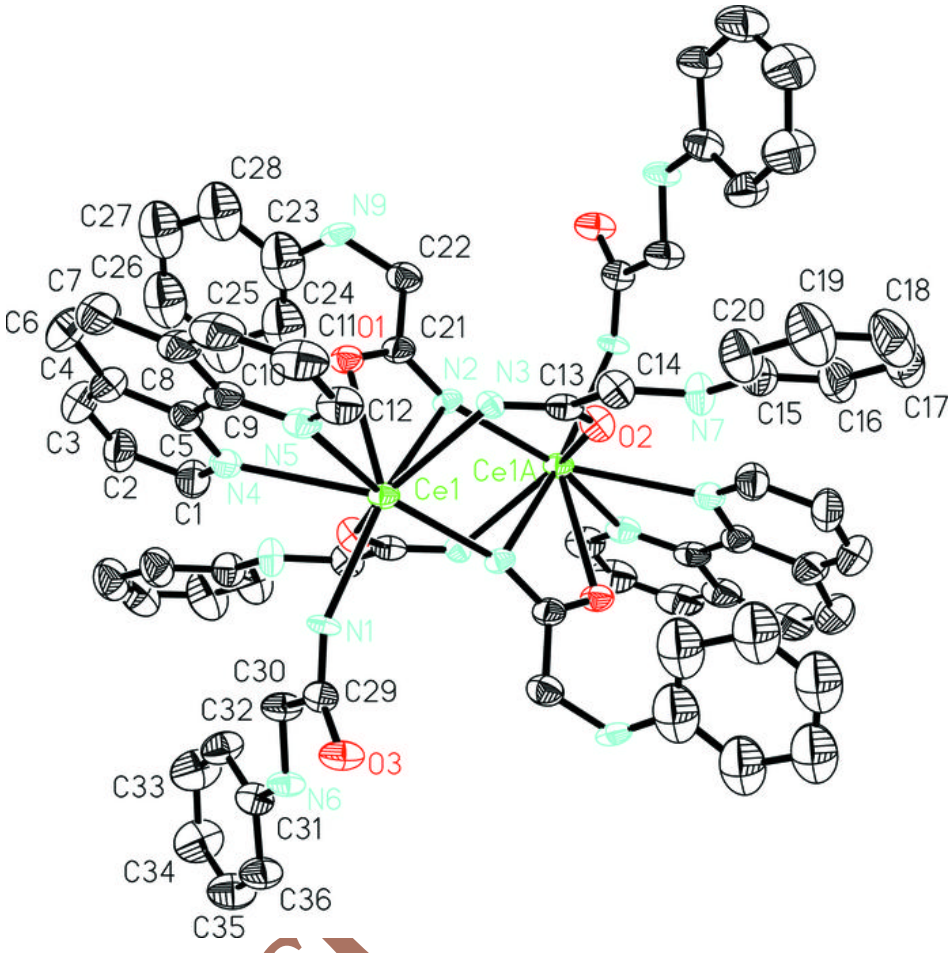
C28
C27
C23
N9
C22
C7
C26
C25
C24
C6
C11
O1
C21
C4
C8
C10
N2
N3
C13
C14
C19
C18
C20
C12
C9
O2
N7
C15
C16
C17
C3
C5
N5
C2
N4
Ce1
Ce1A
C1
N1
C30
C29
C32
O3
C33
N6
C31
C34
C36
C35

Fig. 2