

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
<i>trans</i> -Bis[1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehyde)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato- $\kappa^2 O, O'$)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- $\kappa^2 O, O'$)manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II) naphthalene-1,5-disulfonate dihydrate	Liu <i>et al.</i> (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato}-trinitratolutetium(III)copper(II)	Sui <i>et al.</i> (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato- $\kappa^2 O, O'$)iron(II)	Yang <i>et al.</i> (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer <i>et al.</i> (2007a)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer <i>et al.</i> (2007b)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2007)	Author	10.1107/S1600536807031121	WIHKEE
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]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(nitrilomethylidene)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen <i>et al.</i> (2007)	Author	10.1107/S1600536807032540	WIHRIP
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li <i>et al.</i> (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato-1 $\kappa^4 O^1, O^2, O^3, O^4, O^5, O^6, O^7, O^8, O^9, O^{10}$:2 $\kappa^2 O^1, N, N', N'', N'''$ }(methanol-1 κO)- μ -nitrate-1:2 $\kappa^2 O:O'$ -dinitrato-1 $\kappa^4 O, O'$ -cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato}-methanol- μ -nitrate-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato}-methanol- μ -nitrate-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato}-methanol- μ -nitrate-dinitratolutetium(III)zinc(II)	Sui, Sui <i>et al.</i> (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di- μ -chlorido-[chloridonickel(II)]- μ -4,4'-methylenebis(3,5-dimethylpyrazole)- $\kappa^2 N^2, N^2$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
[2,2'-[o-Phenylenebis(nitrilomethylidene)]diphenolato]zinc(II)	Liu <i>et al.</i> (2007a)	Author	10.1107/S1600536807040640	DIKYUS
<i>trans</i> -Bis(ethylenediamine- $\kappa^2 N, N'$)bis(nitrate- κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[<i>N, N'</i> -(o-Phenylene)bis(picolinamido)- $\kappa^4 N, N', N'', N'''$]cobalt(II)	Liu & Zeng (2007a)	Author	10.1107/S1600536807044571	XILFII
[<i>N, N'</i> -(o-Phenylene)dipicolinamide- $\kappa^4 N$]nickel(II)	Liu & Zeng (2007b)	Author	10.1107/S1600536807048386	WINWEW
[2,2'-[o-Phenylenebis(nitrilomethylidene)]diphenolato]manganese(II)	Liu <i>et al.</i> (2007b)	Author	10.1107/S1600536807052993	VIQPIV
<i>N</i> -(2-Amino-3-pyridyl)urea monohydrate	Li <i>et al.</i> (2007)	Author	10.1107/S1600536807047526	SIMFEA
<i>N</i> -(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime- $\kappa^2 N, N'$)(3,5-dinitro-2-oxidobenzooato- $\kappa^2 O^1, O^2$)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ -Acetato-tri- μ -ferrocenecarboxylatobis[(<i>N, N</i> -dimethylformamide)-copper(II)]	Liu, Lin <i>et al.</i> (2007)	Journal	10.1107/S1600536807059041	HIQQEE

Table 1 (continued)

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

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**{6,6'-Dimethoxy-2,2'-[ethane-1,2-diyl-bis(nitrilomethylidene)]diphenolato-1κ⁴O¹,O^{1'},O⁶,O^{6'}:2κ⁴O¹,N,N',O^{1'}}-
(methanol-1κO)-μ-nitrato-1:2κ²O:O'-
dinitrato-1κ⁴O,O'-cerium(III)zinc(II)**

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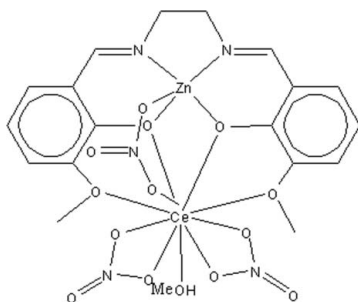
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.025; wR factor = 0.072; data-to-parameter ratio = 17.4.

In the title heteronuclear $\text{Zn}^{\text{II}}-\text{Ce}^{\text{III}}$ complex, $[\text{CeZn}(\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4)(\text{CH}_3\text{O})(\text{NO}_3)_3]$, with the hexadentate Schiff base compartmental ligand N,N' -bis(3-methoxysalicylidene)ethylenediamine (H_2L), the Zn and Ce atoms are triply bridged by two phenolate O atoms provided by the Schiff base ligand and one nitrate. The five-coordinated Zn is in a square-pyramidal geometry with the donor centers of two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The Ce^{III} center has a decacoordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, one methanol O atom, and two O atoms from two nitrates and one from the bridging nitrate. Strong intermolecular $\text{O}-\text{H}\cdots\text{O}$ and some weak $\text{C}-\text{H}\cdots\text{O}$ interactions generate a two-dimensional layer structure.

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, 2007).



Experimental

Crystal data

$[\text{CeZn}(\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4)(\text{CH}_3\text{O})(\text{NO}_3)_3]$	$\beta = 91.629$ (1) $^\circ$
$M_r = 749.91$	$V = 2654.68$ (17) Å ³
Monoclinic, $P2_1/n$	$Z = 4$
$a = 9.6011$ (4) Å	Mo $K\alpha$ radiation
$b = 13.8046$ (5) Å	$\mu = 2.67$ mm ⁻¹
$c = 20.0375$ (7) Å	$T = 293$ (2) K
	$0.28 \times 0.20 \times 0.13$ mm

Data collection

Bruker APEXII area-detector diffractometer	19675 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2004)	6372 independent reflections
$T_{\text{min}} = 0.527$, $T_{\text{max}} = 0.723$	5465 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$	5 restraints
$wR(F^2) = 0.072$	H atom parameters constrained
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.74$ e Å ⁻³
6372 reflections	$\Delta\rho_{\text{min}} = -0.72$ e Å ⁻³
367 parameters	

Table 1

Selected bond lengths (Å).

Ce1—O1	2.4630 (18)	Ce1—O11	2.457 (2)
Ce1—O2	2.4517 (17)	Ce1—O14	2.5301 (19)
Ce1—O3	2.568 (2)	Zn1—O1	2.0212 (17)
Ce1—O4	2.583 (2)	Zn1—O2	2.0136 (19)
Ce1—O6	2.8033 (19)	Zn1—O13	2.0047 (19)
Ce1—O7	2.7957 (19)	Zn1—N1	2.028 (2)
Ce1—O8	2.649 (2)	Zn1—N2	2.068 (2)
Ce1—O9	2.639 (2)		

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O14—H14A \cdots O13 ⁱ	0.875 (18)	1.84 (2)	2.689 (3)	162 (3)
C7—H7 \cdots O8 ⁱⁱ	0.93	2.49	3.393 (3)	165
C5—H5 \cdots O3 ⁱⁱ	0.93	2.57	3.428 (4)	154

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

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: HG2256).

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Article retracted

supplementary materials

Article retracted

Acta Cryst. (2007). E63, m2135-m2136 [doi:10.1107/S1600536807033314]

{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidene)]diphenolato-1κ⁴O¹,O^{1'},O⁶,O^{6'}:2κ⁴O¹,N,N',O^{1'}}(methanol-1κO)-μ-nitrato-1:2κ²O:O'-dinitrato-1κ⁴O,O'-cerium(III)zinc(II)

Y. Sui, X.-N. Fang, P. Hu and J. Lin

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 heterometallic 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 heterometallic Schiff base complexes (Sui *et al.*, 2006; Sui *et al.*, 2007), 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(H₂L).

Complex (I) crystallizes in the space group *P*2₁/*n*, with zinc and cerium triply bridged by two phenolate O atoms provided by a salen-type Schiff base ligand and one nitrate. 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 cerium(III) center in (I) has a decacoordination environment of O atoms. In addition to the phenolate ligands, two methoxy O atoms and one methanol O atoms coordinate to this metal center, two O atoms each from the two nitrates and one of the bridged nitrate O atoms chelate to cerium to complete the decacoordination. The five kinds of Ce—O bond distances are significantly different, the longest being the Ce—O(methoxy) separations and the shortest being the Ce—O(phenolate) and Ce—O11(bridged nitrate).

The zinc(II) is in a square-pyramidal geometry and is five-coordinated by two imine N atoms, two phenolate O atoms and one of the bridged nitrate O atoms. The Zn atom is 0.5822 (2) Å above the mean N₂O₂ plane with an average deviation from the plane of 0.0961 (3) Å, which construct the bottom of square-pyramid. The Zn—O13(nitrate, bridged) separation is 2.0047 (19) Å and the angles of this Zn—O vector with the Zn—N or Zn—O bonds lie between 103.22 (8)° and 115.52 (9)°, which suggesting that the zinc(II) is in a slightly distorted square-pyramidal conformation.

Adjacent molecules are held together by strong interactions (O14—H14A...O13ⁱ = 2.689 (3); symmetry codes: (i) 3/2 - x, y - 1/2, 1/2 - z) and weak interactions (C7—H7...O8ⁱⁱ = 3.393 (3) and C5—H5...O3ⁱⁱ = 3.428 (4); symmetry codes: (ii) 1/2 + x, 1/2 - y, 1/2 + z). these link the molecules into a two-dimensional layer structure (Fig. 2).

Experimental

H₂L was prepared by the 2:1 condensation of 3-methoxysalicylaldehyde and ethylenediamine in methanol. Complex (I) was obtained by the treatment of zinc(II) acetate dihydrate (0.188 g, 1 mmol) with H₂L(0.328 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*.

supplementary materials

Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation at room temperature of a methanol solution. Analysis calculated for $C_{19}H_{22}CeN_5O_{14}Zn$: C 30.43, H 2.96, Ce 18.68, N 9.34, Zn 8.72%; found: C 31.01, H 2.90, Ce 18.60, N 9.38, Zn 8.68%. IR (KBr, cm^{-1}): 1641(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. The methyl group of methanol was constrained as idealized no-rotating CH_3 group.

Figures

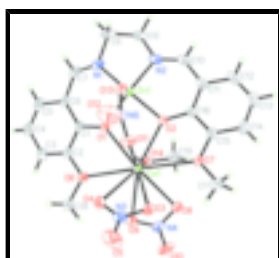


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

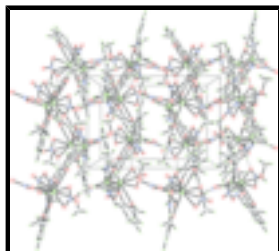


Fig. 2. The packing diagram of (I), viewed along the c axis; hydrogen bonds are shown as dashed lines.

{(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- $1\kappa O$)- μ -nitrate- $1:2\kappa^2O:O^1$ - μ -dinitrate- $1\kappa^4O, O^1$ -cerium(III)zinc(II)

Crystal data

$[CeZn(C_{18}H_{18}N_2O_4)(CH_4O)(NO_3)_3]$

$M_r = 749.91$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2yn$

$a = 9.6011$ (4) Å

$b = 13.8046$ (5) Å

$c = 20.0375$ (7) Å

$\beta = 91.6290$ (10)°

$V = 2654.68$ (17) Å³

$Z = 4$

$F_{000} = 1484$

$D_x = 1.876$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 19675 reflections

$\theta = 1.8$ – 28.3 °

$\mu = 2.67$ mm⁻¹

$T = 293$ (2) K

Block, yellow

$0.28 \times 0.20 \times 0.13$ mm

Data collection

Bruker APEXII area-detector diffractometer	6372 independent reflections
Radiation source: fine-focus sealed tube	5465 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.020$
Detector resolution: 0 pixels mm^{-1}	$\theta_{\text{max}} = 28.3^\circ$
$T = 293(2)$ K	$\theta_{\text{min}} = 1.8^\circ$
φ and ω scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$k = -18 \rightarrow 18$
$T_{\text{min}} = 0.527$, $T_{\text{max}} = 0.723$	$l = -26 \rightarrow 26$
19675 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H-atom parameters constrained
$wR(F^2) = 0.072$	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.8352P]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
6372 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
367 parameters	$\Delta\rho_{\text{max}} = 0.74 \text{ e } \text{\AA}^{-3}$
5 restraints	$\Delta\rho_{\text{min}} = -0.72 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ce1	0.721731 (14)	0.278491 (10)	0.113902 (6)	0.02791 (5)
Zn1	0.68898 (3)	0.37172 (2)	0.273209 (14)	0.03396 (8)
O1	0.82372 (19)	0.28221 (13)	0.22806 (9)	0.0344 (4)

supplementary materials

O2	0.55782 (18)	0.32520 (14)	0.19983 (9)	0.0367 (4)
O3	0.7363 (2)	0.36404 (16)	0.00051 (10)	0.0478 (5)
O7	0.4590 (2)	0.35443 (16)	0.08041 (10)	0.0455 (5)
O6	0.96909 (19)	0.18026 (15)	0.14819 (9)	0.0403 (4)
C1	0.9350 (3)	0.23935 (19)	0.25581 (13)	0.0316 (5)
O4	0.9350 (2)	0.33221 (17)	0.04741 (11)	0.0482 (5)
N1	0.7945 (3)	0.35347 (18)	0.36140 (11)	0.0431 (6)
C11	0.3434 (3)	0.37291 (19)	0.25099 (16)	0.0424 (7)
N2	0.5234 (3)	0.36933 (18)	0.33703 (12)	0.0459 (6)
C16	0.4265 (3)	0.35515 (18)	0.19525 (14)	0.0347 (5)
C6	0.9761 (3)	0.2473 (2)	0.32368 (14)	0.0402 (6)
C12	0.2017 (3)	0.3975 (2)	0.2391 (2)	0.0559 (9)
H12	0.1450	0.4072	0.2754	0.067*
N3	0.8670 (3)	0.3669 (2)	-0.00159 (13)	0.0507 (6)
C2	1.0167 (3)	0.1824 (2)	0.21410 (14)	0.0368 (6)
C15	0.3671 (3)	0.36920 (19)	0.13120 (16)	0.0399 (6)
C14	0.2281 (3)	0.3946 (2)	0.12134 (18)	0.0513 (8)
H14	0.1905	0.4029	0.0784	0.062*
C5	1.0961 (3)	0.1961 (3)	0.34678 (17)	0.0520 (8)
H5	1.1232	0.2002	0.3916	0.062*
C3	1.1328 (3)	0.1340 (2)	0.23810 (17)	0.0490 (7)
H3	1.1850	0.0964	0.2095	0.059*
C7	0.9013 (3)	0.3013 (2)	0.37289 (14)	0.0442 (7)
H7	0.9343	0.2976	0.4169	0.053*
C9	0.5654 (4)	0.3618 (3)	0.40743 (15)	0.0566 (9)
H9A	0.5584	0.2950	0.4221	0.068*
H9B	0.5043	0.4009	0.4342	0.068*
C10	0.3950 (3)	0.3688 (2)	0.31924 (17)	0.0486 (7)
H10	0.3299	0.3656	0.3526	0.058*
O5	0.9252 (3)	0.4002 (3)	-0.04931 (16)	0.1083 (13)
C8	0.7153 (4)	0.3970 (2)	0.41643 (15)	0.0563 (9)
H8A	0.7191	0.4672	0.4141	0.068*
H8B	0.7541	0.3765	0.4594	0.068*
C13	0.1462 (3)	0.4075 (2)	0.1766 (2)	0.0577 (9)
H13	0.0524	0.4230	0.1707	0.069*
O14	0.6427 (2)	0.11821 (14)	0.16096 (10)	0.0422 (4)
O8	0.5705 (2)	0.18208 (16)	0.02343 (10)	0.0459 (5)
O11	0.7636 (2)	0.45076 (15)	0.13802 (10)	0.0477 (5)
O9	0.7877 (2)	0.14445 (16)	0.02635 (11)	0.0485 (5)
N4	0.6690 (3)	0.13210 (17)	0.00004 (12)	0.0453 (6)
C18	1.0647 (3)	0.1421 (3)	0.10137 (17)	0.0554 (8)
H18A	1.1526	0.1748	0.1066	0.083*
H18B	1.0282	0.1519	0.0568	0.083*
H18C	1.0775	0.0740	0.1093	0.083*
C17	0.4079 (4)	0.3800 (3)	0.01437 (17)	0.0621 (9)
H17A	0.3365	0.3352	0.0003	0.093*
H17B	0.4831	0.3775	-0.0162	0.093*
H17C	0.3701	0.4444	0.0150	0.093*
C4	1.1720 (4)	0.1415 (3)	0.30533 (18)	0.0579 (9)

H4	1.2506	0.1088	0.3217	0.069*
O13	0.7477 (2)	0.50345 (14)	0.24266 (9)	0.0413 (4)
N5	0.7785 (3)	0.51482 (18)	0.18155 (12)	0.0470 (6)
O10	0.6498 (3)	0.0758 (2)	-0.04574 (13)	0.0771 (8)
O12	0.8398 (4)	0.6105 (2)	0.16137 (19)	0.1030 (11)
C19	0.5004 (4)	0.0893 (3)	0.1620 (2)	0.0657 (10)
H19A	0.4721	0.0840	0.2074	0.099*
H19B	0.4896	0.0277	0.1402	0.099*
H19C	0.4437	0.1367	0.1391	0.099*
H14A	0.695 (3)	0.087 (2)	0.1905 (13)	0.049 (9)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.03009 (8)	0.03429 (8)	0.01915 (8)	0.00086 (5)	-0.00257 (5)	-0.00135 (5)
Zn1	0.04075 (17)	0.03836 (16)	0.02282 (14)	-0.00119 (12)	0.00205 (12)	-0.00123 (11)
O1	0.0325 (9)	0.0470 (10)	0.0234 (9)	0.0066 (7)	-0.0050 (7)	-0.0011 (7)
O2	0.0292 (9)	0.0485 (11)	0.0323 (10)	0.0051 (8)	0.0012 (8)	-0.0059 (8)
O3	0.0449 (11)	0.0668 (14)	0.0314 (10)	0.0013 (10)	-0.0046 (9)	0.0087 (9)
O7	0.0364 (10)	0.0628 (13)	0.0369 (11)	0.0104 (9)	-0.0079 (9)	-0.0069 (10)
O6	0.0380 (10)	0.0523 (11)	0.0303 (10)	0.0091 (9)	-0.0044 (8)	-0.0048 (8)
C1	0.0313 (12)	0.0369 (12)	0.0260 (12)	-0.0040 (10)	-0.0072 (10)	0.0062 (10)
O4	0.0363 (10)	0.0616 (13)	0.0468 (12)	-0.0019 (9)	0.0006 (9)	0.0098 (10)
N1	0.0595 (15)	0.0469 (13)	0.0228 (11)	-0.0059 (11)	-0.0012 (11)	-0.0014 (10)
C11	0.0387 (14)	0.0346 (13)	0.0548 (18)	-0.0020 (11)	0.0161 (13)	-0.0040 (12)
N2	0.0579 (16)	0.0469 (13)	0.0337 (12)	0.0002 (11)	0.0154 (12)	0.0005 (10)
C16	0.0278 (12)	0.0322 (12)	0.0442 (15)	-0.0009 (9)	0.0031 (11)	-0.0056 (11)
C6	0.0394 (14)	0.0504 (14)	0.0300 (14)	-0.0069 (12)	-0.0106 (11)	0.0108 (12)
C12	0.0385 (16)	0.0444 (16)	0.086 (3)	-0.0001 (13)	0.0260 (17)	-0.0071 (17)
N3	0.0537 (16)	0.0603 (16)	0.0384 (14)	-0.0004 (12)	0.0092 (12)	0.0094 (12)
C2	0.0341 (13)	0.0390 (13)	0.0368 (14)	-0.0009 (11)	-0.0063 (11)	0.0040 (11)
C15	0.0295 (13)	0.0385 (13)	0.0513 (17)	0.0006 (10)	-0.0024 (12)	-0.0082 (12)
C14	0.0320 (14)	0.0501 (17)	0.071 (2)	0.0031 (12)	-0.0101 (15)	-0.0068 (15)
C5	0.0490 (18)	0.068 (2)	0.0384 (16)	0.0002 (15)	-0.0166 (14)	0.0136 (15)
C3	0.0408 (15)	0.0500 (16)	0.056 (2)	0.0112 (13)	-0.0082 (14)	0.0076 (14)
C7	0.0552 (18)	0.0539 (16)	0.0228 (13)	-0.0127 (14)	-0.0128 (13)	0.0054 (12)
C9	0.080 (2)	0.0605 (19)	0.0304 (15)	0.0050 (17)	0.0204 (16)	0.0008 (14)
C10	0.0523 (18)	0.0437 (15)	0.0511 (18)	-0.0002 (13)	0.0241 (15)	-0.0033 (13)
O5	0.091 (2)	0.162 (3)	0.073 (2)	0.005 (2)	0.0358 (18)	0.061 (2)
C8	0.091 (3)	0.0515 (17)	0.0264 (14)	0.0017 (17)	0.0052 (16)	-0.0077 (13)
C13	0.0290 (14)	0.0503 (17)	0.094 (3)	0.0056 (12)	0.0038 (17)	-0.0045 (18)
O14	0.0444 (11)	0.0419 (10)	0.0403 (11)	-0.0039 (9)	-0.0016 (9)	0.0099 (9)
O8	0.0478 (11)	0.0537 (12)	0.0354 (11)	0.0032 (10)	-0.0122 (9)	-0.0040 (9)
O11	0.0688 (14)	0.0416 (10)	0.0328 (9)	-0.0041 (9)	0.0045 (10)	-0.0023 (7)
O9	0.0470 (11)	0.0557 (12)	0.0426 (12)	0.0034 (9)	-0.0028 (10)	-0.0162 (9)
N4	0.0637 (16)	0.0421 (13)	0.0297 (12)	-0.0017 (11)	-0.0074 (12)	-0.0025 (10)
C18	0.0492 (18)	0.071 (2)	0.0459 (18)	0.0189 (15)	0.0047 (15)	-0.0093 (16)
C17	0.059 (2)	0.082 (2)	0.0434 (18)	0.0169 (18)	-0.0169 (16)	-0.0039 (17)

supplementary materials

C4	0.0501 (18)	0.068 (2)	0.054 (2)	0.0132 (16)	-0.0196 (16)	0.0164 (17)
O13	0.0551 (12)	0.0358 (9)	0.0330 (8)	-0.0046 (8)	0.0030 (9)	-0.0026 (7)
N5	0.0596 (15)	0.0440 (12)	0.0374 (10)	0.0027 (11)	0.0040 (11)	-0.0026 (9)
O10	0.103 (2)	0.0703 (16)	0.0568 (15)	0.0007 (15)	-0.0205 (15)	-0.0352 (13)
O12	0.140 (3)	0.0671 (18)	0.104 (3)	-0.0115 (19)	0.035 (2)	0.0014 (18)
C19	0.0525 (19)	0.074 (2)	0.070 (2)	-0.0207 (17)	-0.0022 (18)	0.0150 (19)

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

Ce1—O1	2.4630 (18)	C12—H12	0.9300
Ce1—O2	2.4517 (17)	N3—O5	1.212 (3)
Ce1—O3	2.568 (2)	C2—C3	1.375 (4)
Ce1—O4	2.583 (2)	C15—C14	1.388 (4)
Ce1—O6	2.8033 (19)	C14—C13	1.388 (5)
Ce1—O7	2.7957 (19)	C14—H14	0.9300
Ce1—O8	2.649 (2)	C5—C4	1.351 (5)
Ce1—O9	2.639 (2)	C5—H5	0.9300
Ce1—O11	2.457 (2)	C3—C4	1.392 (5)
Ce1—O14	2.5301 (19)	C3—H3	0.9300
Zn1—O1	2.0212 (17)	C7—H7	0.9300
Zn1—O2	2.0136 (19)	C9—C8	1.525 (5)
Zn1—O13	2.0047 (19)	C9—H9A	0.9700
Zn1—N1	2.028 (2)	C9—H9B	0.9700
Zn1—N2	2.068 (2)	C10—H10	0.9300
O1—C1	1.329 (3)	C8—H8A	0.9700
O2—C16	1.328 (3)	C8—H8B	0.9700
O3—N3	1.258 (3)	C13—H13	0.9300
O7—C15	1.381 (3)	O14—C19	1.423 (4)
O7—C17	1.442 (4)	O14—H14A	0.875 (18)
O6—C2	1.385 (3)	O8—N4	1.270 (3)
O6—C18	1.432 (3)	O11—N5	1.248 (3)
C1—C2	1.403 (4)	O9—N4	1.254 (3)
C1—C6	1.409 (4)	N4—O10	1.212 (3)
O4—N3	1.258 (3)	C18—H18A	0.9600
N1—C7	1.268 (4)	C18—H18B	0.9600
N1—C8	1.484 (4)	C18—H18C	0.9600
C11—C16	1.412 (4)	C17—H17A	0.9600
C11—C12	1.415 (4)	C17—H17B	0.9600
C11—C10	1.442 (5)	C17—H17C	0.9600
N2—C10	1.274 (4)	C4—H4	0.9300
N2—C9	1.460 (4)	O13—N5	1.278 (3)
C16—C15	1.403 (4)	N5—O12	1.506 (4)
C6—C5	1.418 (4)	C19—H19A	0.9600
C6—C7	1.444 (4)	C19—H19B	0.9600
C12—C13	1.354 (5)	C19—H19C	0.9600
O2—Ce1—O11	73.26 (6)	O2—C16—C11	123.8 (3)
O2—Ce1—O1	65.70 (6)	C15—C16—C11	118.4 (2)
O11—Ce1—O1	74.86 (6)	C1—C6—C5	118.6 (3)
O2—Ce1—O14	76.29 (7)	C1—C6—C7	124.6 (3)

O11—Ce1—O14	145.29 (7)	C5—C6—C7	116.7 (3)
O1—Ce1—O14	77.74 (6)	C13—C12—C11	122.1 (3)
O2—Ce1—O3	123.54 (7)	C13—C12—H12	118.9
O11—Ce1—O3	73.52 (7)	C11—C12—H12	118.9
O1—Ce1—O3	141.44 (7)	O5—N3—O3	121.4 (3)
O14—Ce1—O3	139.14 (7)	O5—N3—O4	121.3 (3)
O2—Ce1—O4	145.16 (7)	O3—N3—O4	117.2 (2)
O11—Ce1—O4	72.31 (7)	C3—C2—O6	124.4 (3)
O1—Ce1—O4	99.96 (7)	C3—C2—C1	121.7 (3)
O14—Ce1—O4	133.94 (7)	O6—C2—C1	113.9 (2)
O3—Ce1—O4	49.29 (7)	O7—C15—C14	124.4 (3)
O2—Ce1—O9	145.30 (7)	O7—C15—C16	113.7 (2)
O11—Ce1—O9	140.19 (7)	C14—C15—C16	122.0 (3)
O1—Ce1—O9	122.37 (6)	C13—C14—C15	118.9 (3)
O14—Ce1—O9	73.43 (7)	C13—C14—H14	120.6
O3—Ce1—O9	73.39 (7)	C15—C14—H14	120.6
O4—Ce1—O9	69.50 (7)	C4—C5—C6	121.7 (3)
O2—Ce1—O8	105.22 (6)	C4—C5—H5	119.2
O11—Ce1—O8	134.76 (7)	C6—C5—H5	119.2
O1—Ce1—O8	147.33 (6)	C2—C3—C4	119.8 (3)
O14—Ce1—O8	69.59 (7)	C2—C3—H3	120.1
O3—Ce1—O8	70.61 (7)	C4—C3—H3	120.1
O4—Ce1—O8	102.61 (7)	N1—C7—C6	125.8 (3)
O9—Ce1—O8	47.93 (7)	N1—C7—H7	117.1
O2—Ce1—O7	58.48 (6)	C6—C7—H7	117.1
O11—Ce1—O7	79.96 (7)	N2—C9—C8	109.0 (2)
O1—Ce1—O7	123.18 (6)	N2—C9—H9A	109.9
O14—Ce1—O7	98.00 (7)	C8—C9—H9A	109.9
O3—Ce1—O7	71.74 (6)	N2—C9—H9B	109.9
O4—Ce1—O7	119.44 (7)	C8—C9—H9B	109.9
O9—Ce1—O7	109.59 (6)	H9A—C9—H9B	108.3
O8—Ce1—O7	63.32 (6)	N2—C10—C11	124.7 (3)
O2—Ce1—O6	120.75 (6)	N2—C10—H10	117.7
O11—Ce1—O6	106.70 (7)	C11—C10—H10	117.7
O1—Ce1—O6	58.05 (6)	N1—C8—C9	106.5 (3)
O14—Ce1—O6	75.33 (6)	N1—C8—H8A	110.4
O3—Ce1—O6	111.86 (6)	C9—C8—H8A	110.4
O4—Ce1—O6	65.60 (6)	N1—C8—H8B	110.4
O9—Ce1—O6	66.80 (6)	C9—C8—H8B	110.4
O8—Ce1—O6	111.63 (6)	H8A—C8—H8B	108.6
O7—Ce1—O6	173.00 (6)	C12—C13—C14	120.5 (3)
O13—Zn1—O2	103.99 (8)	C12—C13—H13	119.7
O13—Zn1—O1	103.22 (8)	C14—C13—H13	119.7
O2—Zn1—O1	82.71 (7)	C19—O14—Ce1	123.3 (2)
O13—Zn1—N1	103.95 (9)	C19—O14—H14A	112 (2)
O2—Zn1—N1	152.06 (9)	Ce1—O14—H14A	121 (2)
O1—Zn1—N1	90.21 (9)	N4—O8—Ce1	97.26 (15)
O13—Zn1—N2	115.52 (9)	N5—O11—Ce1	146.97 (17)
O2—Zn1—N2	88.33 (9)	N4—O9—Ce1	98.18 (16)

supplementary materials

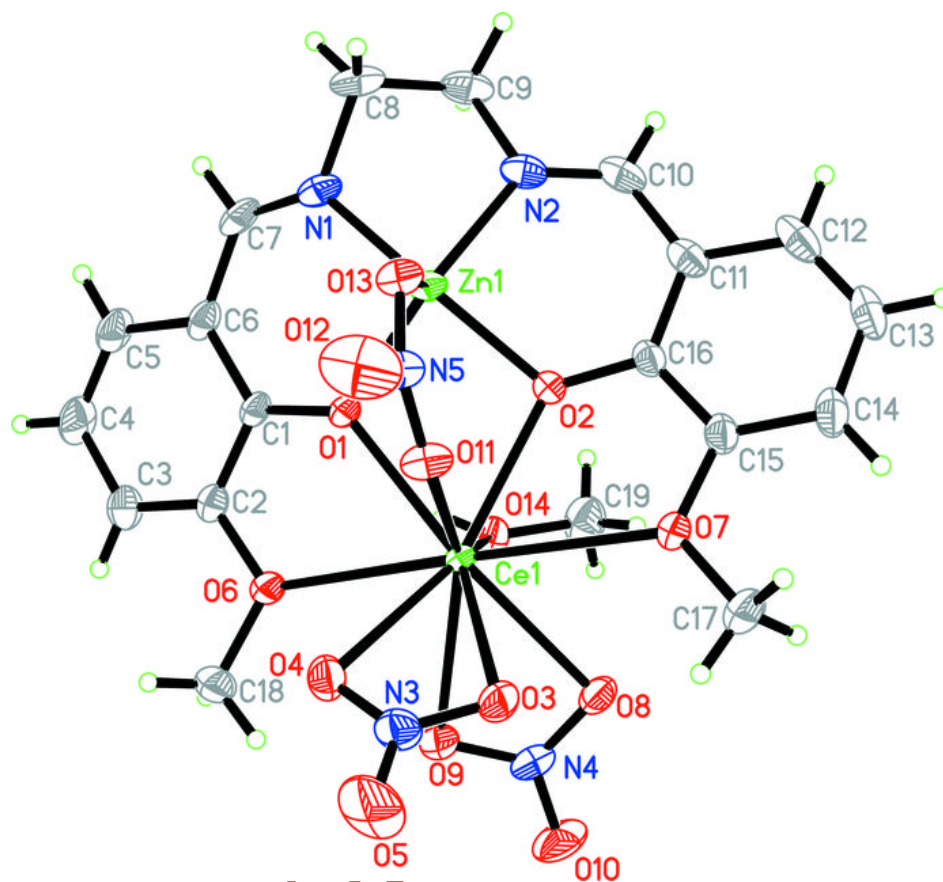
O1—Zn1—N2	141.25 (9)	O10—N4—O9	121.5 (3)
N1—Zn1—N2	80.39 (11)	O10—N4—O8	121.9 (3)
C1—O1—Zn1	127.01 (16)	O9—N4—O8	116.6 (2)
C1—O1—Ce1	132.29 (16)	O6—C18—H18A	109.5
Zn1—O1—Ce1	100.71 (7)	O6—C18—H18B	109.5
C16—O2—Zn1	121.61 (16)	H18A—C18—H18B	109.5
C16—O2—Ce1	131.35 (17)	O6—C18—H18C	109.5
Zn1—O2—Ce1	101.31 (7)	H18A—C18—H18C	109.5
N3—O3—Ce1	97.10 (16)	H18B—C18—H18C	109.5
C15—O7—C17	115.6 (2)	O7—C17—H17A	109.5
C15—O7—Ce1	118.02 (16)	O7—C17—H17B	109.5
C17—O7—Ce1	126.38 (18)	H17A—C17—H17B	109.5
C2—O6—C18	115.6 (2)	O7—C17—H17C	109.5
C2—O6—Ce1	118.50 (15)	H17A—C17—H17C	109.5
C18—O6—Ce1	124.90 (17)	H17B—C17—H17C	109.5
O1—C1—C2	117.1 (2)	C5—C4—C3	120.0 (3)
O1—C1—C6	124.7 (2)	C5—C4—H4	120.0
C2—C1—C6	118.2 (2)	C3—C4—H4	120.0
N3—O4—Ce1	96.36 (16)	N5—O13—Zn1	118.62 (17)
C7—N1—C8	121.6 (3)	O11—N5—O13	123.9 (2)
C7—N1—Zn1	127.6 (2)	O11—N5—O12	118.2 (2)
C8—N1—Zn1	110.1 (2)	O13—N5—O12	117.9 (2)
C16—C11—C12	118.0 (3)	O14—C19—H19A	109.5
C16—C11—C10	123.8 (3)	O14—C19—H19B	109.5
C12—C11—C10	118.1 (3)	H19A—C19—H19B	109.5
C10—N2—C9	120.6 (3)	O14—C19—H19C	109.5
C10—N2—Zn1	125.6 (2)	H19A—C19—H19C	109.5
C9—N2—Zn1	113.8 (2)	H19B—C19—H19C	109.5
O2—C16—C15	117.8 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O14—H14A...O13 ⁱ	0.875 (18)	1.84 (2)	2.689 (3)	162 (3)
C7—H7...O8 ⁱⁱ	0.93	2.49	3.393 (3)	165
C5—H5...O3 ⁱⁱ	0.93	2.57	3.428 (4)	154
C17—H17B...O3	0.96	2.45	3.180 (4)	133
C18—H18B...O9	0.96	2.37	3.018 (4)	124

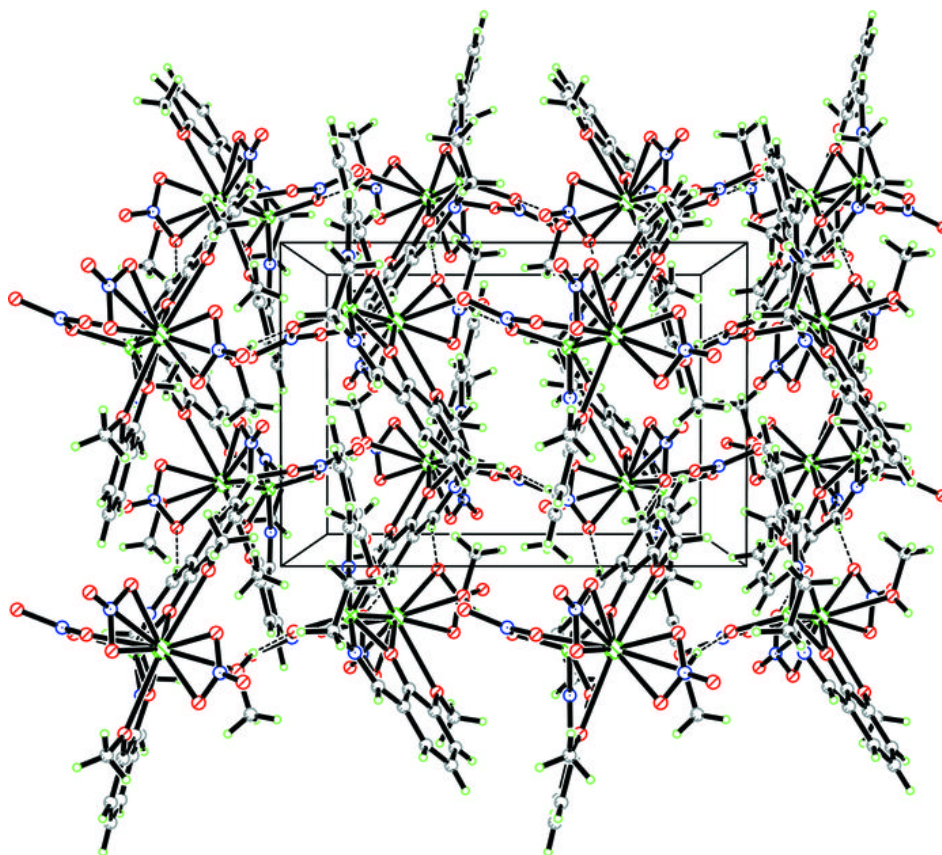
Symmetry codes: (i) $-x+3/2, y-1/2, -z+1/2$; (ii) $x+1/2, -y+1/2, z+1/2$.

Fig. 1



Article

Fig. 2



Article