

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

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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
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i>	Liu & Xie (2007a)	10.1107/S1600536807026852	EDUMAS
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')copper(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807028255	EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNOF₂</i>	Liu Wang, Wang & Xie (2007a)	10.1107/S1600536807027195	ICSD 240891
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')cobalt(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807031224	WIHJED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxy)acetato-κ²O:O']bis[(1,10-phenanthroline-κ²N,N')-(2-pyridyloxy)acetato-κO]neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Liu & Zhu (2007j)	10.1107/S1600536807040068	KIKQAX
<i>2-Hydroxy-3,5-dinitrobenzamide monohydrate</i>	Liu & Zhu (2007k)	10.1107/S1600536807039712	KIKQEB
<i>2-(1-Hydroxy-2-pyridyl)acetamide monohydrate</i>	Liu & Zhu (2007l)	10.1107/S1600536807040652	CIKQOD
<i>Bis(2,2'-bipyridine-κN,N')bis(thiocyanato-κN)iron(II)</i>	Liu & Zhu (2007a)	10.1107/S1600536807043486	XIFXOA
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III)]</i>	Liu & Zhu (2007b)	10.1107/S1600536807045485	XILNAI
<i>3-Hydroxy-2,4,6-trinitropyridine monohydrate</i>	Liu & Zhu (2007m)	10.1107/S1600536807045230	PILNOO
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]</i>	Liu & Zhu (2007d)	10.1107/S1600536807050969	GIMZOS
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)</i>	Liu & Zhu (2007e)	10.1107/S1600536807051756	WINFAB
<i>2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate</i>	Liu & Zhu (2007n)	10.1107/S1600536807048477	GINFEP
<i>2-(Benzoylhydrazinocarbonyl)benzoic acid</i>	Liu & Zhu (2007o)	10.1107/S160053680705204X	TINZIA
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)</i>	Liu & Zhu (2007f)	10.1107/S1600536807054529	HIPZIQ
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')nickel(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')copper(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ²N,N')cobalt(II)]-μ-acetamidato-κ²O:N]</i>	Liu & Zhu (2007i)	10.1107/S1600536807060631	YIQMER
<i>N'-Benzoyl-4-nitronicotinohydrazide</i>	Liu & Zhu (2007p)	10.1107/S1600536807053068	CIPVON
<i>N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide</i>	Liu & Zhu (2007q)	10.1107/S1600536807054876	RIRWEV

Table 1 (continued)

Title	Reference	DOI	Refcode
<i>Ethylenediammonium sulfate</i>	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
<i>Ethylenediammonium perchlorate</i>	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
<i>catena-Poly[[[nitrate-κO](1,10-phenanthroline-κ²N,N')manganese(II)]-μ-nitrate-κ²O:O']</i>	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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Tetrakis[μ -(2-pyridyloxy)acetato- κ^2 O:O']bis[(1,10-phenanthroline- κ^2 N,N')[(2-pyridyloxy)acetato- κ O]-neodymium(III)]

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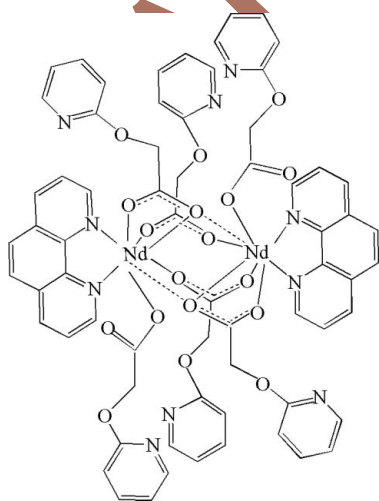
Received 18 July 2007; accepted 19 July 2007

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.011$ Å; R factor = 0.042; wR factor = 0.128; data-to-parameter ratio = 16.8.

The molecule of the title compound, $[\text{Nd}_2(\text{C}_7\text{H}_6\text{NO}_3)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]$, has an inversion centre midway between the two Nd^{III} ions, which are bridged by two tridentate and two bidentate carboxylate groups. Each Nd atom is seven-coordinated by two N atoms of a 1,10-phenanthroline ligand and five O atoms of (2-pyridyloxy)acetate ligands. In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds lead to a supramolecular network.

Related literature

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



Experimental

Crystal data

$[\text{Nd}_2(\text{C}_7\text{H}_6\text{NO}_3)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]$
 $M_r = 1561.66$
 Monoclinic, $P2_1/n$
 $a = 20.1233$ (11) Å
 $b = 8.3987$ (12) Å
 $c = 20.6864$ (13) Å
 $\beta = 107.207$ (6)°
 $V = 3339.7$ (6) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.62$ mm⁻¹
 $T = 273$ (2) K
 $0.33 \times 0.13 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.620$, $T_{\text{max}} = 0.880$
 25069 measured reflections
 6771 independent reflections
 4723 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.128$
 $S = 0.99$
 6771 reflections
 403 parameters
 3 restraints
 H atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.67$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.67$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Nd1—O1	2.544 (3)	Nd1—O5 ⁱ	2.519 (3)
Nd1—O2	2.784 (4)	Nd1—O8 ⁱⁱ	2.522 (3)
Nd1—O2 ⁱ	2.439 (3)	Nd1—N1	2.742 (4)
Nd1—O3	2.387 (3)	Nd1—N2	2.701 (4)
Nd1—O4	2.471 (3)		
O1—Nd1—O2	48.39 (9)	O3—Nd1—N1	77.25 (12)
O1—Nd1—O3	138.63 (11)	O4—Nd1—N1	127.42 (11)
O1—Nd1—O4	73.88 (11)	O1—Nd1—N2	73.72 (11)
O2—Nd1—O3	139.46 (10)	O2—Nd1—N2	118.03 (10)
O2—Nd1—O4	65.28 (10)	O3—Nd1—N2	96.98 (11)
O3—Nd1—O4	145.80 (11)	O4—Nd1—N2	80.97 (11)
O1—Nd1—N1	63.12 (11)	N1—Nd1—N2	59.65 (13)
O2—Nd1—N1	102.23 (11)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C10—H10 ⁱⁱⁱ ···O1 ⁱⁱⁱ	0.93	2.32	3.198 (7)	157
C14—H14B···O3 ^{iv}	0.97	2.37	3.317 (6)	164
C12—H12···O8 ⁱⁱ	0.93	2.46	3.051 (7)	122
C1—H1···O5 ⁱ	0.93	2.44	3.120 (7)	130

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: HK2296).

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Article retracted

supplementary materials

Article retracted

Acta Cryst. (2007). E63, m2196-m2197 [doi:10.1107/S1600536807035349]

Tetrakis[μ -(2-pyridyloxy)acetato- $\kappa^2 O:O'$]bis{(1,10-phenanthroline- $\kappa^2 N,N'$)}(2-pyridyloxy)acetato- κO]neodymium(III)}

T. Liu, Z.-W. Wang, Y.-X. Wang and Z.-P. Xie

Comment

The crystal structures of tetrakis(μ -(2-pyridyloxy)acetato)bis[(1,10-phenanthroline)((2-pyridyloxy)acetato)lanthanum(III)], (II), (Liu *et al.*, 2007a) and tetrakis(μ -(2-pyridyloxy)acetato) bis[(1,10-phenanthroline)((2-pyridyloxy)acetato)praseodymium(III)], (III), (Liu *et al.*, 2007b) have previously been reported. 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).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). It has an inversion centre between the two Nd^{III} ions, in which they are bridged by the two terdentate and the two bidentate carboxylate groups. Each Nd atom is seven-coordinated by the two N atoms of 1,10-phenanthroline (phen) ligand and the five O atoms of 2-pyridyloxy-acetic acid ligands. The Nd—O and Nd—N bonds are in the range of [2.387 (3)–2.784 (4) Å] and [2.701 (4)–2.742 (4) Å], respectively (Table 1), as in (II) and (III).

In the crystal structure, intermolecular C—H \cdots O hydrogen bonds (Table 2) lead to a supramolecular network structure (Fig. 2), in which they may be effective in the stabilization of the structure, as in (II) and (III).

The 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. Neodymium (III) chloride hexahydrate (143.4 mg, 0.4 mmol), phen (79.2 mg, 0.4 mmol), phenoxyacetic acid (182.6 mg, 1.2 mmol) and distilled water (6 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure for 7 d at 433 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. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å, for aromatic and methylene H atoms, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

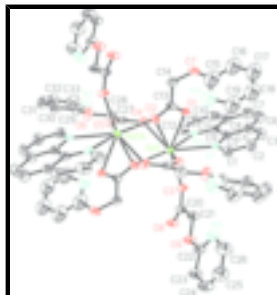


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $2 - x, -y, 2 - z$]. H atoms have been omitted for clarity.

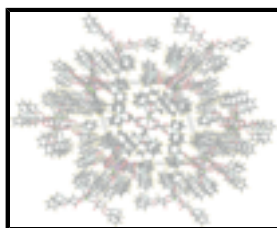


Fig. 2. Packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Tetrakis[μ -(2-pyridyloxy)acetato- κ^2 O:O']bis{(1,10-phenanthroline- κ^2 N,N')}[(2-pyridyloxy)acetato- κ O]neodymium(III)

Crystal data

[Nd₂(C₇H₆NO₃)₆(C₁₂H₈N₂)₂]

$M_r = 1561.66$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 20.1233$ (11) Å

$b = 8.3987$ (12) Å

$c = 20.6864$ (13) Å

$\beta = 107.207$ (6)°

$V = 3339.7$ (6) Å³

$Z = 2$

$F_{000} = 1564$

$D_x = 1.553$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 8971 reflections

$\theta = 2.6$ – 26.0 °

$\mu = 1.62$ mm⁻¹

$T = 273$ (2) K

Plate, colourless

$0.33 \times 0.13 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

φ and ω scans

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

$T_{\min} = 0.620$, $T_{\max} = 0.880$

25069 measured reflections

6771 independent reflections

4723 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\text{max}} = 26.4$ °

$\theta_{\text{min}} = 2.1$ °

$h = -25$ → 24

$k = -10$ → 10

$l = -25$ → 25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.128$	$w = 1/[\sigma^2(F_o^2) + (0.0839P)^2]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
6771 reflections	$(\Delta/\sigma)_{\max} = 0.002$
403 parameters	$\Delta\rho_{\max} = 1.67 \text{ e } \text{\AA}^{-3}$
3 restraints	$\Delta\rho_{\min} = -0.67 \text{ e } \text{\AA}^{-3}$
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	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd1	0.931198 (12)	0.19065 (3)	0.964296 (11)	0.03913 (11)
O1	0.84635 (15)	-0.0360 (4)	0.91890 (15)	0.0436 (7)
O2	0.94655 (17)	-0.1384 (4)	0.97708 (16)	0.0493 (8)
O3	0.93994 (17)	0.4208 (4)	1.03403 (15)	0.0473 (8)
O4	0.97062 (17)	0.0607 (4)	0.87489 (15)	0.0466 (8)
O5	1.06707 (17)	-0.0828 (4)	0.92160 (15)	0.0487 (8)
O6	1.11849 (19)	-0.0172 (5)	0.82196 (18)	0.0659 (10)
O7	0.7848 (2)	-0.3263 (4)	0.8976 (2)	0.0616 (10)
O8	1.00768 (19)	0.6128 (4)	1.09070 (16)	0.0556 (9)
O9	0.9869 (2)	0.5278 (4)	1.20624 (16)	0.0612 (10)
N1	0.7969 (2)	0.2338 (5)	0.9666 (2)	0.0474 (10)
N2	0.8341 (2)	0.3065 (4)	0.8546 (2)	0.0478 (10)
N3	1.1131 (4)	0.1068 (9)	0.7156 (3)	0.113 (2)
N4	0.7850 (5)	-0.2799 (8)	1.0109 (5)	0.1287 (16)
N5	0.9273 (3)	0.3784 (9)	1.2711 (3)	0.0954 (18)
C1	0.7784 (3)	0.1916 (6)	1.0202 (3)	0.0624 (15)
H1	0.8130	0.1695	1.0603	0.075*

supplementary materials

C2	0.7091 (3)	0.1788 (8)	1.0193 (4)	0.081 (2)
H2	0.6978	0.1479	1.0579	0.097*
C3	0.6580 (3)	0.2123 (9)	0.9608 (4)	0.089 (2)
H3	0.6116	0.2042	0.9597	0.106*
C4	0.6741 (3)	0.2567 (9)	0.9048 (4)	0.0740 (18)
C5	0.7462 (3)	0.2669 (6)	0.9090 (3)	0.0519 (13)
C6	0.6226 (4)	0.2959 (11)	0.8403 (5)	0.109 (3)
H6	0.5754	0.2866	0.8361	0.131*
C7	0.6423 (4)	0.3443 (10)	0.7882 (4)	0.102 (3)
H7	0.6083	0.3728	0.7486	0.122*
C8	0.7131 (3)	0.3546 (8)	0.7900 (3)	0.0695 (17)
C9	0.7665 (3)	0.3093 (5)	0.8510 (3)	0.0520 (13)
C10	0.7361 (4)	0.4039 (8)	0.7369 (3)	0.085 (2)
H10	0.7040	0.4395	0.6973	0.102*
C11	0.8034 (4)	0.4016 (8)	0.7411 (3)	0.0791 (19)
H11	0.8179	0.4344	0.7045	0.095*
C12	0.8525 (3)	0.3495 (7)	0.8009 (3)	0.0627 (15)
H12	0.8992	0.3452	0.8028	0.075*
C13	0.8839 (3)	-0.1511 (6)	0.9390 (2)	0.0435 (11)
C14	0.8574 (3)	-0.3142 (6)	0.9194 (3)	0.0545 (13)
H14A	0.8753	-0.3513	0.8834	0.065*
H14B	0.8753	-0.3843	0.9579	0.065*
C15	0.7520 (7)	-0.3150 (9)	0.9438 (7)	0.1287 (16)
C16	0.6802 (6)	-0.3400 (10)	0.9208 (6)	0.1287 (16)
H16	0.6594	-0.3615	0.8752	0.154*
C17	0.6397 (6)	-0.3341 (10)	0.9629 (6)	0.1287 (16)
H17	0.5923	-0.3556	0.9479	0.154*
C18	0.6728 (6)	-0.2943 (10)	1.0291 (6)	0.1287 (16)
H18	0.6457	-0.2852	1.0583	0.154*
C19	0.7388 (6)	-0.2688 (11)	1.0536 (6)	0.1287 (16)
H19	0.7572	-0.2429	1.0991	0.154*
C20	0.9695 (3)	0.4990 (6)	1.0865 (2)	0.0435 (11)
C21	0.9488 (3)	0.4452 (7)	1.1475 (2)	0.0559 (13)
H21A	0.8995	0.4640	1.1396	0.067*
H21B	0.9572	0.3318	1.1541	0.067*
C22	0.9747 (3)	0.4893 (6)	1.2653 (2)	0.0540 (13)
C23	1.0147 (3)	0.5696 (8)	1.3221 (3)	0.0700 (16)
H23	1.0482	0.6423	1.3183	0.084*
C24	1.0049 (4)	0.5417 (9)	1.3835 (3)	0.090 (2)
H24	1.0313	0.5967	1.4214	0.108*
C25	0.9566 (4)	0.4339 (11)	1.3898 (3)	0.102 (3)
H25	0.9493	0.4168	1.4316	0.123*
C26	0.9193 (5)	0.3518 (11)	1.3346 (4)	0.104 (3)
H26	0.8876	0.2755	1.3394	0.125*
C27	1.0287 (3)	0.0030 (5)	0.8773 (2)	0.0426 (11)
C28	1.0524 (3)	0.0515 (7)	0.8172 (3)	0.0551 (13)
H28B	1.0185	0.0165	0.7758	0.066*
H28A	1.0557	0.1666	0.8157	0.066*
C29	1.1461 (3)	0.0138 (7)	0.7707 (3)	0.0615 (14)

C30	1.2081 (3)	-0.0571 (8)	0.7763 (3)	0.0766 (18)
H30	1.2291	-0.1193	0.8141	0.092*
C31	1.2402 (4)	-0.0377 (9)	0.7267 (5)	0.093 (2)
H31	1.2827	-0.0869	0.7308	0.111*
C32	1.2103 (5)	0.0519 (9)	0.6726 (5)	0.104 (3)
H32	1.2324	0.0651	0.6394	0.125*
C33	1.1489 (5)	0.1231 (11)	0.6652 (4)	0.108 (3)
H33	1.1291	0.1842	0.6268	0.130*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.04630 (17)	0.03256 (17)	0.03352 (16)	-0.00149 (11)	0.00407 (10)	0.00062 (10)
O1	0.0453 (17)	0.0325 (18)	0.0453 (18)	0.0007 (14)	0.0014 (14)	-0.0035 (14)
O2	0.0472 (19)	0.0473 (19)	0.0442 (19)	-0.0032 (16)	-0.0004 (15)	0.0077 (15)
O3	0.069 (2)	0.0305 (17)	0.0406 (18)	-0.0048 (16)	0.0131 (15)	-0.0036 (14)
O4	0.058 (2)	0.0430 (19)	0.0386 (17)	0.0057 (17)	0.0135 (15)	0.0010 (15)
O5	0.061 (2)	0.047 (2)	0.0393 (18)	0.0069 (17)	0.0160 (15)	0.0100 (15)
O6	0.068 (2)	0.081 (3)	0.055 (2)	0.018 (2)	0.0287 (19)	0.0201 (19)
O7	0.059 (2)	0.044 (2)	0.070 (3)	-0.0138 (17)	-0.0001 (19)	-0.0070 (17)
O8	0.083 (3)	0.047 (2)	0.0369 (18)	-0.026 (2)	0.0179 (17)	-0.0040 (15)
O9	0.087 (3)	0.058 (2)	0.0380 (19)	-0.027 (2)	0.0185 (18)	-0.0061 (16)
N1	0.048 (2)	0.037 (2)	0.049 (2)	0.0042 (18)	0.0030 (19)	-0.0083 (18)
N2	0.062 (3)	0.036 (2)	0.036 (2)	0.0044 (19)	0.0001 (18)	0.0002 (17)
N3	0.143 (6)	0.116 (5)	0.100 (5)	-0.007 (5)	0.069 (5)	0.020 (4)
N4	0.154 (4)	0.086 (2)	0.172 (4)	0.015 (3)	0.088 (4)	0.028 (3)
N5	0.098 (4)	0.115 (5)	0.077 (4)	-0.034 (4)	0.031 (3)	0.001 (4)
C1	0.059 (3)	0.071 (4)	0.056 (3)	0.008 (3)	0.015 (3)	-0.003 (3)
C2	0.060 (4)	0.107 (6)	0.083 (5)	0.002 (4)	0.031 (4)	-0.013 (4)
C3	0.046 (3)	0.105 (6)	0.114 (7)	-0.005 (3)	0.021 (4)	-0.017 (5)
C4	0.052 (3)	0.081 (4)	0.073 (4)	0.006 (3)	-0.007 (3)	-0.017 (4)
C5	0.053 (3)	0.036 (3)	0.057 (3)	0.008 (2)	0.002 (2)	-0.009 (2)
C6	0.064 (5)	0.139 (9)	0.098 (7)	0.016 (5)	-0.017 (4)	-0.035 (6)
C7	0.077 (5)	0.108 (6)	0.084 (5)	0.039 (4)	-0.033 (4)	-0.023 (5)
C8	0.074 (4)	0.060 (4)	0.050 (4)	0.018 (3)	-0.019 (3)	-0.011 (3)
C9	0.059 (3)	0.033 (3)	0.046 (3)	0.007 (2)	-0.012 (2)	-0.004 (2)
C10	0.116 (6)	0.068 (5)	0.044 (4)	0.016 (4)	-0.019 (4)	0.000 (3)
C11	0.118 (6)	0.072 (5)	0.035 (3)	0.001 (4)	0.003 (3)	0.011 (3)
C12	0.081 (4)	0.048 (3)	0.049 (3)	-0.002 (3)	0.005 (3)	0.008 (2)
C13	0.048 (3)	0.048 (3)	0.031 (2)	-0.005 (2)	0.006 (2)	-0.003 (2)
C14	0.062 (3)	0.044 (3)	0.052 (3)	0.002 (2)	0.009 (3)	-0.008 (2)
C15	0.154 (4)	0.086 (2)	0.172 (4)	0.015 (3)	0.088 (4)	0.028 (3)
C16	0.154 (4)	0.086 (2)	0.172 (4)	0.015 (3)	0.088 (4)	0.028 (3)
C17	0.154 (4)	0.086 (2)	0.172 (4)	0.015 (3)	0.088 (4)	0.028 (3)
C18	0.154 (4)	0.086 (2)	0.172 (4)	0.015 (3)	0.088 (4)	0.028 (3)
C19	0.154 (4)	0.086 (2)	0.172 (4)	0.015 (3)	0.088 (4)	0.028 (3)
C20	0.060 (3)	0.032 (3)	0.038 (3)	-0.001 (2)	0.014 (2)	0.001 (2)
C21	0.077 (4)	0.049 (3)	0.043 (3)	-0.020 (3)	0.020 (2)	-0.004 (2)

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C22	0.072 (3)	0.052 (3)	0.039 (3)	-0.005 (3)	0.018 (2)	0.003 (2)
C23	0.086 (4)	0.071 (4)	0.050 (3)	-0.020 (3)	0.016 (3)	-0.011 (3)
C24	0.122 (6)	0.100 (5)	0.039 (3)	-0.019 (5)	0.011 (3)	-0.011 (3)
C25	0.127 (6)	0.138 (7)	0.050 (4)	-0.028 (6)	0.039 (4)	0.009 (4)
C26	0.128 (7)	0.132 (7)	0.066 (5)	-0.054 (6)	0.048 (5)	-0.002 (4)
C27	0.055 (3)	0.033 (3)	0.038 (3)	-0.006 (2)	0.011 (2)	-0.003 (2)
C28	0.065 (3)	0.055 (3)	0.047 (3)	0.005 (3)	0.019 (2)	0.012 (2)
C29	0.073 (4)	0.064 (4)	0.056 (3)	-0.008 (3)	0.032 (3)	0.005 (3)
C30	0.079 (4)	0.090 (5)	0.071 (4)	0.001 (4)	0.038 (3)	0.000 (4)
C31	0.093 (5)	0.091 (6)	0.113 (6)	-0.006 (4)	0.060 (5)	-0.008 (5)
C32	0.140 (7)	0.081 (5)	0.131 (7)	-0.018 (5)	0.100 (6)	-0.007 (5)
C33	0.163 (8)	0.099 (6)	0.093 (6)	0.010 (6)	0.083 (6)	0.028 (5)

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

Nd1—O1	2.544 (3)	C6—H6	0.9300
Nd1—O2	2.784 (4)	C7—C8	1.418 (11)
Nd1—O2 ⁱ	2.439 (3)	C7—H7	0.9300
Nd1—O3	2.387 (3)	C8—C10	1.376 (10)
Nd1—O4	2.471 (3)	C8—C9	1.444 (7)
Nd1—O5 ⁱ	2.519 (3)	C10—C11	1.332 (9)
Nd1—O8 ⁱⁱ	2.522 (3)	C10—H10	0.9300
Nd1—N1	2.742 (4)	C11—C12	1.406 (8)
Nd1—N2	2.701 (4)	C11—H11	0.9300
O1—C13	1.222 (6)	C12—H12	0.9300
O2—C13	1.278 (6)	C13—C14	1.482 (7)
O2—Nd1 ⁱ	2.439 (3)	C14—H14A	0.9700
O3—C20	1.258 (5)	C14—H14B	0.9700
O4—C27	1.252 (5)	C15—C16	1.398 (15)
O5—C27	1.239 (5)	C16—C17	1.358 (12)
O5—Nd1 ⁱ	2.519 (3)	C16—H16	0.9300
O6—C29	1.360 (6)	C17—C18	1.374 (15)
O6—C28	1.427 (6)	C17—H17	0.9300
O7—C15	1.316 (11)	C18—C19	1.292 (14)
O7—C14	1.399 (6)	C18—H18	0.9300
O8—C20	1.213 (6)	C19—H19	0.9300
O8—Nd1 ⁱⁱ	2.522 (3)	C20—C21	1.509 (6)
O9—C22	1.354 (6)	C21—H21A	0.9700
O9—C21	1.413 (6)	C21—H21B	0.9700
N1—C1	1.318 (7)	C22—C23	1.388 (7)
N1—C5	1.348 (6)	C23—C24	1.362 (8)
N2—C12	1.321 (7)	C23—H23	0.9300
N2—C9	1.340 (7)	C24—C25	1.363 (10)
N3—C29	1.380 (9)	C24—H24	0.9300
N3—C33	1.439 (9)	C25—C26	1.355 (10)
N4—C15	1.382 (14)	C25—H25	0.9300
N4—C19	1.462 (12)	C26—H26	0.9300
N5—C22	1.365 (8)	C27—C28	1.514 (7)

N5—C26	1.387 (8)	C28—H28B	0.9700
C1—C2	1.394 (8)	C28—H28A	0.9700
C1—H1	0.9300	C29—C30	1.356 (8)
C2—C3	1.365 (10)	C30—C31	1.375 (9)
C2—H2	0.9300	C30—H30	0.9300
C3—C4	1.345 (10)	C31—C32	1.336 (11)
C3—H3	0.9300	C31—H31	0.9300
C4—C5	1.431 (8)	C32—C33	1.339 (11)
C4—C6	1.464 (10)	C32—H32	0.9300
C5—C9	1.422 (8)	C33—H33	0.9300
C6—C7	1.318 (12)		
O1—Nd1—O2	48.39 (9)	C5—C9—C8	118.6 (5)
O1—Nd1—O3	138.63 (11)	C11—C10—C8	121.3 (6)
O1—Nd1—O4	73.88 (11)	C11—C10—H10	119.4
O2—Nd1—O3	139.46 (10)	C8—C10—H10	119.4
O2—Nd1—O4	65.28 (10)	C10—C11—C12	119.9 (6)
O3—Nd1—O4	145.80 (11)	C10—C11—H11	120.1
O1—Nd1—N1	63.12 (11)	C12—C11—H11	120.1
O2—Nd1—N1	102.23 (11)	N2—C12—C11	121.7 (6)
O3—Nd1—N1	77.25 (12)	N2—C12—H12	119.1
O4—Nd1—N1	127.42 (11)	C11—C12—H12	119.1
O1—Nd1—N2	73.72 (11)	O1—C13—O2	122.8 (4)
O2—Nd1—N2	118.03 (10)	O1—C13—C14	120.1 (4)
O3—Nd1—N2	96.98 (11)	O2—C13—C14	117.1 (5)
O4—Nd1—N2	80.97 (11)	O7—C14—C13	114.4 (4)
N1—Nd1—N2	59.65 (13)	O7—C14—H14A	108.7
O3—Nd1—O2 ⁱ	87.83 (12)	C13—C14—H14A	108.7
O2 ⁱ —Nd1—O4	78.04 (11)	O7—C14—H14B	108.7
O3—Nd1—O5 ⁱ	75.33 (10)	C13—C14—H14B	108.7
O2 ⁱ —Nd1—O5 ⁱ	74.76 (11)	H14A—C14—H14B	107.6
O4—Nd1—O5 ⁱ	128.61 (11)	O7—C15—N4	123.3 (11)
O3—Nd1—O8 ⁱⁱ	77.52 (11)	O7—C15—C16	115.6 (12)
O2 ⁱ —Nd1—O8 ⁱⁱ	77.72 (12)	N4—C15—C16	121.1 (11)
O4—Nd1—O8 ⁱⁱ	69.15 (11)	C17—C16—C15	122.1 (13)
O5 ⁱ —Nd1—O8 ⁱⁱ	141.70 (11)	C17—C16—H16	118.9
O2 ⁱ —Nd1—O1	121.12 (12)	C15—C16—H16	118.9
O5 ⁱ —Nd1—O1	84.18 (11)	C16—C17—C18	116.2 (12)
O8 ⁱⁱ —Nd1—O1	133.38 (10)	C16—C17—H17	121.9
O2 ⁱ —Nd1—N2	148.81 (12)	C18—C17—H17	121.9
O5 ⁱ —Nd1—N2	136.30 (12)	C19—C18—C17	124.8 (12)
O8 ⁱⁱ —Nd1—N2	73.35 (12)	C19—C18—H18	117.6
O2 ⁱ —Nd1—N1	150.42 (12)	C17—C18—H18	117.6
O5 ⁱ —Nd1—N1	76.80 (12)	C18—C19—N4	121.1 (12)
O8 ⁱⁱ —Nd1—N1	122.43 (13)	C18—C19—H19	119.5
O2 ⁱ —Nd1—O2	72.96 (13)	N4—C19—H19	119.5

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O5 ⁱ —Nd1—O2	65.40 (10)	O8—C20—O3	126.9 (4)
O8 ⁱⁱ —Nd1—O2	129.58 (11)	O8—C20—C21	120.2 (4)
C13—O1—Nd1	100.8 (3)	O3—C20—C21	112.8 (4)
C13—O2—Nd1 ⁱ	163.1 (3)	O9—C21—C20	111.0 (4)
C13—O2—Nd1	87.9 (3)	O9—C21—H21A	109.4
Nd1 ⁱ —O2—Nd1	107.04 (12)	C20—C21—H21A	109.4
C20—O3—Nd1	151.1 (3)	O9—C21—H21B	109.4
C27—O4—Nd1	130.0 (3)	C20—C21—H21B	109.4
C27—O5—Nd1 ⁱ	137.2 (3)	H21A—C21—H21B	108.0
C29—O6—C28	117.2 (4)	O9—C22—N5	124.1 (5)
C15—O7—C14	117.4 (7)	O9—C22—C23	115.7 (5)
C20—O8—Nd1 ⁱⁱ	150.1 (3)	N5—C22—C23	120.2 (5)
C22—O9—C21	117.5 (4)	C24—C23—C22	119.9 (6)
C1—N1—C5	118.2 (5)	C24—C23—H23	120.0
C1—N1—Nd1	120.2 (3)	C22—C23—H23	120.0
C5—N1—Nd1	120.2 (3)	C23—C24—C25	120.5 (6)
C12—N2—C9	118.8 (4)	C23—C24—H24	119.7
C12—N2—Nd1	119.4 (4)	C25—C24—H24	119.7
C9—N2—Nd1	121.6 (3)	C26—C25—C24	119.3 (6)
C29—N3—C33	115.5 (7)	C26—C25—H25	120.3
C15—N4—C19	114.6 (10)	C24—C25—H25	120.3
C22—N5—C26	118.3 (6)	C25—C26—N5	121.8 (7)
N1—C1—C2	122.6 (6)	C25—C26—H26	119.1
N1—C1—H1	118.7	N5—C26—H26	119.1
C2—C1—H1	118.7	O5—C27—O4	128.7 (4)
C3—C2—C1	119.0 (6)	O5—C27—C28	119.0 (4)
C3—C2—H2	120.5	O4—C27—C28	112.3 (4)
C1—C2—H2	120.5	O6—C28—C27	110.4 (4)
C4—C3—C2	120.7 (6)	O6—C28—H28B	109.6
C4—C3—H3	119.6	C27—C28—H28B	109.6
C2—C3—H3	119.6	O6—C28—H28A	109.6
C3—C4—C5	117.6 (6)	C27—C28—H28A	109.6
C3—C4—C6	124.1 (7)	H28B—C28—H28A	108.1
C5—C4—C6	118.3 (7)	C30—C29—O6	115.3 (5)
N1—C5—C9	117.9 (5)	C30—C29—N3	121.7 (6)
N1—C5—C4	121.9 (5)	O6—C29—N3	123.0 (5)
C9—C5—C4	120.2 (5)	C29—C30—C31	120.5 (7)
C7—C6—C4	120.7 (8)	C29—C30—H30	119.8
C7—C6—H6	119.6	C31—C30—H30	119.8
C4—C6—H6	119.6	C32—C31—C30	119.8 (7)
C6—C7—C8	122.7 (7)	C32—C31—H31	120.1
C6—C7—H7	118.6	C30—C31—H31	120.1
C8—C7—H7	118.6	C31—C32—C33	121.3 (7)
C10—C8—C7	124.8 (6)	C31—C32—H32	119.4
C10—C8—C9	116.0 (6)	C33—C32—H32	119.4
C7—C8—C9	119.3 (7)	C32—C33—N3	121.2 (8)
N2—C9—C5	119.2 (4)	C32—C33—H33	119.4
N2—C9—C8	122.2 (5)	N3—C33—H33	119.4

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

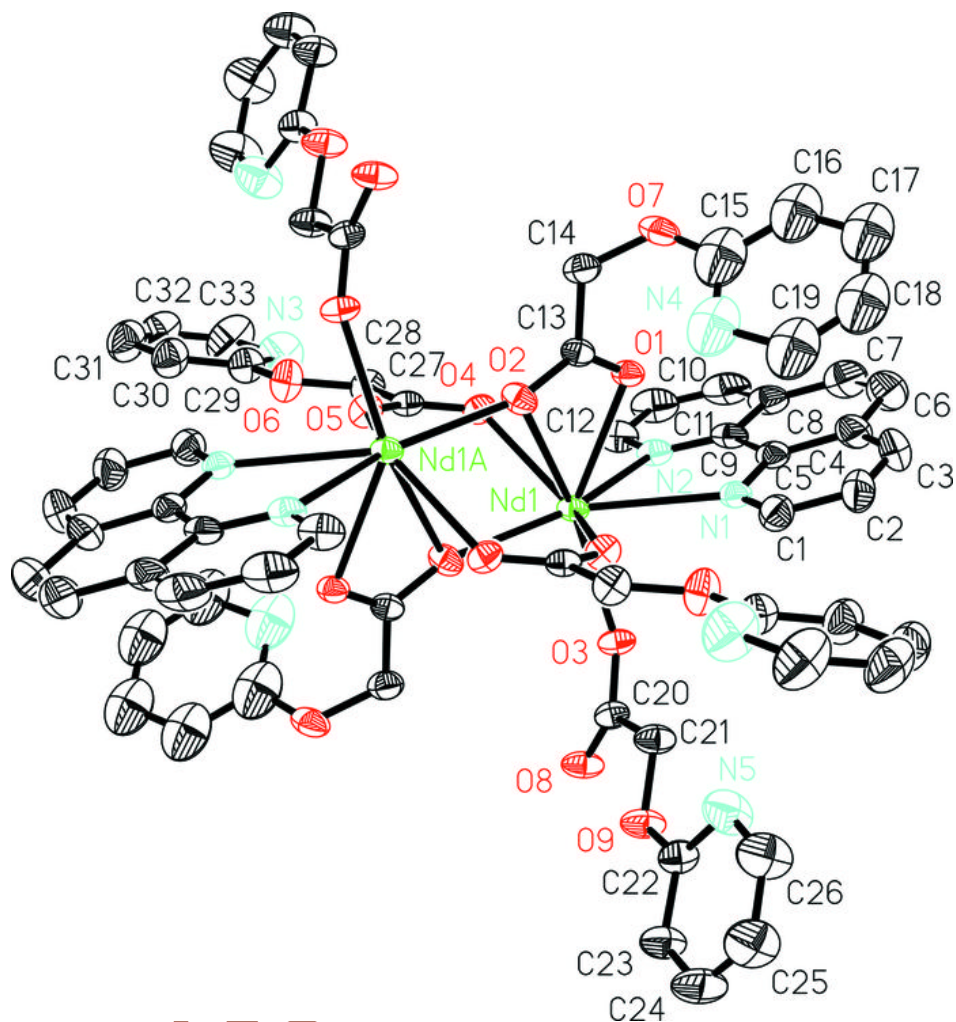
Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C10—H10...O1 ⁱⁱⁱ	0.93	2.32	3.198 (7)	157
C14—H14B...O3 ^{iv}	0.97	2.37	3.317 (6)	164
C12—H12...O8 ⁱⁱ	0.93	2.46	3.051 (7)	122
C1—H1...O5 ⁱ	0.93	2.44	3.120 (7)	130

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

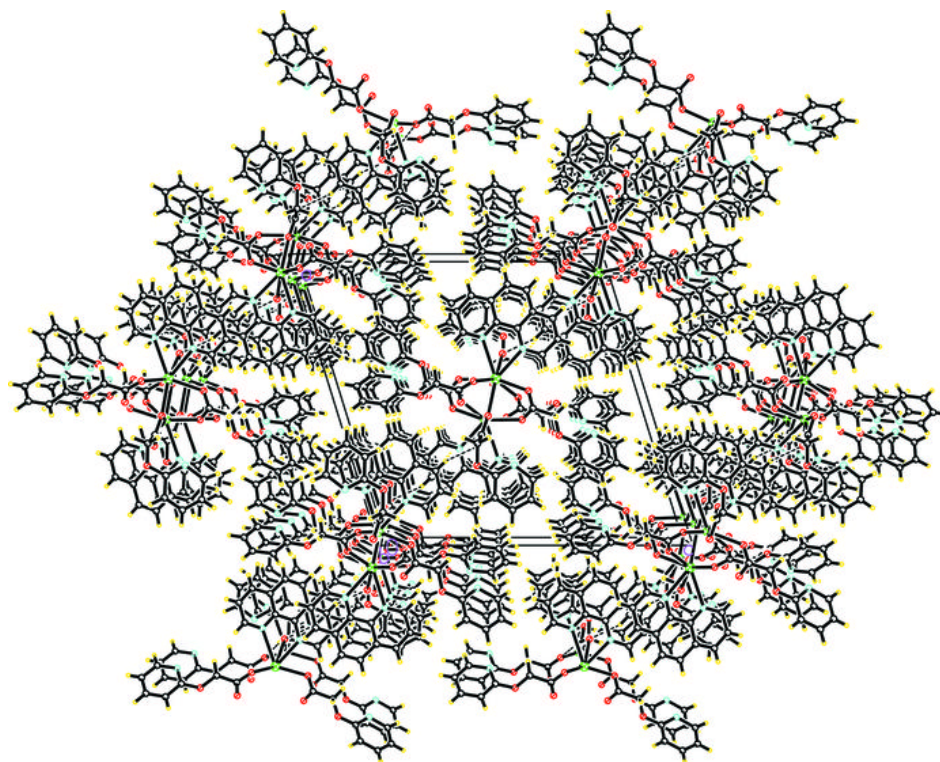
Article retracted

Fig. 1



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Fig. 2



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