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

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

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

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

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

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(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)

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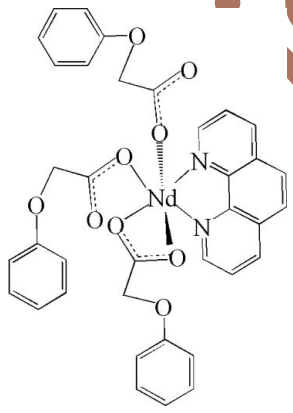
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.011 Å; R factor = 0.041; wR factor = 0.112; data-to-parameter ratio = 17.2.

In the molecule of the title compound, $[Nd(C_8H_7O_3)_3(C_{12}H_8N_2)]$, the Nd^{III} atom is six-coordinated by two N atoms of the 1,10-phenanthroline (phen) ligand and four O atoms of the three phenoxyacetate ligands. In the crystal structure, intermolecular C—H···O hydrogen bonds lead to a supramolecular network.

Related literature

For bond length data, see: Allen *et al.* (1987). For a related structure, see: Zhong *et al.* (2007).



Experimental

Crystal data

$[Nd(C_8H_7O_3)_3(C_{12}H_8N_2)]$
M_r = 777.85
Monoclinic, $P2_1/n$
a = 20.103 (5) Å
b = 8.5028 (17) Å
c = 20.7887 (14) Å
β = 106.997 (4)°
V = 3398.3 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 273 (2) K
0.33 × 0.13 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.626, T_{max} = 0.885
25585 measured reflections
6951 independent reflections
4794 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.01
6951 reflections
403 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O1	2.484 (3)	Nd1—O4	2.818 (4)
Nd1—O2	2.412 (3)	Nd1—N1	2.743 (4)
Nd1—O3	2.564 (3)	Nd1—N2	2.718 (4)
O1—Nd1—O2	145.95 (10)	O3—Nd1—N1	63.59 (11)
O1—Nd1—O3	73.37 (10)	O4—Nd1—N1	102.31 (10)
O1—Nd1—O4	65.19 (9)	O1—Nd1—N2	80.90 (11)
O2—Nd1—O3	139.00 (10)	O2—Nd1—N2	96.80 (10)
O2—Nd1—O4	139.50 (9)	O3—Nd1—N2	74.13 (10)
O3—Nd1—O4	48.10 (9)	O4—Nd1—N2	118.24 (10)
O1—Nd1—N1	127.33 (11)	N1—Nd1—N2	59.81 (12)
O2—Nd1—N1	77.16 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C30—H30B···O2^{i}	0.97	2.40	3.347 (6)	164
C12—H12···O8^{ii}	0.93	2.59	3.438 (7)	152
C12—H12···O6^{ii}	0.93	2.47	3.057 (6)	122
C10—H10···O3^{iii}	0.93	2.34	3.215 (6)	156
C1—H1···O5^{iv}	0.93	2.44	3.130 (6)	132

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

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: HK2277).

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supplementary materials

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(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)

H. Zhong, X.-M. Yang, Q.-Y. Luo and Y.-P. Xu

Comment

The crystal structure of tri(phenoxyacetic acid)(1,10-phenanthroline-N,*N*') cerium(III), (II), has recently been reported (Zhong *et al.*, 2007). 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 that of (II). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The six-coordinate environment of the Nd atom is completed by two N atoms of the 1,10-phenanthroline (phen) ligand and four O atoms of the three phenoxyacetic acid ligand (Table 1). The Nd—O and Nd—N bonds are in the range of [2.412 (3)–2.818 (4) Å] and [2.718 (4)–2.743 (4) Å], respectively (Table 1).

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

The both compounds, (I) and (II), 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 (107.3 mg, 0.3 mmol), phen (59.4 mg, 0.3 mmol), phenoxyacetic acid (91.3 mg, 0.6 mmol) and distilled water (3 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 423 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, which 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_{iso}(H) = 1.2U_{eq}(C).

Figures

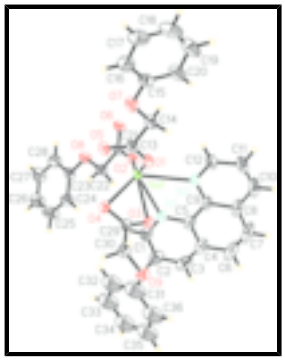

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

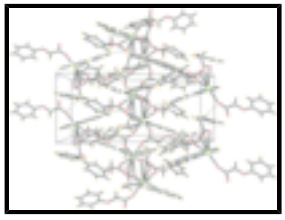

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

(1,10-Phenanthroline-κ^2*N*,*N*')tris(phenoxyacetato)-κ*O*;κ*O*;κ*O*,*O*'- neodymium(III)

Crystal data

$[Nd(C_8H_7O_3)_3(C_{12}H_8N_2)]$	F_{000} = 1564
M_r = 777.85	D_x = 1.520 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9077 reflections
a = 20.103 (5) Å	θ = 2.5–27.0º
b = 8.5028 (17) Å	μ = 1.59 mm^{-1}
c = 20.7887 (14) Å	T = 273 (2) K
β = 106.997 (4)º	Block, colorless
V = 3398.3 (11) Å^3	0.33 × 0.13 × 0.08 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	6951 independent reflections
Radiation source: fine-focus sealed tube	4794 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 273(2) K	θ_{max} = 26.5º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→24
T_{min} = 0.626, T_{max} = 0.885	k = −10→10
25585 measured reflections	l = −26→25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.9706P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.002$
6951 reflections	$\Delta\rho_{max} = 1.04$ e Å^{-3}
403 parameters	$\Delta\rho_{min} = -0.63$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Nd1	0.931203 (12)	0.19066 (3)	0.964281 (11)	0.03943 (10)
O1	0.97063 (16)	0.0607 (4)	0.87482 (14)	0.0468 (7)
O2	0.93999 (16)	0.4207 (3)	1.03415 (14)	0.0474 (7)
O3	0.84628 (14)	−0.0359 (3)	0.91886 (14)	0.0439 (7)
O4	0.94655 (15)	−0.1382 (4)	0.97728 (15)	0.0497 (8)
O5	1.06695 (16)	−0.0827 (4)	0.92164 (14)	0.0495 (8)
O6	1.00778 (18)	0.6127 (4)	1.09087 (15)	0.0567 (9)
O7	1.11832 (18)	−0.0166 (4)	0.82194 (17)	0.0667 (10)
O8	0.98695 (18)	0.5275 (4)	1.20633 (15)	0.0617 (9)
O9	0.78466 (18)	−0.3261 (4)	0.89805 (19)	0.0627 (10)
N1	0.79683 (19)	0.2343 (5)	0.9669 (2)	0.0476 (9)
N2	0.8341 (2)	0.3069 (4)	0.85460 (18)	0.0482 (9)
C1	0.7784 (3)	0.1918 (6)	1.0198 (3)	0.0635 (14)
H1	0.8131	0.1688	1.0593	0.076*
C2	0.7093 (3)	0.1795 (8)	1.0198 (4)	0.0833 (19)
H2	0.6978	0.1502	1.0583	0.100*
C3	0.6583 (3)	0.2123 (9)	0.9604 (4)	0.093 (2)

H3	0.6118	0.2026	0.9588	0.111*
C4	0.6745 (3)	0.2577 (8)	0.9049 (3)	0.0744 (17)
C5	0.7462 (3)	0.2674 (6)	0.9088 (3)	0.0527 (12)
C6	0.6227 (4)	0.2962 (10)	0.8401 (4)	0.109 (3)
H6	0.5755	0.2863	0.8360	0.131*
C7	0.6420 (4)	0.3441 (10)	0.7881 (4)	0.104 (3)
H7	0.6080	0.3721	0.7488	0.125*
C8	0.7134 (3)	0.3546 (7)	0.7900 (3)	0.0707 (17)
C9	0.7662 (3)	0.3100 (5)	0.8510 (2)	0.0519 (12)
C10	0.7358 (4)	0.4037 (8)	0.7368 (3)	0.087 (2)
H10	0.7036	0.4389	0.6976	0.105*
C11	0.8038 (4)	0.4014 (7)	0.7409 (3)	0.0795 (18)
H11	0.8187	0.4337	0.7046	0.095*
C12	0.8526 (3)	0.3493 (6)	0.8011 (2)	0.0626 (14)
H12	0.8993	0.3447	0.8030	0.075*
C13	1.0286 (2)	0.0034 (5)	0.8772 (2)	0.0427 (10)
C14	1.0524 (3)	0.0512 (6)	0.8173 (2)	0.0549 (12)
H14A	1.0186	0.0165	0.7761	0.066*
H14B	1.0557	0.1649	0.8157	0.066*
C15	1.1459 (3)	0.0143 (7)	0.7703 (3)	0.0625 (14)
C16	1.2078 (3)	−0.0571 (8)	0.7766 (3)	0.0792 (17)
H16	1.2284	−0.1192	0.8139	0.095*
C17	1.2402 (4)	−0.0364 (9)	0.7267 (4)	0.094 (2)
H17	1.2829	−0.0841	0.7307	0.113*
C18	1.2100 (5)	0.0526 (9)	0.6724 (4)	0.103 (3)
H18	1.2320	0.0648	0.6390	0.124*
C19	1.1488 (5)	0.1241 (10)	0.6655 (4)	0.107 (3)
H19	1.1286	0.1852	0.6277	0.129*
C20	1.1150 (4)	0.1061 (8)	0.7159 (3)	0.0832 (19)
H20	1.0728	0.1556	0.7120	0.100*
C21	0.9694 (2)	0.4987 (5)	1.0865 (2)	0.0438 (10)
C22	0.9488 (3)	0.4453 (6)	1.1474 (2)	0.0554 (12)
H22A	0.8994	0.4632	1.1397	0.066*
H22B	0.9574	0.3333	1.1540	0.066*
C23	0.9745 (3)	0.4892 (6)	1.2653 (2)	0.0550 (12)
C24	0.9277 (3)	0.3802 (8)	1.2720 (3)	0.0724 (16)
H24	0.9013	0.3251	1.2345	0.087*
C25	0.9193 (4)	0.3515 (10)	1.3342 (3)	0.105 (3)
H25	0.8878	0.2752	1.3388	0.126*
C26	0.9568 (4)	0.4343 (10)	1.3899 (3)	0.103 (2)
H26	0.9496	0.4169	1.4315	0.123*
C27	1.0044 (4)	0.5414 (9)	1.3836 (3)	0.089 (2)
H27	1.0306	0.5959	1.4213	0.107*
C28	1.0143 (3)	0.5704 (7)	1.3218 (3)	0.0712 (15)
H28	1.0472	0.6436	1.3178	0.085*
C29	0.8838 (2)	−0.1507 (6)	0.9391 (2)	0.0445 (11)
C30	0.8574 (3)	−0.3145 (5)	0.9194 (3)	0.0557 (12)
H30A	0.8753	−0.3508	0.8835	0.067*
H30B	0.8754	−0.3839	0.9576	0.067*

C31	0.7525 (6)	−0.3138 (9)	0.9448 (6)	0.1243 (14)
C32	0.7840 (5)	−0.2778 (9)	1.0118 (6)	0.1243 (14)
H32	0.8316	−0.2608	1.0285	0.149*
C33	0.7406 (5)	−0.2683 (9)	1.0529 (6)	0.1243 (14)
H33	0.7595	−0.2444	1.0983	0.149*
C34	0.6740 (5)	−0.2923 (9)	1.0290 (6)	0.1243 (14)
H34	0.6474	−0.2803	1.0585	0.149*
C35	0.6393 (5)	−0.3341 (9)	0.9635 (5)	0.1243 (14)
H35	0.5920	−0.3572	0.9496	0.149*
C36	0.6802 (5)	−0.3391 (9)	0.9200 (5)	0.1243 (14)
H36	0.6598	−0.3592	0.8745	0.149*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.04609 (15)	0.03354 (15)	0.03390 (14)	−0.00157 (11)	0.00426 (9)	0.00058 (10)
O1	0.0562 (19)	0.0452 (19)	0.0387 (16)	0.0066 (16)	0.0134 (14)	0.0014 (14)
O2	0.068 (2)	0.0318 (16)	0.0408 (17)	−0.0052 (15)	0.0138 (14)	−0.0046 (13)
O3	0.0444 (16)	0.0331 (17)	0.0466 (17)	0.0008 (14)	0.0015 (13)	−0.0033 (13)
O4	0.0462 (18)	0.0494 (19)	0.0449 (18)	−0.0033 (15)	0.0000 (14)	0.0073 (14)
O5	0.0603 (19)	0.0485 (19)	0.0409 (17)	0.0073 (16)	0.0166 (14)	0.0100 (15)
O6	0.084 (2)	0.048 (2)	0.0386 (17)	−0.0261 (19)	0.0183 (16)	−0.0031 (15)
O7	0.068 (2)	0.083 (3)	0.057 (2)	0.017 (2)	0.0291 (18)	0.0200 (19)
O8	0.087 (2)	0.060 (2)	0.0387 (18)	−0.0270 (19)	0.0193 (17)	−0.0062 (15)
O9	0.058 (2)	0.045 (2)	0.072 (2)	−0.0135 (16)	−0.0015 (18)	−0.0068 (17)
N1	0.047 (2)	0.040 (2)	0.048 (2)	0.0041 (17)	0.0034 (18)	−0.0080 (17)
N2	0.061 (2)	0.036 (2)	0.038 (2)	0.0031 (18)	−0.0008 (17)	0.0002 (16)
C1	0.057 (3)	0.073 (4)	0.059 (3)	0.008 (3)	0.015 (3)	−0.002 (3)
C2	0.057 (3)	0.112 (6)	0.086 (5)	0.003 (3)	0.029 (3)	−0.013 (4)
C3	0.048 (3)	0.105 (6)	0.121 (6)	−0.004 (3)	0.020 (4)	−0.017 (5)
C4	0.052 (3)	0.084 (4)	0.073 (4)	0.006 (3)	−0.003 (3)	−0.018 (3)
C5	0.051 (3)	0.036 (3)	0.062 (3)	0.007 (2)	0.001 (2)	−0.011 (2)
C6	0.061 (4)	0.139 (8)	0.102 (6)	0.016 (4)	−0.018 (4)	−0.030 (6)
C7	0.079 (5)	0.109 (6)	0.087 (5)	0.038 (4)	−0.034 (4)	−0.022 (5)
C8	0.074 (4)	0.061 (3)	0.053 (3)	0.018 (3)	−0.018 (3)	−0.011 (3)
C9	0.059 (3)	0.034 (3)	0.046 (3)	0.006 (2)	−0.011 (2)	−0.004 (2)
C10	0.119 (6)	0.068 (4)	0.046 (3)	0.018 (4)	−0.021 (3)	0.001 (3)
C11	0.117 (5)	0.071 (4)	0.038 (3)	−0.002 (4)	0.003 (3)	0.011 (3)
C12	0.080 (4)	0.051 (3)	0.047 (3)	−0.002 (3)	0.005 (3)	0.008 (2)
C13	0.056 (3)	0.033 (2)	0.037 (2)	−0.007 (2)	0.011 (2)	−0.0030 (19)
C14	0.064 (3)	0.056 (3)	0.047 (3)	0.005 (3)	0.019 (2)	0.011 (2)
C15	0.070 (3)	0.067 (4)	0.059 (3)	−0.008 (3)	0.033 (3)	0.001 (3)
C16	0.079 (4)	0.096 (5)	0.073 (4)	0.002 (4)	0.037 (3)	−0.002 (4)
C17	0.092 (5)	0.097 (6)	0.113 (6)	−0.006 (4)	0.062 (4)	−0.008 (5)
C18	0.138 (7)	0.083 (5)	0.126 (7)	−0.017 (5)	0.096 (6)	−0.005 (5)
C19	0.156 (7)	0.101 (5)	0.091 (5)	0.010 (6)	0.077 (5)	0.027 (4)
C20	0.100 (5)	0.089 (5)	0.078 (4)	0.007 (4)	0.053 (4)	0.023 (4)
C21	0.058 (3)	0.034 (2)	0.038 (2)	−0.001 (2)	0.013 (2)	0.0013 (19)

C22	0.074 (3)	0.051 (3)	0.043 (3)	−0.018 (3)	0.019 (2)	−0.004 (2)
C23	0.073 (3)	0.054 (3)	0.037 (3)	−0.002 (3)	0.015 (2)	0.003 (2)
C24	0.078 (4)	0.088 (4)	0.053 (3)	−0.033 (3)	0.022 (3)	−0.004 (3)
C25	0.127 (6)	0.134 (7)	0.067 (4)	−0.056 (5)	0.048 (4)	−0.003 (4)
C26	0.126 (6)	0.140 (7)	0.051 (4)	−0.026 (5)	0.040 (4)	0.009 (4)
C27	0.117 (5)	0.104 (5)	0.041 (3)	−0.021 (4)	0.013 (3)	−0.010 (3)
C28	0.086 (4)	0.073 (4)	0.051 (3)	−0.020 (3)	0.016 (3)	−0.011 (3)
C29	0.048 (3)	0.049 (3)	0.032 (2)	−0.006 (2)	0.0055 (19)	−0.0039 (19)
C30	0.061 (3)	0.043 (3)	0.056 (3)	0.002 (2)	0.008 (2)	−0.007 (2)
C31	0.136 (3)	0.086 (2)	0.173 (4)	0.014 (2)	0.080 (3)	0.027 (3)
C32	0.136 (3)	0.086 (2)	0.173 (4)	0.014 (2)	0.080 (3)	0.027 (3)
C33	0.136 (3)	0.086 (2)	0.173 (4)	0.014 (2)	0.080 (3)	0.027 (3)
C34	0.136 (3)	0.086 (2)	0.173 (4)	0.014 (2)	0.080 (3)	0.027 (3)
C35	0.136 (3)	0.086 (2)	0.173 (4)	0.014 (2)	0.080 (3)	0.027 (3)
C36	0.136 (3)	0.086 (2)	0.173 (4)	0.014 (2)	0.080 (3)	0.027 (3)

Geometric parameters (Å, °)

Nd1—O1	2.484 (3)	C11—C12	1.416 (7)
Nd1—O2	2.412 (3)	C11—H11	0.9300
Nd1—O3	2.564 (3)	C12—H12	0.9300
Nd1—O4	2.818 (4)	C13—C14	1.515 (6)
Nd1—N1	2.743 (4)	C14—H14A	0.9700
Nd1—N2	2.718 (4)	C14—H14B	0.9700
Nd1—O4^{i}	2.443 (3)	C15—C16	1.358 (8)
Nd1—O5^{i}	2.533 (3)	C15—C20	1.366 (8)
Nd1—O6^{ii}	2.537 (3)	C16—C17	1.387 (8)
O1—C13	1.251 (5)	C16—H16	0.9300
O2—C21	1.264 (5)	C17—C18	1.347 (10)
O3—C29	1.231 (5)	C17—H17	0.9300
O4—C29	1.282 (5)	C18—C19	1.343 (10)
O4—Nd1^{i}	2.443 (3)	C18—H18	0.9300
O5—C13	1.252 (5)	C19—C20	1.413 (8)
O5—Nd1^{i}	2.533 (3)	C19—H19	0.9300
O6—C21	1.225 (5)	C20—H20	0.9300
O6—Nd1^{ii}	2.537 (3)	C21—C22	1.513 (6)
O7—C15	1.369 (6)	C22—H22A	0.9700
O7—C14	1.422 (6)	C22—H22B	0.9700
O8—C23	1.361 (5)	C23—C24	1.357 (7)
O8—C22	1.424 (5)	C23—C28	1.395 (7)
O9—C31	1.318 (10)	C24—C25	1.375 (8)
O9—C30	1.401 (6)	C24—H24	0.9300
N1—C1	1.310 (6)	C25—C26	1.376 (9)
N1—C5	1.362 (6)	C25—H25	0.9300
N2—C12	1.322 (6)	C26—C27	1.354 (9)
N2—C9	1.345 (6)	C26—H26	0.9300
C1—C2	1.394 (8)	C27—C28	1.379 (8)
C1—H1	0.9300	C27—H27	0.9300

C2—C3	1.383 (10)	C28—H28	0.9300
C2—H2	0.9300	C29—C30	1.505 (6)
C3—C4	1.344 (9)	C30—H30A	0.9700
C3—H3	0.9300	C30—H30B	0.9700
C4—C5	1.422 (8)	C31—C32	1.386 (14)
C4—C6	1.479 (9)	C31—C36	1.410 (13)
C5—C9	1.421 (7)	C32—C33	1.390 (11)
C6—C7	1.316 (11)	C32—H32	0.9300
C6—H6	0.9300	C33—C34	1.300 (12)
C7—C8	1.427 (10)	C33—H33	0.9300
C7—H7	0.9300	C34—C35	1.383 (13)
C8—C10	1.375 (9)	C34—H34	0.9300
C8—C9	1.446 (6)	C35—C36	1.388 (11)
C10—C11	1.346 (9)	C35—H35	0.9300
C10—H10	0.9300	C36—H36	0.9300
O1—Nd1—O2	145.95 (10)	C12—C11—H11	120.4
O1—Nd1—O3	73.37 (10)	N2—C12—C11	122.5 (6)
O1—Nd1—O4	65.19 (9)	N2—C12—H12	118.8
O2—Nd1—O3	139.00 (10)	C11—C12—H12	118.8
O2—Nd1—O4	139.50 (9)	O1—C13—O5	128.5 (4)
O3—Nd1—O4	48.10 (9)	O1—C13—C14	112.2 (4)
O1—Nd1—N1	127.33 (11)	O5—C13—C14	119.3 (4)
O2—Nd1—N1	77.16 (11)	O7—C14—C13	110.3 (4)
O3—Nd1—N1	63.59 (11)	O7—C14—H14A	109.6
O4—Nd1—N1	102.31 (10)	C13—C14—H14A	109.6
O1—Nd1—N2	80.90 (11)	O7—C14—H14B	109.6
O2—Nd1—N2	96.80 (10)	C13—C14—H14B	109.6
O3—Nd1—N2	74.13 (10)	H14A—C14—H14B	108.1
O4—Nd1—N2	118.24 (10)	C16—C15—C20	121.1 (5)
N1—Nd1—N2	59.81 (12)	C16—C15—O7	114.2 (5)
O2—Nd1—O4^{i}	87.86 (11)	C20—C15—O7	124.7 (5)
O4^{i}—Nd1—O1	78.25 (10)	C15—C16—C17	119.3 (6)
O2—Nd1—O5^{i}	75.61 (10)	C15—C16—H16	120.3
O4^{i}—Nd1—O5^{i}	74.40 (10)	C17—C16—H16	120.3
O1—Nd1—O5^{i}	128.26 (10)	C18—C17—C16	120.2 (7)
O2—Nd1—O6^{ii}	77.15 (10)	C18—C17—H17	119.9
O4^{i}—Nd1—O6^{ii}	78.23 (11)	C16—C17—H17	119.9
O1—Nd1—O6^{ii}	69.68 (10)	C19—C18—C17	121.1 (7)
O5^{i}—Nd1—O6^{ii}	141.73 (10)	C19—C18—H18	119.4
O4^{i}—Nd1—O3	120.72 (11)	C17—C18—H18	119.4
O5^{i}—Nd1—O3	84.18 (10)	C18—C19—C20	119.8 (7)
O6^{ii}—Nd1—O3	133.35 (10)	C18—C19—H19	120.1
O4^{i}—Nd1—N2	148.77 (11)	C20—C19—H19	120.1
O5^{i}—Nd1—N2	136.69 (11)	C15—C20—C19	118.4 (6)
O6^{ii}—Nd1—N2	72.83 (12)	C15—C20—H20	120.8

O4^{i}—Nd1—N1	150.26 (11)	C19—C20—H20	120.8
O5^{i}—Nd1—N1	77.04 (11)	O6—C21—O2	127.2 (4)
O6^{ii}—Nd1—N1	121.92 (12)	O6—C21—C22	119.7 (4)
O4^{i}—Nd1—O4	72.85 (11)	O2—C21—C22	112.9 (4)
O5^{i}—Nd1—O4	65.13 (10)	O8—C22—C21	111.2 (4)
O6^{ii}—Nd1—O4	130.06 (10)	O8—C22—H22A	109.4
C13—O1—Nd1	129.9 (3)	C21—C22—H22A	109.4
C21—O2—Nd1	151.3 (3)	O8—C22—H22B	109.4
C29—O3—Nd1	101.2 (3)	C21—C22—H22B	109.4
C29—O4—Nd1^{i}	163.0 (3)	H22A—C22—H22B	108.0
C29—O4—Nd1	87.8 (3)	C24—C23—O8	124.8 (4)
Nd1^{i}—O4—Nd1	107.15 (11)	C24—C23—C28	119.8 (5)
C13—O5—Nd1^{i}	137.8 (3)	O8—C23—C28	115.4 (5)
C21—O6—Nd1^{ii}	149.9 (3)	C23—C24—C25	119.8 (6)
C15—O7—C14	116.8 (4)	C23—C24—H24	120.1
C23—O8—C22	117.6 (4)	C25—C24—H24	120.1
C31—O9—C30	116.8 (6)	C24—C25—C26	120.9 (6)
C1—N1—C5	118.7 (4)	C24—C25—H25	119.6
C1—N1—Nd1	120.1 (3)	C26—C25—H25	119.6
C5—N1—Nd1	119.7 (3)	C27—C26—C25	119.5 (6)
C12—N2—C9	118.5 (4)	C27—C26—H26	120.3
C12—N2—Nd1	119.7 (3)	C25—C26—H26	120.3
C9—N2—Nd1	121.5 (3)	C26—C27—C28	120.6 (6)
N1—C1—C2	123.2 (5)	C26—C27—H27	119.7
N1—C1—H1	118.4	C28—C27—H27	119.7
C2—C1—H1	118.4	C27—C28—C23	119.5 (6)
C3—C2—C1	117.6 (6)	C27—C28—H28	120.2
C3—C2—H2	121.2	C23—C28—H28	120.2
C1—C2—H2	121.2	O3—C29—O4	122.7 (4)
C4—C3—C2	121.5 (6)	O3—C29—C30	120.6 (4)
C4—C3—H3	119.2	O4—C29—C30	116.8 (4)
C2—C3—H3	119.2	O9—C30—C29	113.9 (4)
C3—C4—C5	117.6 (6)	O9—C30—H30A	108.8
C3—C4—C6	124.2 (7)	C29—C30—H30A	108.8
C5—C4—C6	118.1 (7)	O9—C30—H30B	108.8
N1—C5—C9	118.7 (4)	C29—C30—H30B	108.8
N1—C5—C4	121.4 (5)	H30A—C30—H30B	107.7
C9—C5—C4	120.0 (5)	O9—C31—C32	125.5 (10)
C7—C6—C4	121.2 (7)	O9—C31—C36	113.3 (10)
C7—C6—H6	119.4	C32—C31—C36	121.2 (10)
C4—C6—H6	119.4	C31—C32—C33	116.6 (10)
C6—C7—C8	122.2 (6)	C31—C32—H32	121.7
C6—C7—H7	118.9	C33—C32—H32	121.7
C8—C7—H7	118.9	C34—C33—C32	121.0 (11)
C10—C8—C7	124.0 (6)	C34—C33—H33	119.5
C10—C8—C9	117.1 (6)	C32—C33—H33	119.5
C7—C8—C9	118.8 (6)	C33—C34—C35	125.7 (10)

N2—C9—C5	118.8 (4)	C33—C34—H34	117.1
N2—C9—C8	121.8 (5)	C35—C34—H34	117.1
C5—C9—C8	119.4 (5)	C34—C35—C36	115.1 (10)
C11—C10—C8	120.7 (5)	C34—C35—H35	122.4
C11—C10—H10	119.6	C36—C35—H35	122.4
C8—C10—H10	119.6	C35—C36—C31	120.1 (11)
C10—C11—C12	119.2 (6)	C35—C36—H36	119.9
C10—C11—H11	120.4	C31—C36—H36	119.9

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*
C30—H30B···O2^{iii}	0.97	2.40	3.347 (6)	164
C12—H12···O8^{ii}	0.93	2.59	3.438 (7)	152
C12—H12···O6^{ii}	0.93	2.47	3.057 (6)	122
C10—H10···O3^{iv}	0.93	2.34	3.215 (6)	156
C1—H1···O5^{i}	0.93	2.44	3.130 (6)	132

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

Fig. 1

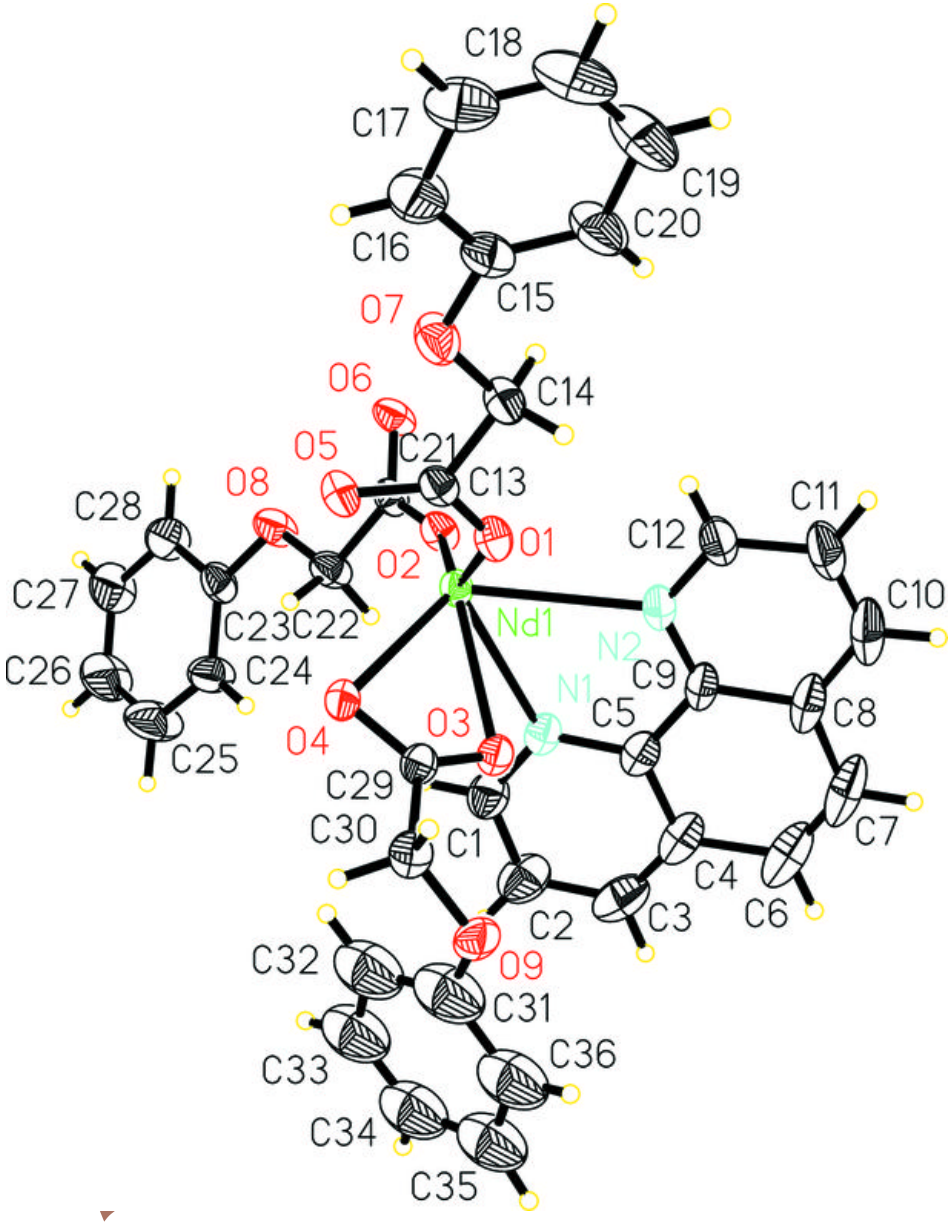
C18
C17
C19
C20
C16
C15
O7
O6
C14
O5
C21
O8
C13
C28
C11
C12
O1
O2
C27
C10
Nd1
N2
C23
C22
C26
C24
C9
N1
C5
C8
O4
O3
C25
C29
C30
C1
C7
C4
C6
C3
C2
C32
O9
C31
C36
C33
C34
C35

Fig. 2