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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(3-phenylpropanoato-κO)neodymium(III)

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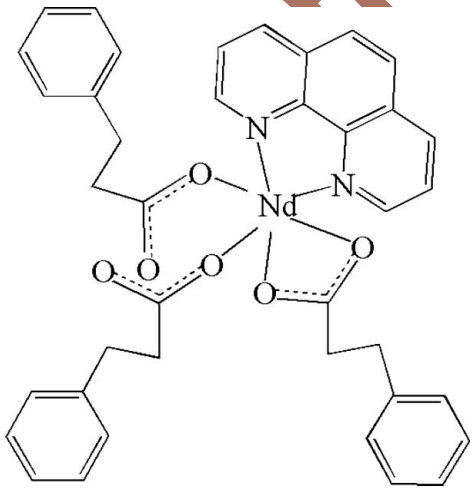
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.015 Å; R factor = 0.043; wR factor = 0.188; data-to-parameter ratio = 18.2.

The Nd^{III} atom in the title complex, $[Nd(C_9H_9O_2)_3(C_{12}H_8N_2)]$, is coordinated by two N atoms of the 1,10-phenanthroline (phen) ligand and four O atoms of the three 3-phenylpropanoate ligands. This mononuclear complex is further extended into a supramolecular network structure *via* nonclassical hydrogen bonds between CH groups of 1,10-phenanthroline or 3-phenylpropanoate and O atoms of neighbouring 3-phenylpropanoate molecules.

Related literature

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



Experimental

Crystal data

$[Nd(C_9H_9O_2)_3(C_{12}H_8N_2)]$
M_r = 771.93
Monoclinic, $P2_1/n$
a = 19.9971 (13) Å
b = 8.7352 (14) Å
c = 20.9978 (12) Å
β = 106.903 (8)°
V = 3509.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 273 (2) K
0.33 × 0.12 × 0.08 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.632, T_{max} = 0.886
25068 measured reflections
6782 independent reflections
4739 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.188
S = 1.02
6782 reflections
373 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.39 e Å^{-3}
$\Delta\rho_{min}$ = −1.12 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O1	2.606 (4)	Nd1—O5	2.465 (5)
Nd1—O2	2.898 (6)	Nd1—O6^{ii}	2.576 (5)
Nd1—O2^{i}	2.429 (5)	Nd1—N1	2.729 (6)
Nd1—O3	2.511 (5)	Nd1—N2	2.731 (6)
Nd1—O4^{i}	2.563 (4)		
O1—Nd1—O2	47.14 (14)	O3—Nd1—N1	127.13 (17)
O1—Nd1—O3	72.53 (15)	O5—Nd1—N1	77.14 (17)
O1—Nd1—O5	139.94 (16)	O1—Nd1—N2	75.58 (16)
O2—Nd1—O3	64.78 (15)	O2—Nd1—N2	118.64 (15)
O2—Nd1—O5	140.06 (14)	O3—Nd1—N2	80.61 (17)
O3—Nd1—O5	145.90 (16)	O5—Nd1—N2	96.29 (16)
O1—Nd1—N1	64.66 (17)	N1—Nd1—N2	60.29 (19)
O2—Nd1—N1	102.65 (17)		

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···O4^{i}	0.93	2.44	3.132 (10)	132
C12—H12···O6^{ii}	0.93	2.50	3.066 (10)	119
C32—H32B···O5^{iii}	0.97	2.46	3.411 (9)	165
C10—H10···O1^{iv}	0.93	2.38	3.259 (10)	158

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

Data collection: *APEX2* (Bruker, 2005); 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: AT2346).

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supplementary materials

Acta Cryst. (2007). E**63**, m2209-m2210 [**doi:10.1107/S1600536807035350**]

(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)

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

Comment

The crystal structure of (1,10-phenanthroline-*N*,*N*')tri(benzenepropanoic acid)lanthanum(III), (II), has previously 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 the two N atoms of 1,10-phenanthroline ligand and four O atoms of three 3-phenylpropanoate ligands (Table 1). The Nd—O bond lengths are in the range 2.429 (5) to 2.898 (6) Å. The Nd—N bond lengths are in the range 2.729 (6) to 2.731 (6) Å. C—H···O non-classical hydrogen bonds between C—H groups of 1,10-phenanthroline or 3-phenylpropanoate and O atoms of neighbouring 3-phenylpropanoate molecules, with an average C···O distances of 3.217 (10) Å, generate a layered hydrogen-bonded network (Fig. 2 and Table 2). The non-classical hydrogen-bonding interactions link the mononuclear complex into a supramolecular network structure, as in (II). The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound (I) were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Neodymium (III) nitrate hexahydrate (219.1 mg, 0.5 mmol), phen (99 mg, 0.5 mmol), 3-phenylpropanoate (150.2 mg, 1 mmol) and distilled water (4 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 colourless solution was decanted from small colourless 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 − 0.97 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

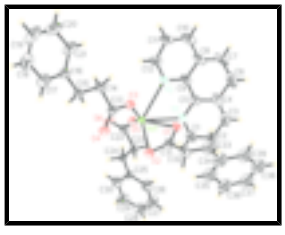

Fig. 1. View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

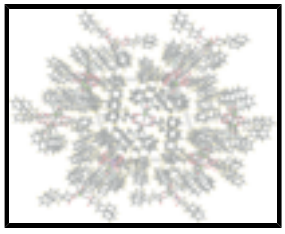

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

(1,10-Phenanthroline-κ^2*N*,*N*')tris(3-phenylpropanoato- κ*O*)neodymium(III)

Crystal data

$[Nd(C_9H_9O_2)_3(C_{12}H_8N_2)]$	F_{000} = 1564
M_r = 771.93	D_x = 1.461 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8997 reflections
a = 19.9971 (13) Å	θ = 2.5–26.5º
b = 8.7352 (14) Å	μ = 1.53 mm^{-1}
c = 20.9978 (12) Å	T = 273 (2) K
β = 106.903 (8)º	Plane, colourless
V = 3509.4 (6) Å^3	0.33 × 0.12 × 0.08 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	6782 independent reflections
Radiation source: fine-focus sealed tube	4739 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 273(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −24→24
T_{min} = 0.632, T_{max} = 0.886	k = −10→10
25068 measured reflections	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
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.188	$w = 1/[\sigma^2(F_o^2) + (0.1501P)^2 + 0.285P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.002
6782 reflections	$\Delta\rho_{max}$ = 1.39 e Å^{-3}

373 parameters
4 restraints
Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -1.12$ 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}
Nd1	0.931203 (18)	0.19073 (4)	0.964289 (16)	0.04101 (18)
O1	0.8463 (2)	−0.0366 (5)	0.9193 (2)	0.0471 (11)
O2	0.9471 (3)	−0.1386 (7)	0.9774 (2)	0.0533 (12)
O3	0.9709 (2)	0.0612 (6)	0.8749 (2)	0.0500 (11)
O4	1.0666 (3)	−0.0829 (6)	0.9216 (2)	0.0542 (12)
O5	0.9402 (2)	0.4211 (5)	1.0341 (2)	0.0504 (11)
O6	1.0077 (3)	0.6123 (6)	1.0912 (2)	0.0600 (14)
N1	0.7968 (3)	0.2347 (8)	0.9665 (3)	0.0513 (14)
N2	0.8347 (3)	0.3068 (6)	0.8547 (3)	0.0500 (15)
C1	0.7782 (5)	0.1907 (9)	1.0201 (5)	0.068 (2)
H1	0.8131	0.1682	1.0591	0.081*
C2	0.7094 (5)	0.1773 (12)	1.0197 (6)	0.090 (3)
H2	0.6979	0.1455	1.0574	0.108*
C3	0.6574 (5)	0.2131 (13)	0.9607 (7)	0.094 (4)
H3	0.6107	0.2056	0.9595	0.113*
C4	0.6742 (5)	0.2587 (14)	0.9054 (5)	0.083 (3)
C5	0.7466 (4)	0.2672 (9)	0.9098 (4)	0.0562 (19)
C6	0.6188 (6)	0.2947 (17)	0.8414 (8)	0.127 (6)
H6	0.5716	0.2846	0.8378	0.152*
C7	0.6419 (6)	0.3455 (15)	0.7860 (6)	0.103 (4)
H7	0.6091	0.3736	0.7464	0.124*
C8	0.7127 (5)	0.3530 (12)	0.7910 (4)	0.075 (3)
C9	0.7667 (4)	0.3100 (8)	0.8500 (4)	0.055 (2)
C10	0.7369 (7)	0.4016 (12)	0.7367 (5)	0.093 (3)
H10	0.7049	0.4326	0.6972	0.111*
C11	0.8055 (6)	0.4031 (12)	0.7421 (4)	0.084 (3)
H11	0.8215	0.4398	0.7075	0.101*
C12	0.8525 (5)	0.3482 (9)	0.8007 (4)	0.066 (2)
H12	0.8992	0.3401	0.8021	0.079*

C13	1.0280 (4)	0.0023 (8)	0.8771 (3)	0.0452 (15)
C14	1.0519 (4)	0.0502 (9)	0.8171 (3)	0.0515 (10)
H14A	1.0175	0.0179	0.7764	0.062*
H14B	1.0558	0.1608	0.8162	0.062*
C15	1.1170 (4)	−0.0168 (9)	0.8210 (3)	0.0515 (10)
H15A	1.1502	0.0165	0.8622	0.062*
H15B	1.1121	−0.1269	0.8239	0.062*
C16	1.1456 (4)	0.0136 (9)	0.7692 (3)	0.0515 (10)
C17	1.2069 (5)	−0.0570 (13)	0.7758 (5)	0.086 (3)
H17	1.2269	−0.1185	0.8125	0.103*
C18	1.2403 (6)	−0.0364 (15)	0.7261 (7)	0.099 (3)
H18	1.2830	−0.0833	0.7300	0.119*
C19	1.2092 (7)	0.0548 (14)	0.6709 (7)	0.115 (5)
H19	1.2313	0.0670	0.6379	0.139*
C20	1.1489 (8)	0.1242 (16)	0.6647 (6)	0.114 (4)
H20	1.1287	0.1832	0.6271	0.137*
C21	1.1142 (6)	0.1086 (13)	0.7161 (5)	0.089 (3)
H21	1.0728	0.1600	0.7136	0.107*
C22	0.9694 (4)	0.4984 (8)	1.0862 (3)	0.0468 (16)
C23	0.9485 (4)	0.4455 (8)	1.1469 (3)	0.0481 (9)
H23B	0.8987	0.4610	1.1389	0.058*
H23A	0.9579	0.3368	1.1536	0.058*
C24	0.9859 (4)	0.5271 (8)	1.2062 (3)	0.0481 (9)
H24A	1.0354	0.5150	1.2116	0.058*
H24B	0.9752	0.6351	1.1984	0.058*
C25	0.9743 (4)	0.4887 (8)	1.2652 (3)	0.0481 (9)
C26	0.9278 (5)	0.3793 (13)	1.2715 (4)	0.076 (3)
H26	0.9024	0.3238	1.2346	0.091*
C27	0.9187 (8)	0.3518 (18)	1.3335 (6)	0.119 (5)
H27	0.8874	0.2767	1.3378	0.143*
C28	0.9560 (6)	0.4354 (16)	1.3898 (5)	0.103 (4)
H28	0.9476	0.4197	1.4306	0.124*
C29	1.0051 (6)	0.5407 (13)	1.3840 (4)	0.094 (3)
H29	1.0317	0.5926	1.4215	0.113*
C30	1.0153 (5)	0.5704 (11)	1.3217 (4)	0.076 (2)
H30	1.0481	0.6420	1.3175	0.091*
C31	0.8831 (4)	−0.1523 (9)	0.9389 (3)	0.0471 (16)
C32	0.8573 (4)	−0.3127 (8)	0.9194 (4)	0.057 (2)
H32A	0.8755	−0.3463	0.8836	0.069*
H32B	0.8766	−0.3798	0.9571	0.069*
C33	0.7864 (7)	−0.3302 (12)	0.8992 (7)	0.1029 (15)
H33A	0.7670	−0.2563	0.8643	0.123*
H33B	0.7759	−0.4313	0.8798	0.123*
C34	0.7536 (7)	−0.3141 (9)	0.9460 (8)	0.1029 (15)
C35	0.7827 (7)	−0.2751 (13)	1.0104 (7)	0.1029 (15)
H35	0.8303	−0.2549	1.0265	0.123*
C36	0.7376 (6)	−0.2651 (14)	1.0551 (7)	0.1029 (15)
H36	0.7549	−0.2397	1.0999	0.123*
C37	0.6714 (7)	−0.2947 (12)	1.0267 (7)	0.1029 (15)

H37	0.6425	−0.2882	1.0541	0.123*
C38	0.6392 (7)	−0.3341 (12)	0.9616 (7)	0.1029 (15)
H38	0.5918	−0.3573	0.9464	0.123*
C39	0.6804 (7)	−0.3368 (12)	0.9214 (7)	0.1029 (15)
H39	0.6605	−0.3541	0.8761	0.123*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.0460 (3)	0.0368 (3)	0.0352 (2)	−0.00139 (14)	0.00398 (16)	0.00061 (13)
O1	0.043 (2)	0.039 (3)	0.051 (3)	−0.002 (2)	0.000 (2)	−0.003 (2)
O2	0.052 (3)	0.053 (3)	0.046 (3)	−0.002 (2)	0.001 (2)	0.007 (2)
O3	0.057 (3)	0.050 (3)	0.044 (3)	0.003 (2)	0.016 (2)	0.002 (2)
O4	0.062 (3)	0.057 (3)	0.045 (3)	0.007 (3)	0.018 (2)	0.013 (2)
O5	0.066 (3)	0.039 (3)	0.044 (3)	−0.002 (2)	0.013 (2)	−0.006 (2)
O6	0.083 (4)	0.058 (3)	0.040 (3)	−0.028 (3)	0.019 (2)	−0.001 (2)
N1	0.048 (3)	0.049 (4)	0.050 (4)	0.005 (3)	0.004 (3)	−0.006 (3)
N2	0.060 (4)	0.047 (4)	0.034 (3)	0.005 (3)	0.001 (3)	0.001 (2)
C1	0.058 (5)	0.085 (7)	0.060 (5)	0.011 (4)	0.016 (4)	−0.004 (4)
C2	0.055 (5)	0.131 (10)	0.087 (7)	−0.004 (5)	0.026 (5)	−0.015 (6)
C3	0.051 (5)	0.117 (10)	0.110 (10)	−0.009 (5)	0.018 (6)	−0.014 (7)
C4	0.054 (5)	0.094 (7)	0.083 (7)	0.005 (5)	−0.005 (5)	−0.022 (6)
C5	0.058 (4)	0.034 (4)	0.068 (5)	0.008 (3)	0.005 (4)	−0.007 (3)
C6	0.049 (6)	0.188 (17)	0.127 (12)	0.001 (7)	0.000 (7)	−0.022 (10)
C7	0.073 (7)	0.140 (10)	0.068 (7)	0.042 (6)	−0.023 (5)	0.005 (7)
C8	0.077 (6)	0.074 (6)	0.051 (5)	0.019 (5)	−0.017 (4)	−0.009 (4)
C9	0.063 (5)	0.041 (4)	0.046 (4)	0.002 (3)	−0.008 (4)	−0.007 (3)
C10	0.122 (9)	0.077 (7)	0.053 (6)	0.013 (6)	−0.017 (5)	−0.006 (5)
C11	0.116 (8)	0.085 (7)	0.037 (4)	0.001 (6)	0.001 (5)	0.012 (4)
C12	0.083 (6)	0.052 (5)	0.054 (5)	−0.003 (4)	0.007 (4)	0.009 (4)
C13	0.052 (4)	0.040 (4)	0.042 (4)	−0.008 (3)	0.010 (3)	−0.001 (3)
C14	0.055 (2)	0.057 (3)	0.046 (2)	0.006 (2)	0.0212 (19)	0.0120 (19)
C15	0.055 (2)	0.057 (3)	0.046 (2)	0.006 (2)	0.0212 (19)	0.0120 (19)
C16	0.055 (2)	0.057 (3)	0.046 (2)	0.006 (2)	0.0212 (19)	0.0120 (19)
C17	0.085 (6)	0.111 (8)	0.073 (6)	0.006 (6)	0.042 (5)	−0.003 (6)
C18	0.086 (7)	0.114 (10)	0.111 (9)	−0.011 (7)	0.051 (7)	−0.011 (7)
C19	0.147 (11)	0.089 (8)	0.157 (12)	−0.016 (8)	0.118 (10)	−0.005 (8)
C20	0.163 (12)	0.110 (9)	0.098 (9)	0.018 (9)	0.083 (9)	0.036 (7)
C21	0.109 (8)	0.089 (7)	0.091 (7)	0.001 (6)	0.064 (6)	0.018 (6)
C22	0.057 (4)	0.035 (4)	0.046 (4)	0.000 (3)	0.013 (3)	0.001 (3)
C23	0.066 (2)	0.046 (2)	0.0334 (19)	−0.0147 (19)	0.0161 (17)	−0.0033 (16)
C24	0.066 (2)	0.046 (2)	0.0334 (19)	−0.0147 (19)	0.0161 (17)	−0.0033 (16)
C25	0.066 (2)	0.046 (2)	0.0334 (19)	−0.0147 (19)	0.0161 (17)	−0.0033 (16)
C26	0.075 (6)	0.103 (7)	0.051 (5)	−0.034 (5)	0.019 (4)	−0.010 (5)
C27	0.144 (11)	0.157 (11)	0.073 (7)	−0.058 (10)	0.058 (8)	−0.003 (8)
C28	0.124 (9)	0.140 (11)	0.056 (6)	−0.017 (8)	0.041 (6)	0.008 (6)
C29	0.125 (9)	0.107 (8)	0.046 (5)	−0.012 (7)	0.017 (5)	−0.004 (5)
C30	0.084 (6)	0.083 (6)	0.056 (5)	−0.028 (5)	0.014 (4)	−0.012 (4)

C31	0.047 (4)	0.056 (4)	0.034 (3)	−0.001 (3)	0.005 (3)	−0.002 (3)
C32	0.053 (4)	0.059 (5)	0.053 (5)	0.006 (3)	0.004 (4)	−0.008 (3)
C33	0.103 (3)	0.083 (3)	0.130 (4)	0.001 (3)	0.044 (3)	0.018 (3)
C34	0.103 (3)	0.083 (3)	0.130 (4)	0.001 (3)	0.044 (3)	0.018 (3)
C35	0.103 (3)	0.083 (3)	0.130 (4)	0.001 (3)	0.044 (3)	0.018 (3)
C36	0.103 (3)	0.083 (3)	0.130 (4)	0.001 (3)	0.044 (3)	0.018 (3)
C37	0.103 (3)	0.083 (3)	0.130 (4)	0.001 (3)	0.044 (3)	0.018 (3)
C38	0.103 (3)	0.083 (3)	0.130 (4)	0.001 (3)	0.044 (3)	0.018 (3)
C39	0.103 (3)	0.083 (3)	0.130 (4)	0.001 (3)	0.044 (3)	0.018 (3)

Geometric parameters (Å, °)

Nd1—O1	2.606 (4)	C15—H15B	0.9700
Nd1—O2	2.898 (6)	C16—C17	1.344 (11)
Nd1—O2^{i}	2.429 (5)	C16—C21	1.385 (12)
Nd1—O3	2.511 (5)	C17—C18	1.403 (14)
Nd1—O4^{i}	2.563 (4)	C17—H17	0.9300
Nd1—O5	2.465 (5)	C18—C19	1.395 (17)
Nd1—O6^{ii}	2.576 (5)	C18—H18	0.9300
Nd1—N1	2.729 (6)	C19—C20	1.320 (16)
Nd1—N2	2.731 (6)	C19—H19	0.9300
O1—C31	1.248 (9)	C20—C21	1.450 (13)
O2—C31	1.305 (8)	C20—H20	0.9300
O2—Nd1^{i}	2.429 (5)	C21—H21	0.9300
O3—C13	1.241 (8)	C22—C23	1.525 (9)
O4—C13	1.266 (8)	C23—C24	1.440 (9)
O4—Nd1^{i}	2.563 (4)	C23—H23B	0.9700
O5—C22	1.273 (8)	C23—H23A	0.9700
O6—C22	1.241 (8)	C24—C25	1.366 (9)
O6—Nd1^{ii}	2.576 (5)	C24—H24A	0.9700
N1—C1	1.339 (11)	C24—H24B	0.9700
N1—C5	1.346 (9)	C25—C26	1.368 (11)
N2—C12	1.333 (10)	C25—C30	1.422 (10)
N2—C9	1.337 (10)	C26—C27	1.385 (13)
C1—C2	1.378 (12)	C26—H26	0.9300
C1—H1	0.9300	C27—C28	1.406 (16)
C2—C3	1.401 (16)	C27—H27	0.9300
C2—H2	0.9300	C28—C29	1.378 (15)
C3—C4	1.359 (16)	C28—H28	0.9300
C3—H3	0.9300	C29—C30	1.405 (12)
C4—C5	1.426 (12)	C29—H29	0.9300
C4—C6	1.505 (16)	C30—H30	0.9300
C5—C9	1.473 (12)	C31—C32	1.508 (10)
C6—C7	1.442 (18)	C32—C33	1.364 (14)
C6—H6	0.9300	C32—H32A	0.9700
C7—C8	1.390 (15)	C32—H32B	0.9700
C7—H7	0.9300	C33—C34	1.337 (17)
C8—C10	1.426 (15)	C33—H33A	0.9700

C8—C9	1.436 (11)	C33—H33B	0.9700
C10—C11	1.344 (14)	C34—C35	1.352 (19)
C10—H10	0.9300	C34—C39	1.418 (18)
C11—C12	1.398 (12)	C35—C36	1.482 (17)
C11—H11	0.9300	C35—H35	0.9300
C12—H12	0.9300	C36—C37	1.309 (17)
C13—C14	1.529 (9)	C36—H36	0.9300
C14—C15	1.408 (9)	C37—C38	1.374 (18)
C14—H14A	0.9700	C37—H37	0.9300
C14—H14B	0.9700	C38—C39	1.342 (16)
C15—C16	1.393 (9)	C38—H38	0.9300
C15—H15A	0.9700	C39—H39	0.9300
O1—Nd1—O2	47.14 (14)	C13—C14—H14B	109.6
O1—Nd1—O3	72.53 (15)	H14A—C14—H14B	108.2
O1—Nd1—O5	139.94 (16)	C16—C15—C14	117.3 (6)
O2—Nd1—O3	64.78 (15)	C16—C15—H15A	108.0
O2—Nd1—O5	140.06 (14)	C14—C15—H15A	108.0
O3—Nd1—O5	145.90 (16)	C16—C15—H15B	108.0
O1—Nd1—N1	64.66 (17)	C14—C15—H15B	108.0
O2—Nd1—N1	102.65 (17)	H15A—C15—H15B	107.2
O3—Nd1—N1	127.13 (17)	C17—C16—C21	122.9 (8)
O5—Nd1—N1	77.14 (17)	C17—C16—C15	113.7 (7)
O1—Nd1—N2	75.58 (16)	C21—C16—C15	123.4 (7)
O2—Nd1—N2	118.64 (15)	C16—C17—C18	118.8 (10)
O3—Nd1—N2	80.61 (17)	C16—C17—H17	120.6
O5—Nd1—N2	96.29 (16)	C18—C17—H17	120.6
N1—Nd1—N2	60.29 (19)	C19—C18—C17	119.8 (11)
$O2^{i}$—Nd1—O5	87.93 (18)	C19—C18—H18	120.1
$O2^{i}$—Nd1—O3	78.68 (16)	C17—C18—H18	120.1
$O2^{i}$—Nd1—$O4^{i}$	73.59 (16)	C20—C19—C18	121.3 (10)
O5—Nd1—$O4^{i}$	76.45 (16)	C20—C19—H19	119.4
O3—Nd1—$O4^{i}$	127.61 (16)	C18—C19—H19	119.4
$O2^{i}$—Nd1—$O6^{ii}$	79.37 (18)	C19—C20—C21	120.2 (12)
O5—Nd1—$O6^{ii}$	76.17 (16)	C19—C20—H20	119.9
O3—Nd1—$O6^{ii}$	70.63 (16)	C21—C20—H20	119.9
$O4^{i}$—Nd1—$O6^{ii}$	141.85 (16)	C16—C21—C20	117.0 (10)
$O2^{i}$—Nd1—O1	119.47 (18)	C16—C21—H21	121.5
$O4^{i}$—Nd1—O1	83.77 (16)	C20—C21—H21	121.5
$O6^{ii}$—Nd1—O1	133.62 (15)	O6—C22—O5	127.9 (6)
$O2^{i}$—Nd1—N1	149.95 (17)	O6—C22—C23	119.0 (6)
$O4^{i}$—Nd1—N1	77.58 (17)	O5—C22—C23	112.9 (6)
$O6^{ii}$—Nd1—N1	120.85 (19)	C24—C23—C22	111.9 (6)
$O2^{i}$—Nd1—N2	148.54 (18)	C24—C23—H23B	109.2
$O4^{i}$—Nd1—N2	137.72 (18)	C22—C23—H23B	109.2
$O6^{ii}$—Nd1—N2	71.52 (18)	C24—C23—H23A	109.2

O2^{i}—Nd1—O2	72.54 (19)	C22—C23—H23A	109.2
O4^{i}—Nd1—O2	64.85 (15)	H23B—C23—H23A	107.9
O6^{ii}—Nd1—O2	130.74 (16)	C25—C24—C23	118.7 (6)
C31—O1—Nd1	103.7 (4)	C25—C24—H24A	107.6
C31—O2—Nd1^{i}	162.4 (5)	C23—C24—H24A	107.6
C31—O2—Nd1	88.4 (4)	C25—C24—H24B	107.6
Nd1^{i}—O2—Nd1	107.46 (19)	C23—C24—H24B	107.6
C13—O3—Nd1	130.3 (4)	H24A—C24—H24B	107.1
C13—O4—Nd1^{i}	138.3 (4)	C24—C25—C26	124.0 (6)
C22—O5—Nd1	151.6 (5)	C24—C25—C30	115.2 (7)
C22—O6—Nd1^{ii}	149.2 (4)	C26—C25—C30	120.8 (7)
C1—N1—C5	119.1 (7)	C25—C26—C27	119.4 (9)
C1—N1—Nd1	119.3 (5)	C25—C26—H26	120.3
C5—N1—Nd1	120.0 (5)	C27—C26—H26	120.3
C12—N2—C9	116.7 (7)	C26—C27—C28	121.2 (10)
C12—N2—Nd1	121.4 (5)	C26—C27—H27	119.4
C9—N2—Nd1	121.7 (5)	C28—C27—H27	119.4
N1—C1—C2	122.6 (9)	C29—C28—C27	119.3 (9)
N1—C1—H1	118.7	C29—C28—H28	120.4
C2—C1—H1	118.7	C27—C28—H28	120.4
C1—C2—C3	118.0 (10)	C28—C29—C30	120.4 (9)
C1—C2—H2	121.0	C28—C29—H29	119.8
C3—C2—H2	121.0	C30—C29—H29	119.8
C4—C3—C2	121.1 (9)	C29—C30—C25	118.7 (8)
C4—C3—H3	119.5	C29—C30—H30	120.6
C2—C3—H3	119.5	C25—C30—H30	120.6
C3—C4—C5	117.3 (9)	O1—C31—O2	120.5 (7)
C3—C4—C6	121.6 (10)	O1—C31—C32	122.7 (6)
C5—C4—C6	121.1 (11)	O2—C31—C32	116.8 (7)
N1—C5—C4	121.9 (8)	C33—C32—C31	115.5 (7)
N1—C5—C9	119.3 (7)	C33—C32—H32A	108.4
C4—C5—C9	118.8 (8)	C31—C32—H32A	108.4
C7—C6—C4	117.4 (10)	C33—C32—H32B	108.4
C7—C6—H6	121.3	C31—C32—H32B	108.4
C4—C6—H6	121.3	H32A—C32—H32B	107.5
C8—C7—C6	120.8 (9)	C34—C33—C32	116.6 (13)
C8—C7—H7	119.6	C34—C33—H33A	108.1
C6—C7—H7	119.6	C32—C33—H33A	108.1
C7—C8—C10	121.9 (9)	C34—C33—H33B	108.1
C7—C8—C9	123.1 (10)	C32—C33—H33B	108.1
C10—C8—C9	115.0 (9)	H33A—C33—H33B	107.3
N2—C9—C8	124.2 (8)	C33—C34—C35	127.0 (14)
N2—C9—C5	117.1 (6)	C33—C34—C39	113.1 (15)
C8—C9—C5	118.6 (8)	C35—C34—C39	119.9 (13)
C11—C10—C8	120.8 (9)	C34—C35—C36	119.0 (13)
C11—C10—H10	119.6	C34—C35—H35	120.5
C8—C10—H10	119.6	C36—C35—H35	120.5

C10—C11—C12	118.5 (9)	C37—C36—C35	114.8 (14)
C10—C11—H11	120.7	C37—C36—H36	122.6
C12—C11—H11	120.7	C35—C36—H36	122.6
N2—C12—C11	124.5 (9)	C36—C37—C38	128.5 (14)
N2—C12—H12	117.8	C36—C37—H37	115.7
C11—C12—H12	117.8	C38—C37—H37	115.7
O3—C13—O4	128.9 (6)	C39—C38—C37	115.7 (13)
O3—C13—C14	111.1 (6)	C39—C38—H38	122.2
O4—C13—C14	120.0 (6)	C37—C38—H38	122.2
C15—C14—C13	110.1 (6)	C38—C39—C34	121.8 (15)
C15—C14—H14A	109.6	C38—C39—H39	119.1
C13—C14—H14A	109.6	C34—C39—H39	119.1
C15—C14—H14B	109.6		

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···O4^{i}	0.93	2.44	3.132 (10)	132
C12—H12···O6^{ii}	0.93	2.50	3.066 (10)	119
C32—H32B···O5^{iii}	0.97	2.46	3.411 (9)	165
C10—H10···O1^{iv}	0.93	2.38	3.259 (10)	158

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

Fig. 1

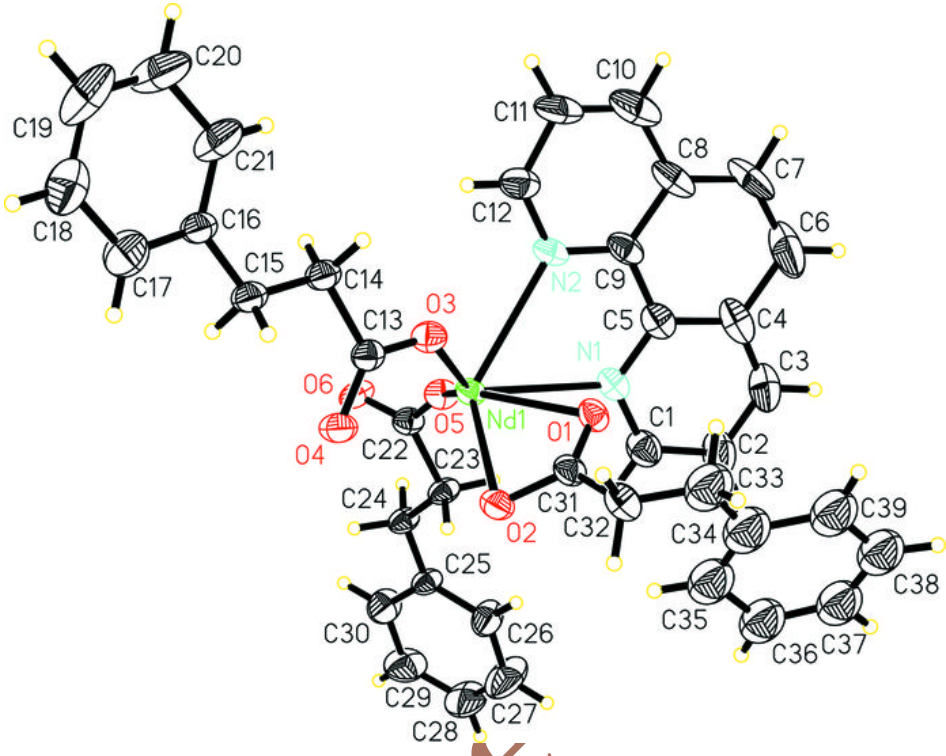

Fig. 2