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Crystal structures of [$Ln(NO_3)_3(\mu_2$-bpydo)$_2$], where Ln = Ce, Pr or Nd, and bpydo = 4,4′-bipyridine N,N'-dioxide: layered coordination networks containing 4^4 grids

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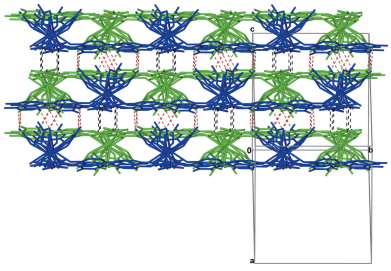
Three isostructural coordination networks of Ce, Pr, and Nd nitrate with 4,4′-bipyridine N,N'-dioxide (bpydo) are reported, namely poly[[tris(nitrato-κ^2O,O')cerium(III)]-bis(μ_2-4,4′-bipyridine N,N'-dioxide-$\kappa^2N:N'$)], [$Ce(NO_3)_3(C_{10}H_8N_2O_2)_2$], poly[[tris(nitrato-$\kappa^2O,O'$)praeseodymium(III)]-bis(μ_2-4,4′-bipyridine N,N'-dioxide-$\kappa^2N:N'$)], [$Pr(NO_3)_3(C_{10}H_8N_2O_2)_2$], and poly[[tris(nitrato-κ^2O,O')neodymium(III)]-bis(μ_2-4,4′-bipyridine N,N'-dioxide-$\kappa^2N:N'$], [$Nd(NO_3)_3(C_{10}H_8N_2O_2)_2$]. All three compounds are isostructural to the previously reported La analogue. The asymmetric unit of [$Ln(NO_3)_3(\mu_2$-bpydo)$_2$] contains one lanthanide cation, two bpydo ligands, and three nitrate anions. Both bpydo ligands act as end-to-end μ_2-bridges and display nearly ideal *cis* and *gauche* conformations, respectively. The bpydo ligands link the ten-coordinate Ln^{III} cations, forming interdigitating 4^4 grid-like layers extending parallel to ($\bar{1}$01), where interdigitation of layers is promoted by C—H···O interactions between nitrate anions and bpydo ligands. The interdigitated layers are linked to sets of neighboring layers *via* further C—H···O and π–π interactions.

1. Chemical context

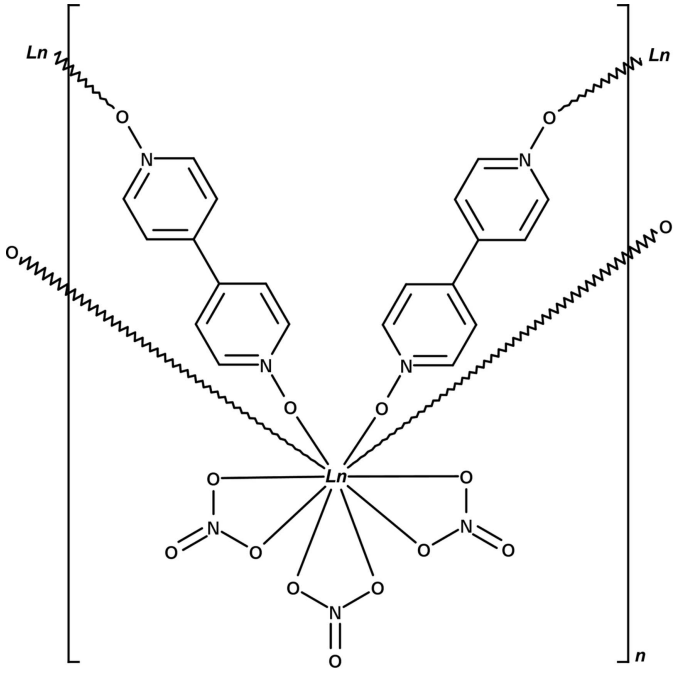
The use of aromatic N,N'-dioxide ligands such as 4,4′-bipyridine N,N'-dioxide (bpydo) in the synthesis of lanthanide compounds comprising coordination networks has been of recent interest (Dillner *et al.*, 2010*a*,*b*; Hill *et al.*, 2004, 2005*a*,*b*; Long *et al.*, 2000, 2002). The coordination modes of aromatic N,N'-dioxide ligands are flexible; they may act as terminal ligands, end-on or end-to-end μ_2-bridges, μ_3-bridges, or μ_4-bridges (Lu *et al.*, 2002; Ma *et al.*, 2001, 2003; Zhang *et al.*, 2004*a*,*b*). When acting as end-to-end μ_2-bridges, these ligands can display *cis*, *gauche*, or *trans* conformations where the ideal conformations have M—O···O—M torsion angles of 0, 90 and 180°, respectively (Sun *et al.*, 2004). Furthermore, aromatic N,N'-dioxide ligands are able to participate in a variety of hydrogen-bonding interactions (González Mantero *et al.*, 2006). Structure prediction with these ligands can be difficult, not only due to their flexible bonding modes and various hydrogen-bonding interactions, but also due to the influences of solvent and anion (Hill *et al.*, 2005*a*).



2. Structural commentary

Three isostructural coordination networks of Ce, Pr, and Nd nitrate with 4,4′-bipyridine N,N'-dioxide (bpydo), [$Ln(NO_3)_3(\mu_2$-bpydo)$_2$] [Ln = Ce (I), Pr (II), and Nd (III)] are

reported. All three compounds are isostructural to the previously reported La analogue (Hill *et al.*, 2004).



(I) *Ln* = Ce
(II) *Ln* = Pr
(III) *Ln* = Nd

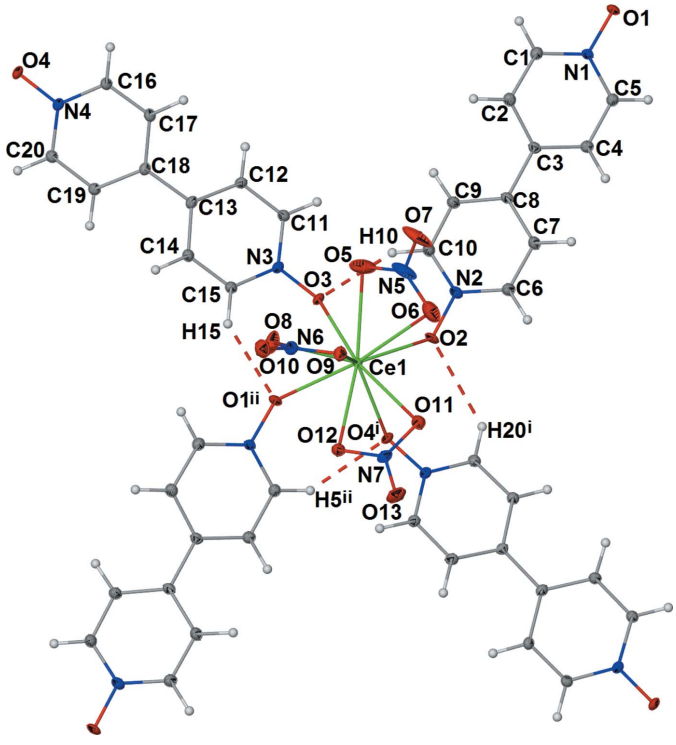


Figure 1
Coordination sphere around the Ce^{III} cation in the structure of (I), with displacement ellipsoids drawn at the 50% probability level. Dashed lines represent C—H···O interactions between neighboring bpydo ligands within the coordination sphere. [Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, y-1, z$.]

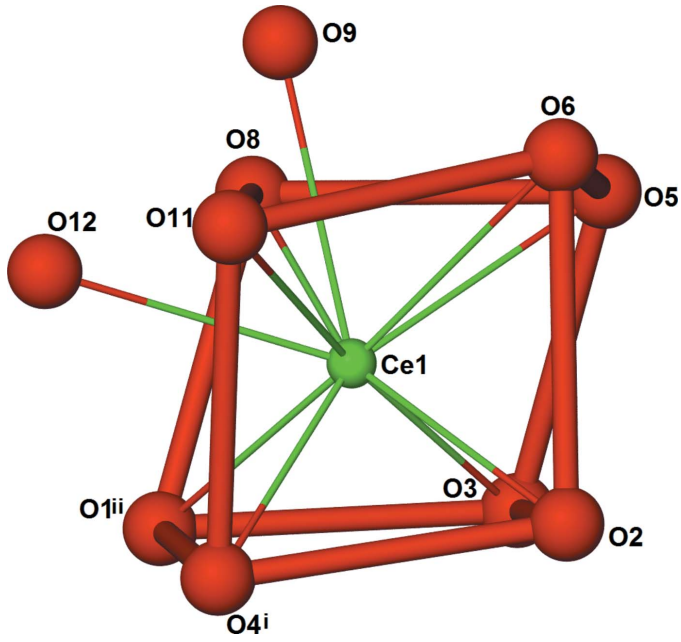


Figure 2
LnO_{10} coordination environment forming a distorted bicapped square prism. [Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, y-1, z$.]

The asymmetric unit of $[Ln(NO_3)_3(\mu_2\text{-bpydo})_2]$ contains one lanthanide cation, two end-to-end bridging μ_2-bpydo ligands, and three chelating nitrate anions. All atoms in the asymmetric unit lie on general positions (Fig. 1). The Ln^{III} atoms have a coordination sphere defined by six oxygen atoms from chelating nitrate anions and four oxygen atoms from bpydo ligands. The ten oxygen atoms in the LnO_{10} coordina-

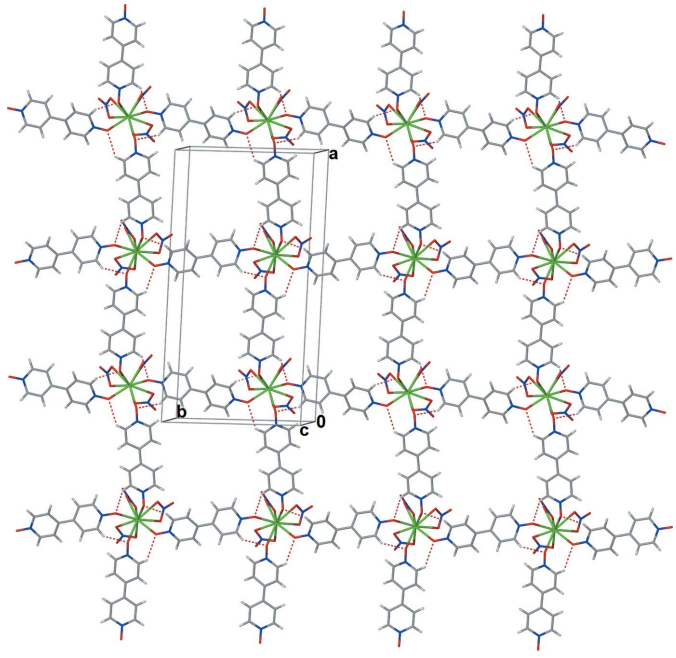


Figure 3
Diagram showing the 4^4 grid-like layers that lie parallel to $(\bar{1}01)$ in (I). Dashed lines represent C—H···O interactions between neighboring bpydo ligands within the Ce^{III} coordination sphere.

Table 1
Selected geometric parameters (Å, °) for (I)–(III).

Dihedral angles are reported between the mean planes defined by the indicated aromatic rings. *Cg*1 is the centroid of the N3/C11–C15 ring.

		(I)	(II)	(III)
Ln···*Ln* distances				
	*Ln*1···*Ln*1^{iii}	13.3398 (13)	13.3127 (9)	13.3035 (5)
	*Ln*1···*Ln*1^{iv}	13.2996 (11)	13.2634 (8)	13.2558 (4)
Dihedral angles				
	N1/C1–C5···N2/C6–C10	27.387 (58)	28.041 (62)	28.471 (109)
	N3/C11–C15···N4/C16–C20	22.560 (50)	22.552 (55)	22.677 (93)
Torsion angles				
	*Ln*1—O2···O1—*Ln*1^{iii}	92.53 (6)	91.80 (6)	91.75 (11)
	*Ln*1—O3···O4—*Ln*1^{iv}	5.38 (7)	4.86 (8)	4.87 (14)
π–π interactions for *Cg*1···*Cg*1^{x}				
	Centroid–centroid distance	3.7535 (10)	3.7465 (10)	3.7344 (17)
	Interplanar distance	3.2830 (6)	3.2790 (7)	3.2815 (11)
	Slippage	1.820	1.810	1.783
	*Cg*1—H15^{x} distance	3.305	3.312	3.311

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

Table 2
Selected bond lengths (Å) in compounds (I)–(III).

	Compound	(I)	(II)	(III)
Ln—O bond lengths involving bpydo ligands				
	*Ln*1—O1^{ii}	2.5464 (11)	2.5360 (12)	2.526 (2)
	*Ln*1—O2	2.5192 (11)	2.5009 (12)	2.488 (2)
	*Ln*1—O3	2.4685 (11)	2.4558 (11)	2.451 (2)
	*Ln*1—O4^{i}	2.4692 (11)	2.4554 (12)	2.448 (2)
	Average *Ln*—O distances	2.501	2.487	2.478
Ln—O bond lengths involving chelating nitrate anions				
	*Ln*1—O5	2.5929 (13)	2.5750 (13)	2.555 (2)
	*Ln*1—O6	2.6573 (13)	2.6443 (14)	2.640 (2)
	*Ln*1—O8	2.6004 (12)	2.5832 (13)	2.573 (2)
	*Ln*1—O9	2.6428 (12)	2.6242 (13)	2.615 (2)
	*Ln*1—O11	2.6231 (12)	2.6036 (12)	2.585 (2)
	*Ln*1—O12	2.6333 (11)	2.6147 (12)	2.597 (2)
	Average *Ln*—O distances	2.625	2.608	2.594

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

tion environment form a distorted bi-capped square prism (Fig. 2). One of the ligands bridges in a nearly perfect *cis* conformation with an *Ln*1—O3···O4—*Ln*1^{iv} torsion angle of approximately 5° and a dihedral angle between the rings of approximately 33°. The other ligand bridges in a nearly perfect *gauche* conformation with an *Ln*1—O2···O1—*Ln*1^{iii} torsion angle of approximately 92° and a dihedral angle between the rings of approximately 28° (see Table 1). The bpydo ligands link the *Ln*^{III} atoms, forming 4^4 grid-like layers that are parallel to $(\bar{1}01)$ (Fig. 3). Each layer interdigitates with a symmetry-equivalent second layer related by a twofold screw axis. The nitrate anions chelate to the metal cations on one side of the 4^4 grid and are directed towards the square void of the symmetry-related interdigitated 4^4 grid (Fig. 4).

While a roughly linear decrease in cell volume for a series of isostructural lanthanide compounds due to the lanthanide contraction may be expected (see, for example, He *et al.*, 2005; Ji *et al.*, 2012), deviations from a linear trend as observed for compounds (I)–(III) are not unprecedented, and the gradual decrease in *Ln*—*X* bond lengths and bridged *Ln*···*Ln* distances provides evidence of the lanthanide contraction (see, for example, Jia *et al.*, 2013; Li *et al.*, 2004, 2015). Recent studies on several series of isostructural lanthanide compounds have shown that the lanthanide contraction can be observed by the quadratic decay of the *Ln*—O bond lengths with increasing atomic number (Quadrelli, 2002; Seitz *et al.*, 2007; Xu *et al.*, 2013). An examination of both the *Ln*—O_{bpydo} and *Ln*—$O_{nitrate}$ distances for compounds (I)–(III) shows the expected gradual decrease in the *Ln*—O bond lengths from Ce (I) to Nd (III) due to the lanthanide contraction (Table 2). The gradual decrease in bpydo-bridged *Ln*···*Ln* distances within the layers is also consistent with the radius contraction from Ce to Nd (Table 1).

3. Supramolecular features

Stabilizing C—H···O interactions (C5—H5···O4^{vii}, C10—H10···O3, C15—H15···O1^{ii}, and C20—H20···O2^{iv}) are observed between neighboring bpydo ligands within the coordination sphere of the *Ln*^{III} cation (see Tables 3–5 for symmetry codes; Fig. 1). The interdigitation of layers is promoted by C—H···O interactions (C1—H1···O5^{v}, C4—

Table 3
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O5^{v}	0.95	2.59	3.342 (2)	136
C4—H4···O13^{vi}	0.95	2.37	3.208 (2)	148
C5—H5···O4^{vii}	0.95	2.38	3.1868 (19)	142
C9—H9···O9^{viii}	0.95	2.62	3.206 (2)	121
C9—H9···O10^{v}	0.95	2.59	3.475 (2)	156
C10—H10···O3	0.95	2.32	3.128 (2)	143
C10—H10···O7^{viii}	0.95	2.58	3.264 (2)	129
C11—H11···O10^{v}	0.95	2.49	3.237 (2)	135
C14—H14···O7^{ix}	0.95	2.22	3.004 (2)	139
C15—H15···O1^{ii}	0.95	2.32	3.1069 (19)	140
C16—H16···O13^{v}	0.95	2.55	3.154 (2)	122
C17—H17···O12^{v}	0.95	2.36	3.2837 (19)	164
C20—H20···O2^{iv}	0.95	2.63	3.3265 (19)	130

Symmetry codes: (ii) $x, y-1, z$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (vi) $-x, -y+1, -z+1$; (vii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (viii) $x, -y+1, z+\frac{1}{2}$; (ix) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 4
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O5^{v}	0.95	2.59	3.331 (2)	135
C4—H4···O13^{vi}	0.95	2.36	3.200 (2)	147
C5—H5···O4^{vii}	0.95	2.37	3.168 (2)	141
C9—H9···O9^{viii}	0.95	2.61	3.204 (2)	121
C9—H9···O10^{v}	0.95	2.58	3.468 (2)	156
C10—H10···O3	0.95	2.31	3.115 (2)	143
C10—H10···O7^{viii}	0.95	2.60	3.277 (3)	129
C11—H11···O10^{v}	0.95	2.50	3.239 (2)	135
C14—H14···O7^{ix}	0.95	2.22	3.002 (2)	139
C15—H15···O1^{ii}	0.95	2.31	3.0924 (19)	140
C16—H16···O13^{v}	0.95	2.56	3.154 (2)	121
C17—H17···O12^{v}	0.95	2.36	3.288 (2)	164
C20—H20···O2^{iv}	0.95	2.62	3.307 (2)	130

Symmetry codes: (ii) $x, y-1, z$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (vi) $-x, -y+1, -z+1$; (vii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (viii) $x, -y+1, z+\frac{1}{2}$; (ix) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 5
Hydrogen-bond geometry (Å, °) for (III).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O5^{v}	0.95	2.61	3.353 (4)	135
C4—H4···O13^{vi}	0.95	2.37	3.206 (4)	147
C5—H5···O4^{vii}	0.95	2.37	3.163 (4)	141
C9—H9···O9^{viii}	0.95	2.63	3.216 (4)	121
C9—H9···O10^{v}	0.95	2.58	3.464 (4)	156
C10—H10···O3	0.95	2.30	3.110 (4)	142
C10—H10···O7^{viii}	0.95	2.61	3.289 (4)	129
C11—H11···O10^{v}	0.95	2.50	3.243 (4)	135
C14—H14···O7^{ix}	0.95	2.21	2.998 (4)	139
C15—H15···O1^{ii}	0.95	2.31	3.091 (4)	139
C16—H16···O13^{v}	0.95	2.56	3.159 (4)	121
C17—H17···O12^{v}	0.95	2.37	3.295 (4)	165
C20—H20···O2^{iv}	0.95	2.61	3.294 (4)	130

Symmetry codes: (ii) $x, y-1, z$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (vi) $-x, -y+1, -z+1$; (vii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (viii) $x, -y+1, z+\frac{1}{2}$; (ix) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

H4···O13^{vi}, C9—H9···O10^{v}, C11—H11···O10^{v}, C14—H14···O7^{ix}, C16—H16···O13^{v}, and C17—H17···O12^{v}) between the ligands of one layer and nitrate anions of the other layer (Fig. 4). Further C—H···O interactions (C9—H9···O9^{viii} and C10—H10···O7^{viii}) and π–π interactions between $Cg1$ and the inversion-related $Cg1^{x}$ link each set of interdigitated layers to symmetry-equivalent sets of layers above and below it [symmetry code: (x) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$; Fig. 5). π–π interactions between the neighboring rings are observed with a centroid-to-centroid distance of 3.7535 (10) Å and an interplanar distance of 3.2830 (6) Å for (I); there is a slippage of 1.820 Å such that H15^{x} of the neighboring *N*-oxide

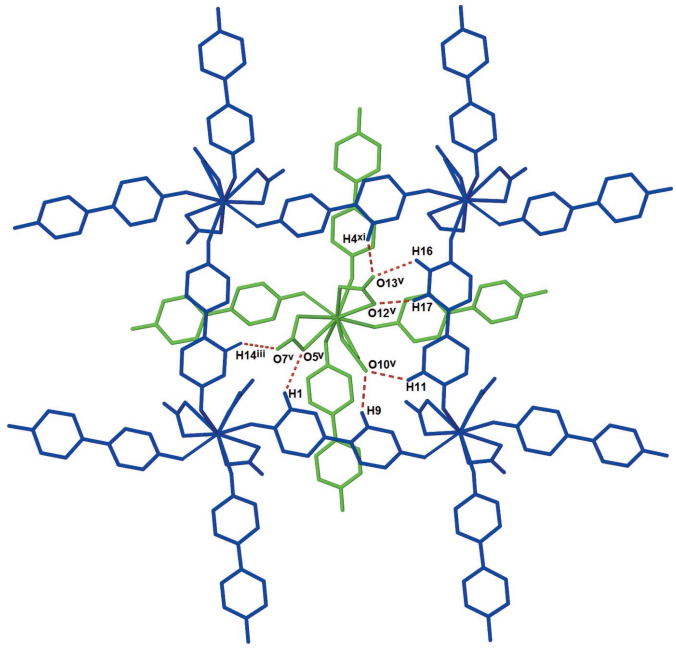


Figure 4
Diagram showing the C—H···O interactions between anions and ligands of interdigitated layers in (I). Individual layers are represented in green and blue. Dashed red lines represent C—H···O interactions between the layers. [Symmetry codes: (iii) $x, y+1, z$; (v) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (xi) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.]

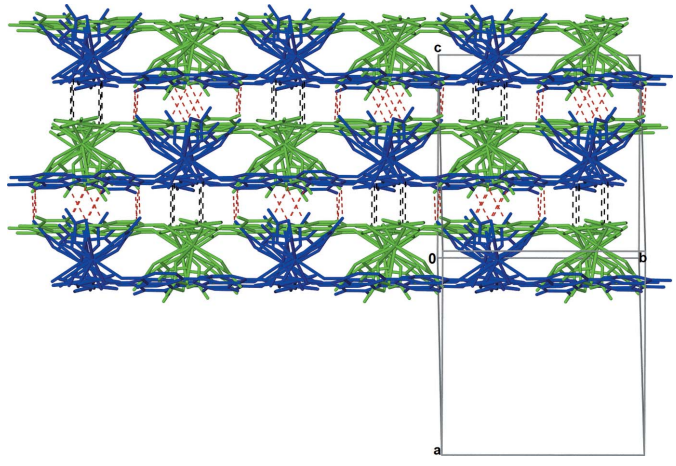


Figure 5
Diagram showing C—H···O interactions and π–π interactions that link each set of interdigitated layers to similar sets of layers above and below it in (I). Individual layers are represented in green and blue. Dashed red lines represent C—H···O interactions, and dashed black lines represent π–π interactions.

Table 6
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$[Ce(NO_3)_3(C_{10}H_8N_2O_2)_2]$	$[Pr(NO_3)_3(C_{10}H_8N_2O_2)_2]$	$[Nd(NO_3)_3(C_{10}H_8N_2O_2)_2]$
M_r	702.52	703.31	706.64
Crystal system, space group	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*
Temperature (K)	173	173	173
a, *b*, *c* (Å)	26.786 (3), 13.3398 (13), 13.7571 (13)	26.7416 (18), 13.3127 (9), 13.7586 (9)	26.7422 (10), 13.3035 (5), 13.7804 (5)
β (°)	105.837 (1)	105.981 (1)	106.065 (1)
V (Å^3)	4729.1 (8)	4708.8 (5)	4711.1 (3)
Z	8	8	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.01	2.16	2.29
Crystal size (mm)	0.55 × 0.45 × 0.38	0.55 × 0.37 × 0.26	0.14 × 0.12 × 0.08
Data collection			
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD	Bruker D8 Quest CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.536, 0.746	0.579, 0.746	0.682, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15990, 7152, 6686	18363, 7241, 6782	47148, 8277, 5419
R_{int}	0.018	0.020	0.115
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.735	0.737	0.777
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.050, 1.05	0.021, 0.052, 1.05	0.051, 0.067, 1.01
No. of reflections	7152	7241	8277
No. of parameters	370	370	370
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.10, −0.65	0.89, −1.06	1.49, −1.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2009, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *X-SEED* (Barbour, 2001).

ring lies nearly centered over the centroid of *Cg*1 at a distance of 3.305 Å [see Table 1 for distances in compounds (II) and (III)].

4. Database survey

A survey of the Cambridge Structural Database (CSD, November 2014; Groom & Allen, 2014) returned hits for 333 structures with 4,4′-bipyridine *N*,*N*′-dioxide. Sixty three structures are reported where bpydo coordinates to a lanthanide metal and acts a as bridging ligand in a coordination network. Of these structures, ten are reported with nitrate as the counter-ion. In $[Tb(bpydo)_2(NO_3)_3]$, linear chains are observed (Long *et al.*, 2002). A one-dimensional network composed of zigzag chains is observed for $[Tb(bpydo)(CH_3OH)(NO_3)_3]$ (Long *et al.*, 2002). In $\{[Ln(bpydo)_{1.5}(NO_3)_3]\cdot CH_2Cl_2\}$ with *Ln* = Eu (Dillner *et al.*, 2010*a*), Gd (Dillner *et al.*, 2010*b*), and Tb (Long *et al.*, 2002), a one-dimensional network composed of ladder-like chains is observed. $[La(bpydo)_2(NO_3)_3]$ is a two-dimensional network composed of sheets with 4^4 topology and is isostructural to the Ce, Pr, and Nd structures reported herein (Hill *et al.*, 2004). In $\{[Er_2(bpydo)_3(NO_3)_6]\cdot 2CH_3OH\}$, $\{[Tb(bpydo)_{1.5}(NO_3)_3]\cdot CH_3OH\cdot 0.8H_2O\}$, and $\{[Tb(bpydo)_{1.5}(NO_3)_3]\cdot 0.4CCl_4\cdot 0.8CH_3OH\}$, two-dimensional networks composed of sheets with 4.8^2 topology are formed (Long *et al.*, 2000, 2002). In $\{[Sm(bpydo)_2(NO_3)_3]\cdot 0.5H_2O\}$, a twofold interpenetrating three-dimensional network is formed (Long *et al.*, 2000).

5. Synthesis and crystallization

4,4′-bipyridine *N*,*N*′-dioxide·H_2O was synthesized from 4,4′-bipyridine according to the method of Simpson *et al.* (1963). All other chemicals were obtained from commercial sources and used without further purification. For the Ce, Pr and Nd compounds, respectively, the appropriate $Ln(NO_3)_3\cdot 6H_2O$ (0.113 mmol) was placed in the bottom of a test tube and covered with CH_2Cl_2 (5 ml). 4,4′-Bipyridine-*N*,*N*′-dioxide·H_2O (0.0376 g, 0.182 mmol) was dissolved in methanol (8 ml), and this solution was layered over the CH_2Cl_2 solution. The two solutions were allowed to slowly mix. Over a period of several weeks the $Ln(NO_3)_3\cdot 6H_2O$ dissolved, and red block-like crystals of $[Ce(\mu_2\text{-bpydo})_2(NO_3)_3]$, yellow block-like crystals of $[Pr(\mu_2\text{-bpydo})_2(NO_3)_3]$, and yellow block-like crystals of $[Nd(\mu_2\text{-bpydo})_2(NO_3)_3]$ were formed.

6. Refinement

All aromatic H atoms were positioned geometrically and refined using a riding model with C—H = 0.95 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. Crystal data, data collection and structure refinement details are summarized in Table 6.

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supporting information

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Crystal structures of [*Ln*(NO$_3$)$_3$(μ_2-bpydo)$_2$], where *Ln* = Ce, Pr or Nd, and bpydo = 4,4′-bipyridine *N*,*N*′-dioxide: layered coordination networks containing 4^4 grids

Michael L. Stromyer, Cassandra P. Lilly, Adam J. Dillner and Jacqueline M. Knaust

Computing details

Data collection: *APEX2* (Bruker, 2009) for (I), (II); *APEX2* (Bruker, 2014) for (III). Cell refinement: *SAINT* (Bruker, 2009) for (I), (II); *SAINT* (Bruker, 2014) for (III). Data reduction: *SAINT* (Bruker, 2009) for (I), (II); *SAINT* (Bruker, 2014) for (III). For all compounds, program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *X-SEED* (Barbour, 2001).

(I) Poly[[tris(nitrato-κ^2O,O')cerium(III)]-bis(μ-4,4′-bipyridine *N*,*N*′-dioxide-κ^2N:*N*′)]

Crystal data

[Ce(NO$_3$)$_3$(C$_{10}$H$_8$N$_2$O$_2$)$_2$]
M_r = 702.52
Monoclinic, *C*2/*c*
a = 26.786 (3) Å
b = 13.3398 (13) Å
c = 13.7571 (13) Å
β = 105.837 (1)°
V = 4729.1 (8) Å^3
Z = 8
F(000) = 2776
D_x = 1.973 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 11055 reflections
θ = 2.5–31.5°
μ = 2.01 mm^{-1}
T = 173 K
Block, red
0.55 × 0.45 × 0.38 mm

Data collection

Bruker APEXII CCD diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.536, T_{max} = 0.746
15990 measured reflections
7152 independent reflections
6686 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 31.5°, θ_{min} = 1.6°
h = −37→37
k = −11→19
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.050
S = 1.05
7152 reflections
370 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0231P)^2 + 5.9858P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.12666 (2)	0.27581 (2)	0.66455 (2)	0.00880 (3)
O1	0.14943 (4)	1.12935 (8)	0.78743 (9)	0.0138 (2)
O2	0.07510 (4)	0.41815 (8)	0.70896 (9)	0.0154 (2)
O3	0.18037 (4)	0.33380 (8)	0.83061 (8)	0.0131 (2)
O4	0.54328 (4)	0.28358 (8)	1.18738 (9)	0.0126 (2)
O5	0.19329 (6)	0.41286 (11)	0.65215 (10)	0.0288 (3)
O6	0.12041 (6)	0.42801 (10)	0.53717 (11)	0.0267 (3)
O7	0.18842 (7)	0.50937 (10)	0.52255 (12)	0.0365 (4)
O8	0.21266 (5)	0.18687 (11)	0.66189 (9)	0.0221 (3)
O9	0.16939 (5)	0.24235 (9)	0.51565 (9)	0.0157 (2)
O10	0.23607 (5)	0.14464 (9)	0.52773 (9)	0.0195 (2)
O11	0.05806 (5)	0.25187 (9)	0.48914 (9)	0.0162 (2)
O12	0.09542 (4)	0.11414 (8)	0.55499 (8)	0.0148 (2)
O13	0.03572 (5)	0.11024 (10)	0.41152 (9)	0.0217 (3)
N1	0.14037 (5)	1.03162 (9)	0.77682 (9)	0.0113 (2)
N2	0.08640 (5)	0.51564 (10)	0.71907 (10)	0.0134 (2)
N3	0.23131 (5)	0.32751 (10)	0.87085 (9)	0.0109 (2)
N4	0.49487 (5)	0.28718 (9)	1.12873 (10)	0.0111 (2)
N5	0.16766 (7)	0.45133 (11)	0.56933 (12)	0.0253 (3)
N6	0.20687 (5)	0.19053 (10)	0.56676 (10)	0.0145 (2)
N7	0.06262 (5)	0.15808 (10)	0.48319 (9)	0.0137 (2)
C1	0.18034 (6)	0.96562 (12)	0.79956 (12)	0.0142 (3)
H1	0.2150	0.9895	0.8219	0.017*
C2	0.17085 (6)	0.86374 (12)	0.79041 (12)	0.0144 (3)
H2	0.1991	0.8180	0.8075	0.017*
C3	0.12012 (6)	0.82731 (11)	0.75622 (11)	0.0121 (3)
C4	0.08022 (6)	0.89772 (12)	0.73462 (12)	0.0137 (3)
H4	0.0452	0.8759	0.7115	0.016*
C5	0.09092 (6)	0.99873 (12)	0.74644 (12)	0.0136 (3)
H5	0.0632	1.0457	0.7331	0.016*
C6	0.05307 (6)	0.58316 (12)	0.66253 (13)	0.0171 (3)
H6	0.0225	0.5606	0.6144	0.021*
C7	0.06325 (6)	0.68421 (12)	0.67436 (12)	0.0165 (3)
H7	0.0393	0.7310	0.6351	0.020*
C8	0.10854 (6)	0.71893 (11)	0.74362 (12)	0.0124 (3)
C9	0.14170 (6)	0.64712 (12)	0.80061 (12)	0.0162 (3)
H9	0.1727	0.6677	0.8485	0.019*
C10	0.12988 (6)	0.54644 (12)	0.78811 (13)	0.0172 (3)
H10	0.1525	0.4984	0.8284	0.021*

C11	0.25885 (6)	0.41124 (11)	0.90585 (11)	0.0128 (3)
H11	0.2421	0.4747	0.8972	0.015*
C12	0.31105 (6)	0.40468 (12)	0.95406 (11)	0.0131 (3)
H12	0.3300	0.4637	0.9793	0.016*
C13	0.33644 (6)	0.31212 (11)	0.96620 (11)	0.0117 (3)
C14	0.30687 (6)	0.22856 (11)	0.92576 (12)	0.0137 (3)
H14	0.3231	0.1647	0.9302	0.016*
C15	0.25463 (6)	0.23682 (11)	0.87958 (12)	0.0132 (3)
H15	0.2349	0.1788	0.8538	0.016*
C16	0.47610 (6)	0.37514 (11)	1.08504 (11)	0.0131 (3)
H16	0.4985	0.4315	1.0918	0.016*
C17	0.42495 (6)	0.38381 (12)	1.03088 (12)	0.0135 (3)
H17	0.4122	0.4460	1.0004	0.016*
C18	0.39170 (6)	0.30199 (11)	1.02043 (11)	0.0115 (3)
C19	0.41282 (6)	0.21126 (11)	1.06413 (12)	0.0125 (3)
H19	0.3915	0.1534	1.0567	0.015*
C20	0.46424 (6)	0.20521 (12)	1.11776 (12)	0.0129 (3)
H20	0.4782	0.1433	1.1471	0.015*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.00749 (4)	0.00690 (4)	0.01083 (4)	−0.00080 (3)	0.00051 (3)	−0.00044 (2)
O1	0.0156 (5)	0.0062 (5)	0.0175 (5)	−0.0020 (4)	0.0008 (4)	−0.0001 (4)
O2	0.0164 (5)	0.0053 (5)	0.0237 (6)	−0.0017 (4)	0.0043 (4)	−0.0023 (4)
O3	0.0069 (4)	0.0139 (5)	0.0155 (5)	0.0001 (4)	−0.0021 (4)	−0.0013 (4)
O4	0.0063 (5)	0.0135 (5)	0.0158 (5)	0.0010 (4)	−0.0008 (4)	0.0013 (4)
O5	0.0369 (8)	0.0279 (7)	0.0231 (6)	−0.0185 (6)	0.0107 (6)	−0.0048 (5)
O6	0.0349 (7)	0.0180 (6)	0.0309 (7)	0.0042 (5)	0.0152 (6)	0.0061 (5)
O7	0.0665 (11)	0.0128 (6)	0.0464 (9)	−0.0089 (7)	0.0427 (8)	−0.0018 (6)
O8	0.0195 (6)	0.0320 (7)	0.0146 (5)	0.0088 (5)	0.0041 (4)	0.0025 (5)
O9	0.0138 (5)	0.0163 (5)	0.0164 (5)	0.0019 (4)	0.0030 (4)	0.0025 (4)
O10	0.0201 (6)	0.0183 (6)	0.0224 (6)	0.0039 (5)	0.0094 (5)	−0.0015 (5)
O11	0.0169 (5)	0.0131 (5)	0.0170 (5)	0.0016 (4)	0.0018 (4)	0.0001 (4)
O12	0.0154 (5)	0.0117 (5)	0.0151 (5)	0.0000 (4)	0.0006 (4)	−0.0010 (4)
O13	0.0184 (6)	0.0261 (6)	0.0167 (5)	−0.0039 (5)	−0.0016 (4)	−0.0090 (5)
N1	0.0129 (6)	0.0079 (5)	0.0118 (5)	−0.0016 (4)	0.0010 (4)	0.0003 (4)
N2	0.0141 (6)	0.0084 (6)	0.0170 (6)	−0.0003 (5)	0.0033 (5)	−0.0013 (5)
N3	0.0083 (5)	0.0115 (6)	0.0115 (5)	0.0001 (4)	0.0002 (4)	−0.0002 (4)
N4	0.0081 (5)	0.0116 (6)	0.0127 (6)	0.0007 (4)	0.0014 (4)	0.0008 (4)
N5	0.0444 (10)	0.0104 (6)	0.0298 (8)	−0.0066 (6)	0.0244 (7)	−0.0040 (6)
N6	0.0132 (6)	0.0139 (6)	0.0163 (6)	−0.0010 (5)	0.0041 (5)	−0.0004 (5)
N7	0.0119 (6)	0.0169 (6)	0.0117 (5)	−0.0021 (5)	0.0023 (4)	−0.0028 (5)
C1	0.0113 (6)	0.0125 (7)	0.0170 (7)	0.0000 (5)	0.0005 (5)	0.0002 (5)
C2	0.0129 (6)	0.0117 (7)	0.0172 (7)	0.0012 (5)	0.0017 (5)	−0.0002 (5)
C3	0.0147 (7)	0.0083 (6)	0.0117 (6)	−0.0010 (5)	0.0012 (5)	−0.0007 (5)
C4	0.0118 (6)	0.0112 (7)	0.0163 (7)	−0.0011 (5)	0.0010 (5)	0.0003 (5)
C5	0.0113 (6)	0.0112 (7)	0.0163 (7)	0.0002 (5)	0.0005 (5)	0.0007 (5)

C6	0.0155 (7)	0.0120 (7)	0.0196 (7)	−0.0009 (6)	−0.0025 (6)	0.0000 (6)
C7	0.0172 (7)	0.0103 (7)	0.0186 (7)	0.0005 (6)	−0.0010 (6)	0.0018 (6)
C8	0.0143 (7)	0.0084 (6)	0.0139 (7)	−0.0009 (5)	0.0029 (5)	−0.0007 (5)
C9	0.0145 (7)	0.0103 (7)	0.0201 (7)	0.0001 (5)	−0.0015 (6)	−0.0015 (6)
C10	0.0134 (7)	0.0105 (7)	0.0237 (8)	0.0010 (6)	−0.0018 (6)	0.0005 (6)
C11	0.0112 (6)	0.0095 (6)	0.0164 (7)	0.0001 (5)	0.0014 (5)	−0.0014 (5)
C12	0.0099 (6)	0.0111 (6)	0.0163 (7)	−0.0008 (5)	0.0002 (5)	−0.0029 (5)
C13	0.0096 (6)	0.0128 (7)	0.0114 (6)	0.0002 (5)	0.0006 (5)	0.0003 (5)
C14	0.0118 (7)	0.0101 (7)	0.0170 (7)	0.0008 (5)	0.0002 (5)	0.0005 (5)
C15	0.0122 (7)	0.0093 (6)	0.0159 (7)	0.0002 (5)	0.0004 (5)	−0.0004 (5)
C16	0.0108 (6)	0.0112 (6)	0.0158 (7)	−0.0002 (5)	0.0010 (5)	0.0028 (5)
C17	0.0115 (6)	0.0116 (6)	0.0161 (7)	0.0009 (5)	0.0017 (5)	0.0033 (5)
C18	0.0094 (6)	0.0124 (6)	0.0118 (6)	0.0007 (5)	0.0014 (5)	0.0009 (5)
C19	0.0114 (6)	0.0104 (6)	0.0145 (7)	−0.0006 (5)	0.0015 (5)	0.0009 (5)
C20	0.0121 (6)	0.0102 (6)	0.0151 (7)	0.0000 (5)	0.0017 (5)	0.0010 (5)

Geometric parameters (Å, º)

Ce1—O3	2.4685 (11)	C1—H1	0.9500
Ce1—O4^{i}	2.4692 (11)	C2—C3	1.398 (2)
Ce1—O2	2.5192 (11)	C2—H2	0.9500
Ce1—O1^{ii}	2.5464 (11)	C3—C4	1.393 (2)
Ce1—O5	2.5929 (13)	C3—C8	1.479 (2)
Ce1—O8	2.6004 (12)	C4—C5	1.378 (2)
Ce1—O11	2.6231 (12)	C4—H4	0.9500
Ce1—O12	2.6333 (11)	C5—H5	0.9500
Ce1—O9	2.6428 (12)	C6—C7	1.376 (2)
Ce1—O6	2.6573 (13)	C6—H6	0.9500
O1—N1	1.3268 (16)	C7—C8	1.401 (2)
O1—Ce1^{iii}	2.5464 (11)	C7—H7	0.9500
O2—N2	1.3339 (16)	C8—C9	1.393 (2)
O3—N3	1.3277 (15)	C9—C10	1.380 (2)
O4—N4	1.3281 (16)	C9—H9	0.9500
O4—Ce1^{iv}	2.4694 (11)	C10—H10	0.9500
O5—N5	1.267 (2)	C11—C12	1.377 (2)
O6—N5	1.260 (2)	C11—H11	0.9500
O7—N5	1.2321 (19)	C12—C13	1.398 (2)
O8—N6	1.2761 (18)	C12—H12	0.9500
O9—N6	1.2629 (18)	C13—C14	1.393 (2)
O10—N6	1.2264 (17)	C13—C18	1.471 (2)
O11—N7	1.2619 (18)	C14—C15	1.374 (2)
O12—N7	1.2718 (17)	C14—H14	0.9500
O13—N7	1.2292 (17)	C15—H15	0.9500
N1—C5	1.3490 (19)	C16—C17	1.374 (2)
N1—C1	1.355 (2)	C16—H16	0.9500
N2—C10	1.350 (2)	C17—C18	1.391 (2)
N2—C6	1.354 (2)	C17—H17	0.9500
N3—C15	1.3517 (19)	C18—C19	1.400 (2)

N3—C11	1.3527 (19)	C19—C20	1.376 (2)
N4—C20	1.3504 (19)	C19—H19	0.9500
N4—C16	1.3512 (19)	C20—H20	0.9500
C1—C2	1.382 (2)		

O3—Ce1—O4^{i}	107.56 (4)	O7—N5—O5	120.87 (18)
O3—Ce1—O2	76.05 (4)	O6—N5—O5	117.48 (14)
O4^{i}—Ce1—O2	68.67 (4)	O10—N6—O9	122.32 (13)
O3—Ce1—O1^{ii}	69.67 (4)	O10—N6—O8	121.08 (14)
O4^{i}—Ce1—O1^{ii}	74.36 (4)	O9—N6—O8	116.59 (13)
O2—Ce1—O1^{ii}	117.72 (4)	O13—N7—O11	121.39 (14)
O3—Ce1—O5	66.55 (4)	O13—N7—O12	120.88 (14)
O4^{i}—Ce1—O5	153.81 (4)	O11—N7—O12	117.72 (12)
O2—Ce1—O5	85.25 (4)	N1—C1—C2	120.25 (14)
O1^{ii}—Ce1—O5	122.70 (4)	N1—C1—H1	119.9
O3—Ce1—O8	82.02 (4)	C2—C1—H1	119.9
O4^{i}—Ce1—O8	133.70 (4)	C1—C2—C3	120.67 (14)
O2—Ce1—O8	153.34 (4)	C1—C2—H2	119.7
O1^{ii}—Ce1—O8	66.84 (4)	C3—C2—H2	119.7
O5—Ce1—O8	72.09 (5)	C4—C3—C2	117.13 (14)
O3—Ce1—O11	167.04 (4)	C4—C3—C8	120.68 (14)
O4^{i}—Ce1—O11	69.34 (4)	C2—C3—C8	122.18 (14)
O2—Ce1—O11	91.27 (4)	C5—C4—C3	120.78 (14)
O1^{ii}—Ce1—O11	119.87 (4)	C5—C4—H4	119.6
O5—Ce1—O11	110.32 (4)	C3—C4—H4	119.6
O8—Ce1—O11	109.41 (4)	N1—C5—C4	120.64 (14)
O3—Ce1—O12	143.16 (4)	N1—C5—H5	119.7
O4^{i}—Ce1—O12	69.69 (4)	C4—C5—H5	119.7
O2—Ce1—O12	130.28 (4)	N2—C6—C7	120.35 (15)
O1^{ii}—Ce1—O12	74.50 (4)	N2—C6—H6	119.8
O5—Ce1—O12	131.05 (4)	C7—C6—H6	119.8
O8—Ce1—O12	76.27 (4)	C6—C7—C8	120.73 (15)
O11—Ce1—O12	48.73 (4)	C6—C7—H7	119.6
O3—Ce1—O9	120.26 (4)	C8—C7—H7	119.6
O4^{i}—Ce1—O9	129.97 (4)	C9—C8—C7	117.14 (14)
O2—Ce1—O9	134.21 (4)	C9—C8—C3	121.68 (14)
O1^{ii}—Ce1—O9	108.00 (4)	C7—C8—C3	121.18 (14)
O5—Ce1—O9	67.46 (4)	C10—C9—C8	120.65 (15)
O8—Ce1—O9	48.65 (4)	C10—C9—H9	119.7
O11—Ce1—O9	67.00 (4)	C8—C9—H9	119.7
O12—Ce1—O9	63.59 (4)	N2—C10—C9	120.55 (14)
O3—Ce1—O6	106.67 (4)	N2—C10—H10	119.7
O4^{i}—Ce1—O6	115.64 (4)	C9—C10—H10	119.7
O2—Ce1—O6	69.15 (4)	N3—C11—C12	120.16 (14)
O1^{ii}—Ce1—O6	169.94 (4)	N3—C11—H11	119.9
O5—Ce1—O6	48.58 (5)	C12—C11—H11	119.9
O8—Ce1—O6	103.65 (4)	C11—C12—C13	120.71 (14)
O11—Ce1—O6	65.43 (4)	C11—C12—H12	119.6

O12—Ce1—O6	107.17 (4)	C13—C12—H12	119.6
O9—Ce1—O6	65.20 (4)	C14—C13—C12	117.02 (14)
N1—O1—Ce1^{iii}	132.64 (9)	C14—C13—C18	120.87 (14)
N2—O2—Ce1	129.52 (9)	C12—C13—C18	122.11 (14)
N3—O3—Ce1	129.72 (9)	C15—C14—C13	121.13 (14)
N4—O4—Ce1^{iv}	134.54 (9)	C15—C14—H14	119.4
N5—O5—Ce1	97.52 (10)	C13—C14—H14	119.4
N5—O6—Ce1	94.62 (10)	N3—C15—C14	120.03 (14)
N6—O8—Ce1	97.86 (9)	N3—C15—H15	120.0
N6—O9—Ce1	96.18 (9)	C14—C15—H15	120.0
N7—O11—Ce1	97.15 (8)	N4—C16—C17	120.61 (14)
N7—O12—Ce1	96.39 (8)	N4—C16—H16	119.7
O1—N1—C5	119.22 (13)	C17—C16—H16	119.7
O1—N1—C1	120.25 (13)	C16—C17—C18	120.36 (14)
C5—N1—C1	120.49 (13)	C16—C17—H17	119.8
O2—N2—C10	119.84 (13)	C18—C17—H17	119.8
O2—N2—C6	119.56 (13)	C17—C18—C19	117.49 (14)
C10—N2—C6	120.56 (14)	C17—C18—C13	120.50 (14)
O3—N3—C15	119.41 (13)	C19—C18—C13	122.01 (14)
O3—N3—C11	119.65 (12)	C20—C19—C18	120.59 (14)
C15—N3—C11	120.89 (13)	C20—C19—H19	119.7
O4—N4—C20	120.08 (12)	C18—C19—H19	119.7
O4—N4—C16	118.99 (12)	N4—C20—C19	120.07 (14)
C20—N4—C16	120.83 (13)	N4—C20—H20	120.0
O7—N5—O6	121.65 (18)	C19—C20—H20	120.0
Ce1—O3—O4—Ce1^{iv}	5.38 (7)	Ce1—O2—O1—Ce1^{iii}	92.53 (6)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O5^{v}	0.95	2.59	3.342 (2)	136
C4—H4···O13^{vi}	0.95	2.37	3.208 (2)	148
C5—H5···O4^{vii}	0.95	2.38	3.1868 (19)	142
C9—H9···O9^{viii}	0.95	2.62	3.206 (2)	121
C9—H9···O10^{v}	0.95	2.59	3.475 (2)	156
C10—H10···O3	0.95	2.32	3.128 (2)	143
C10—H10···O7^{viii}	0.95	2.58	3.264 (2)	129
C11—H11···O10^{v}	0.95	2.49	3.237 (2)	135
C14—H14···O7^{ix}	0.95	2.22	3.004 (2)	139
C15—H15···O1^{ii}	0.95	2.32	3.1069 (19)	140
C16—H16···O13^{v}	0.95	2.55	3.154 (2)	122
C17—H17···O12^{v}	0.95	2.36	3.2837 (19)	164
C20—H20···O2^{iv}	0.95	2.63	3.3265 (19)	130

Symmetry codes: (ii) $x, y-1, z$; (iv) $x+1/2, -y+1/2, z+1/2$; (v) $-x+1/2, y+1/2, -z+3/2$; (vi) $-x, -y+1, -z+1$; (vii) $x-1/2, -y+3/2, z-1/2$; (viii) $x, -y+1, z+1/2$; (ix) $-x+1/2, y-1/2, -z+3/2$.

(II) Poly[[tris(nitrato-κ^2O,O')praeseodymium(III)]-bis(μ-4,4′-bipyridine *N*,*N*′-dioxide-κ^2N:*N*′)]

Crystal data

$[Pr(NO_3)_3(C_{10}H_8N_2O_2)_2]$
M_r = 703.31
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 26.7416 (18) Å
b = 13.3127 (9) Å
c = 13.7586 (9) Å
β = 105.981 (1)°
V = 4708.8 (5) Å^3
Z = 8
F(000) = 2784
D_x = 1.984 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 11450 reflections
θ = 2.5–31.3°
μ = 2.16 mm^{-1}
T = 173 K
Block, yellow
0.55 × 0.37 × 0.26 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.579, T_{max} = 0.746
18363 measured reflections
7241 independent reflections
6782 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 31.6°, θ_{min} = 1.6°
h = −39→38
k = −18→18
l = −19→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.052
S = 1.05
7241 reflections
370 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0248P)^2 + 6.7123P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pr1	0.12674 (2)	0.27553 (2)	0.66470 (2)	0.00790 (3)
O1	0.14910 (4)	1.12982 (8)	0.78780 (9)	0.0121 (2)
O2	0.07540 (5)	0.41686 (8)	0.70889 (10)	0.0138 (2)
O3	0.17985 (4)	0.33321 (9)	0.83058 (9)	0.0115 (2)
O4	0.54388 (4)	0.28390 (8)	1.18793 (9)	0.0111 (2)
O5	0.19376 (6)	0.41071 (11)	0.65327 (11)	0.0253 (3)
O6	0.12068 (6)	0.42773 (10)	0.53849 (11)	0.0236 (3)
O7	0.18928 (7)	0.50822 (10)	0.52428 (13)	0.0324 (4)
O8	0.21197 (5)	0.18554 (11)	0.66227 (10)	0.0196 (3)
O9	0.16890 (5)	0.24298 (10)	0.51644 (10)	0.0144 (2)

O10	0.23564 (5)	0.14508 (10)	0.52791 (10)	0.0181 (2)
O11	0.05832 (5)	0.25265 (10)	0.49034 (9)	0.0144 (2)
O12	0.09581 (4)	0.11451 (9)	0.55595 (9)	0.0135 (2)
O13	0.03605 (5)	0.11082 (10)	0.41182 (10)	0.0198 (3)
N1	0.14024 (5)	1.03189 (10)	0.77697 (10)	0.0100 (2)
N2	0.08667 (5)	0.51456 (10)	0.71901 (11)	0.0117 (2)
N3	0.23089 (5)	0.32704 (10)	0.87050 (10)	0.0096 (2)
N4	0.49530 (5)	0.28712 (10)	1.12884 (11)	0.0097 (2)
N5	0.16820 (7)	0.45013 (11)	0.57063 (13)	0.0219 (3)
N6	0.20645 (5)	0.19037 (11)	0.56710 (11)	0.0129 (3)
N7	0.06291 (5)	0.15870 (11)	0.48410 (10)	0.0124 (3)
C1	0.18032 (6)	0.96583 (12)	0.79944 (13)	0.0127 (3)
H1	0.2151	0.9899	0.8217	0.015*
C2	0.17102 (6)	0.86383 (12)	0.79021 (13)	0.0130 (3)
H2	0.1994	0.8182	0.8072	0.016*
C3	0.12013 (6)	0.82702 (12)	0.75610 (12)	0.0106 (3)
C4	0.07981 (6)	0.89758 (12)	0.73481 (13)	0.0126 (3)
H4	0.0447	0.8756	0.7120	0.015*
C5	0.09060 (6)	0.99871 (12)	0.74667 (12)	0.0120 (3)
H5	0.0628	1.0457	0.7334	0.014*
C6	0.05349 (6)	0.58208 (12)	0.66223 (13)	0.0152 (3)
H6	0.0230	0.5593	0.6138	0.018*
C7	0.06337 (6)	0.68346 (12)	0.67370 (13)	0.0145 (3)
H7	0.0394	0.7301	0.6340	0.017*
C8	0.10860 (6)	0.71840 (11)	0.74358 (13)	0.0109 (3)
C9	0.14177 (6)	0.64669 (12)	0.80127 (13)	0.0149 (3)
H9	0.1727	0.6674	0.8499	0.018*
C10	0.12999 (6)	0.54590 (12)	0.78830 (14)	0.0154 (3)
H10	0.1527	0.4979	0.8288	0.019*
C11	0.25850 (6)	0.41103 (12)	0.90557 (12)	0.0116 (3)
H11	0.2417	0.4746	0.8969	0.014*
C12	0.31102 (6)	0.40482 (12)	0.95382 (13)	0.0120 (3)
H12	0.3300	0.4640	0.9790	0.014*
C13	0.33636 (6)	0.31196 (12)	0.96590 (12)	0.0100 (3)
C14	0.30678 (6)	0.22808 (11)	0.92570 (13)	0.0122 (3)
H14	0.3231	0.1642	0.9302	0.015*
C15	0.25433 (6)	0.23623 (12)	0.87957 (13)	0.0116 (3)
H15	0.2346	0.1780	0.8540	0.014*
C16	0.47654 (6)	0.37537 (12)	1.08487 (12)	0.0117 (3)
H16	0.4990	0.4318	1.0914	0.014*
C17	0.42522 (6)	0.38374 (12)	1.03083 (13)	0.0120 (3)
H17	0.4124	0.4461	1.0005	0.014*
C18	0.39185 (6)	0.30165 (12)	1.02012 (12)	0.0102 (3)
C19	0.41298 (6)	0.21084 (12)	1.06397 (13)	0.0113 (3)
H19	0.3916	0.1528	1.0566	0.014*
C20	0.46461 (6)	0.20508 (12)	1.11778 (13)	0.0116 (3)
H20	0.4787	0.1431	1.1472	0.014*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00728 (4)	0.00661 (4)	0.00934 (5)	−0.00065 (2)	0.00148 (3)	−0.00049 (3)
O1	0.0148 (5)	0.0056 (5)	0.0146 (5)	−0.0022 (4)	0.0018 (4)	−0.0004 (4)
O2	0.0154 (5)	0.0052 (5)	0.0209 (6)	−0.0015 (4)	0.0053 (5)	−0.0021 (4)
O3	0.0063 (4)	0.0124 (5)	0.0137 (5)	0.0004 (4)	−0.0007 (4)	−0.0013 (4)
O4	0.0065 (5)	0.0123 (5)	0.0129 (5)	0.0013 (4)	0.0001 (4)	0.0010 (4)
O5	0.0328 (7)	0.0242 (7)	0.0209 (7)	−0.0155 (6)	0.0106 (6)	−0.0031 (6)
O6	0.0300 (7)	0.0164 (6)	0.0278 (7)	0.0033 (5)	0.0139 (6)	0.0046 (5)
O7	0.0589 (10)	0.0118 (6)	0.0418 (9)	−0.0076 (6)	0.0397 (8)	−0.0016 (6)
O8	0.0178 (6)	0.0292 (7)	0.0122 (6)	0.0078 (5)	0.0046 (5)	0.0029 (5)
O9	0.0129 (5)	0.0150 (5)	0.0146 (6)	0.0029 (4)	0.0029 (4)	0.0024 (5)
O10	0.0188 (6)	0.0181 (6)	0.0205 (6)	0.0040 (5)	0.0105 (5)	−0.0012 (5)
O11	0.0149 (5)	0.0119 (5)	0.0152 (6)	0.0010 (4)	0.0020 (5)	−0.0003 (5)
O12	0.0145 (5)	0.0112 (5)	0.0130 (5)	0.0008 (4)	0.0009 (4)	−0.0001 (4)
O13	0.0181 (6)	0.0232 (7)	0.0154 (6)	−0.0038 (5)	0.0000 (5)	−0.0078 (5)
N1	0.0129 (6)	0.0075 (6)	0.0094 (6)	−0.0014 (4)	0.0024 (5)	0.0000 (5)
N2	0.0128 (6)	0.0068 (6)	0.0157 (6)	−0.0005 (4)	0.0043 (5)	−0.0013 (5)
N3	0.0079 (5)	0.0102 (6)	0.0102 (6)	0.0001 (4)	0.0016 (4)	0.0000 (5)
N4	0.0077 (5)	0.0109 (6)	0.0106 (6)	0.0006 (4)	0.0028 (5)	0.0003 (5)
N5	0.0391 (9)	0.0081 (6)	0.0260 (8)	−0.0043 (6)	0.0216 (7)	−0.0035 (6)
N6	0.0121 (6)	0.0125 (6)	0.0148 (7)	0.0002 (5)	0.0048 (5)	0.0000 (5)
N7	0.0112 (6)	0.0152 (6)	0.0108 (6)	−0.0018 (5)	0.0031 (5)	−0.0029 (5)
C1	0.0107 (6)	0.0121 (7)	0.0146 (7)	0.0003 (5)	0.0022 (6)	−0.0003 (6)
C2	0.0119 (7)	0.0112 (7)	0.0146 (7)	0.0012 (5)	0.0017 (6)	−0.0009 (6)
C3	0.0137 (7)	0.0072 (6)	0.0107 (7)	−0.0007 (5)	0.0031 (5)	0.0000 (5)
C4	0.0113 (6)	0.0105 (7)	0.0149 (7)	−0.0007 (5)	0.0018 (6)	0.0007 (6)
C5	0.0120 (6)	0.0094 (7)	0.0137 (7)	0.0001 (5)	0.0021 (6)	0.0006 (6)
C6	0.0141 (7)	0.0111 (7)	0.0176 (8)	−0.0016 (5)	−0.0005 (6)	0.0007 (6)
C7	0.0157 (7)	0.0101 (7)	0.0152 (8)	−0.0006 (5)	−0.0001 (6)	0.0009 (6)
C8	0.0132 (7)	0.0077 (7)	0.0120 (7)	−0.0002 (5)	0.0037 (6)	−0.0009 (5)
C9	0.0135 (7)	0.0100 (7)	0.0186 (8)	0.0001 (5)	−0.0001 (6)	−0.0010 (6)
C10	0.0132 (7)	0.0095 (7)	0.0205 (8)	0.0013 (5)	−0.0006 (6)	0.0006 (6)
C11	0.0111 (6)	0.0084 (6)	0.0143 (7)	0.0001 (5)	0.0018 (6)	−0.0010 (6)
C12	0.0100 (6)	0.0097 (7)	0.0152 (7)	−0.0013 (5)	0.0019 (5)	−0.0015 (6)
C13	0.0086 (6)	0.0111 (7)	0.0100 (7)	−0.0006 (5)	0.0019 (5)	0.0004 (5)
C14	0.0113 (7)	0.0088 (7)	0.0151 (7)	0.0003 (5)	0.0015 (6)	0.0003 (6)
C15	0.0113 (7)	0.0082 (6)	0.0141 (7)	0.0000 (5)	0.0011 (6)	−0.0001 (6)
C16	0.0100 (6)	0.0099 (7)	0.0148 (7)	−0.0002 (5)	0.0027 (5)	0.0027 (6)
C17	0.0102 (6)	0.0097 (7)	0.0153 (7)	0.0004 (5)	0.0023 (6)	0.0027 (6)
C18	0.0084 (6)	0.0112 (7)	0.0106 (7)	−0.0001 (5)	0.0020 (5)	0.0000 (6)
C19	0.0107 (6)	0.0103 (7)	0.0127 (7)	−0.0008 (5)	0.0029 (5)	0.0003 (6)
C20	0.0113 (6)	0.0101 (7)	0.0131 (7)	0.0005 (5)	0.0029 (6)	0.0011 (6)

Geometric parameters (Å, º)

Pr1—O4^{i}	2.4554 (12)	C1—H1	0.9500
Pr1—O3	2.4558 (11)	C2—C3	1.400 (2)
Pr1—O2	2.5009 (12)	C2—H2	0.9500
Pr1—O1^{ii}	2.5360 (12)	C3—C4	1.399 (2)
Pr1—O5	2.5750 (13)	C3—C8	1.479 (2)
Pr1—O8	2.5832 (13)	C4—C5	1.377 (2)
Pr1—O11	2.6036 (12)	C4—H4	0.9500
Pr1—O12	2.6147 (12)	C5—H5	0.9500
Pr1—O9	2.6242 (13)	C6—C7	1.376 (2)
Pr1—O6	2.6443 (14)	C6—H6	0.9500
O1—N1	1.3261 (17)	C7—C8	1.401 (2)
O1—Pr1^{iii}	2.5360 (12)	C7—H7	0.9500
O2—N2	1.3337 (17)	C8—C9	1.393 (2)
O3—N3	1.3261 (16)	C9—C10	1.379 (2)
O4—N4	1.3300 (17)	C9—H9	0.9500
O4—Pr1^{iv}	2.4554 (12)	C10—H10	0.9500
O5—N5	1.268 (2)	C11—C12	1.381 (2)
O6—N5	1.261 (2)	C11—H11	0.9500
O7—N5	1.233 (2)	C12—C13	1.397 (2)
O8—N6	1.2782 (19)	C12—H12	0.9500
O9—N6	1.2646 (18)	C13—C14	1.392 (2)
O10—N6	1.2229 (18)	C13—C18	1.472 (2)
O11—N7	1.2620 (18)	C14—C15	1.375 (2)
O12—N7	1.2722 (18)	C14—H14	0.9500
O13—N7	1.2319 (18)	C15—H15	0.9500
N1—C5	1.352 (2)	C16—C17	1.373 (2)
N1—C1	1.355 (2)	C16—H16	0.9500
N2—C10	1.348 (2)	C17—C18	1.393 (2)
N2—C6	1.351 (2)	C17—H17	0.9500
N3—C15	1.352 (2)	C18—C19	1.399 (2)
N3—C11	1.353 (2)	C19—C20	1.377 (2)
N4—C20	1.349 (2)	C19—H19	0.9500
N4—C16	1.353 (2)	C20—H20	0.9500
C1—C2	1.380 (2)		

O4^{i}—Pr1—O3	106.95 (4)	O4—N4—C16	118.73 (13)
O4^{i}—Pr1—O2	68.60 (4)	C20—N4—C16	120.89 (14)
O3—Pr1—O2	75.79 (4)	O7—N5—O6	121.81 (18)
O4^{i}—Pr1—O1^{ii}	73.85 (4)	O7—N5—O5	120.86 (18)
O3—Pr1—O1^{ii}	69.44 (4)	O6—N5—O5	117.33 (15)
O2—Pr1—O1^{ii}	117.22 (4)	O7—N5—Pr1	168.42 (12)
O4^{i}—Pr1—O5	154.35 (4)	O6—N5—Pr1	60.94 (9)
O3—Pr1—O5	66.68 (4)	O5—N5—Pr1	57.81 (8)
O2—Pr1—O5	85.82 (5)	O10—N6—O9	122.44 (15)
O1^{ii}—Pr1—O5	122.36 (4)	O10—N6—O8	121.27 (14)
O4^{i}—Pr1—O8	133.11 (4)	O9—N6—O8	116.28 (14)

O3—Pr1—O8	82.56 (4)	O13—N7—O11	121.44 (14)
O2—Pr1—O8	153.82 (4)	O13—N7—O12	120.85 (14)
O1^{ii}—Pr1—O8	66.88 (4)	O11—N7—O12	117.70 (13)
O5—Pr1—O8	72.05 (5)	N1—C1—C2	120.45 (14)
O4^{i}—Pr1—O11	69.62 (4)	N1—C1—H1	119.8
O3—Pr1—O11	166.61 (4)	C2—C1—H1	119.8
O2—Pr1—O11	91.05 (4)	C1—C2—C3	120.60 (15)
O1^{ii}—Pr1—O11	120.17 (4)	C1—C2—H2	119.7
O5—Pr1—O11	110.48 (4)	C3—C2—H2	119.7
O8—Pr1—O11	109.43 (4)	C4—C3—C2	117.20 (14)
O4^{i}—Pr1—O12	69.86 (4)	C4—C3—C8	120.55 (14)
O3—Pr1—O12	143.04 (4)	C2—C3—C8	122.25 (14)
O2—Pr1—O12	130.35 (4)	C5—C4—C3	120.50 (14)
O1^{ii}—Pr1—O12	74.59 (4)	C5—C4—H4	119.8
O5—Pr1—O12	130.84 (4)	C3—C4—H4	119.8
O8—Pr1—O12	75.74 (4)	N1—C5—C4	120.79 (15)
O11—Pr1—O12	49.12 (4)	N1—C5—H5	119.6
O4^{i}—Pr1—O9	130.11 (4)	C4—C5—H5	119.6
O3—Pr1—O9	120.78 (4)	N2—C6—C7	120.78 (15)
O2—Pr1—O9	134.05 (4)	N2—C6—H6	119.6
O1^{ii}—Pr1—O9	108.67 (4)	C7—C6—H6	119.6
O5—Pr1—O9	67.21 (4)	C6—C7—C8	120.43 (15)
O8—Pr1—O9	49.00 (4)	C6—C7—H7	119.8
O11—Pr1—O9	66.91 (4)	C8—C7—H7	119.8
O12—Pr1—O9	63.63 (4)	C9—C8—C7	117.22 (14)
O4^{i}—Pr1—O6	115.98 (4)	C9—C8—C3	121.62 (14)
O3—Pr1—O6	106.61 (4)	C7—C8—C3	121.16 (14)
O2—Pr1—O6	69.19 (4)	C10—C9—C8	120.43 (15)
O1^{ii}—Pr1—O6	170.15 (4)	C10—C9—H9	119.8
O5—Pr1—O6	48.87 (5)	C8—C9—H9	119.8
O8—Pr1—O6	103.98 (4)	N2—C10—C9	120.93 (15)
O11—Pr1—O6	65.42 (4)	N2—C10—H10	119.5
O12—Pr1—O6	107.45 (4)	C9—C10—H10	119.5
O9—Pr1—O6	65.03 (4)	N3—C11—C12	120.32 (14)
O4^{i}—Pr1—N5	139.09 (4)	N3—C11—H11	119.8
O3—Pr1—N5	88.34 (4)	C12—C11—H11	119.8
O2—Pr1—N5	79.39 (4)	C11—C12—C13	120.37 (14)
O1^{ii}—Pr1—N5	146.01 (4)	C11—C12—H12	119.8
O5—Pr1—N5	24.63 (5)	C13—C12—H12	119.8
O8—Pr1—N5	85.53 (5)	C14—C13—C12	117.30 (14)
O11—Pr1—N5	86.73 (5)	C14—C13—C18	120.64 (14)
O12—Pr1—N5	118.82 (4)	C12—C13—C18	122.05 (14)
O9—Pr1—N5	60.42 (4)	C15—C14—C13	121.05 (15)
O6—Pr1—N5	24.63 (5)	C15—C14—H14	119.5
N1—O1—Pr1^{iii}	132.45 (9)	C13—C14—H14	119.5
N2—O2—Pr1	129.47 (9)	N3—C15—C14	120.09 (14)
N3—O3—Pr1	129.16 (9)	N3—C15—H15	120.0
N4—O4—Pr1^{iv}	134.06 (10)	C14—C15—H15	120.0

N5—O5—Pr1	97.56 (10)	N4—C16—C17	120.31 (14)
N5—O6—Pr1	94.43 (10)	N4—C16—H16	119.8
N6—O8—Pr1	97.84 (9)	C17—C16—H16	119.8
N6—O9—Pr1	96.25 (9)	C16—C17—C18	120.61 (15)
N7—O11—Pr1	97.00 (9)	C16—C17—H17	119.7
N7—O12—Pr1	96.18 (9)	C18—C17—H17	119.7
O1—N1—C5	119.07 (13)	C17—C18—C19	117.47 (14)
O1—N1—C1	120.46 (13)	C17—C18—C13	120.49 (14)
C5—N1—C1	120.42 (14)	C19—C18—C13	122.02 (14)
O2—N2—C10	120.08 (13)	C20—C19—C18	120.40 (15)
O2—N2—C6	119.67 (13)	C20—C19—H19	119.8
C10—N2—C6	120.20 (14)	C18—C19—H19	119.8
O3—N3—C15	119.46 (13)	N4—C20—C19	120.27 (15)
O3—N3—C11	119.65 (13)	N4—C20—H20	119.9
C15—N3—C11	120.82 (13)	C19—C20—H20	119.9
O4—N4—C20	120.28 (13)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O5^{v}	0.95	2.59	3.331 (2)	135
C4—H4···O13^{vi}	0.95	2.36	3.200 (2)	147
C5—H5···O4^{vii}	0.95	2.37	3.168 (2)	141
C9—H9···O9^{viii}	0.95	2.61	3.204 (2)	121
C9—H9···O10^{v}	0.95	2.58	3.468 (2)	156
C10—H10···O3	0.95	2.31	3.115 (2)	143
C10—H10···O7^{viii}	0.95	2.60	3.277 (3)	129
C11—H11···O10^{v}	0.95	2.50	3.239 (2)	135
C14—H14···O7^{ix}	0.95	2.22	3.002 (2)	139
C15—H15···O1^{ii}	0.95	2.31	3.0924 (19)	140
C16—H16···O13^{v}	0.95	2.56	3.154 (2)	121
C17—H17···O12^{v}	0.95	2.36	3.288 (2)	164
C20—H20···O2^{iv}	0.95	2.62	3.307 (2)	130

Symmetry codes: (ii) $x, y-1, z$; (iv) $x+1/2, -y+1/2, z+1/2$; (v) $-x+1/2, y+1/2, -z+3/2$; (vi) $-x, -y+1, -z+1$; (vii) $x-1/2, -y+3/2, z-1/2$; (viii) $x, -y+1, z+1/2$; (ix) $-x+1/2, y-1/2, -z+3/2$.

(III) Poly[[tris(nitrato-κ^2O,O')neodymium(III)]-bis(μ-4,4′-bipyridine N,N'-dioxide-$\kappa^2N:N'$}]

Crystal data

$[Nd(NO_3)_3(C_{10}H_8N_2O_2)_2]$
M_r = 706.64
Monoclinic, $C2/c$
a = 26.7422 (10) Å
b = 13.3035 (5) Å
c = 13.7804 (5) Å
β = 106.065 (1)°
V = 4711.1 (3) Å^3
Z = 8

$F(000)$ = 2792
D_x = 1.993 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8852 reflections
θ = 2.5–31.4°
μ = 2.29 mm^{-1}
T = 173 K
Block, yellow
0.14 × 0.12 × 0.08 mm

Data collection

Bruker D8 Quest CMOS diffractometer
Radiation source: I-mu-S microsource X-ray tube
Laterally graded multilayer (Goebel) mirror monochromator
ω and phi scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.682, T_{max} = 0.747
47148 measured reflections
8277 independent reflections
5419 reflections with $I > 2\sigma(I)$
R_{int} = 0.115
θ_{max} = 33.5°, θ_{min} = 2.2°
h = −38→39
k = −20→18
l = −21→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.067
S = 1.01
8277 reflections
370 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0161P)^2 + 13.5513P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.49 e Å^{-3}
$\Delta\rho_{min}$ = −1.29 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Nd1	0.12681 (2)	0.27502 (2)	0.66431 (2)	0.00728 (4)
O1	0.14904 (8)	1.13013 (15)	0.78718 (16)	0.0116 (5)
O2	0.07574 (8)	0.41599 (15)	0.70766 (16)	0.0130 (5)
O3	0.17968 (8)	0.33233 (15)	0.83003 (15)	0.0111 (4)
O4	0.54422 (8)	0.28373 (16)	1.18789 (15)	0.0104 (4)
O5	0.19319 (10)	0.40971 (18)	0.65362 (18)	0.0251 (6)
O6	0.12057 (10)	0.42656 (17)	0.53782 (19)	0.0236 (6)
O7	0.18928 (11)	0.50787 (17)	0.5251 (2)	0.0317 (7)
O8	0.21193 (9)	0.18587 (18)	0.66255 (16)	0.0190 (5)
O9	0.16865 (8)	0.24311 (15)	0.51655 (16)	0.0139 (5)
O10	0.23559 (9)	0.14500 (17)	0.52853 (17)	0.0187 (5)
O11	0.05854 (8)	0.25293 (15)	0.49154 (16)	0.0136 (5)
O12	0.09612 (8)	0.11469 (16)	0.55686 (16)	0.0120 (5)
O13	0.03619 (9)	0.11085 (17)	0.41220 (17)	0.0198 (5)
N1	0.14002 (10)	1.03179 (18)	0.77624 (18)	0.0092 (5)
N2	0.08697 (10)	0.51388 (19)	0.7183 (2)	0.0113 (6)
N3	0.23077 (10)	0.32610 (19)	0.87052 (18)	0.0094 (5)
N4	0.49563 (9)	0.28710 (19)	1.12926 (17)	0.0094 (5)
N5	0.16807 (13)	0.4492 (2)	0.5712 (2)	0.0228 (7)
N6	0.20618 (10)	0.19050 (19)	0.56738 (19)	0.0125 (6)
N7	0.06299 (10)	0.1590 (2)	0.48487 (19)	0.0124 (6)

C1	0.18004 (12)	0.9658 (2)	0.7982 (2)	0.0123 (6)
H1	0.2148	0.9899	0.8201	0.015*
C2	0.17080 (12)	0.8640 (2)	0.7892 (2)	0.0120 (6)
H2	0.1993	0.8185	0.8059	0.014*
C3	0.12022 (12)	0.8270 (2)	0.7557 (2)	0.0097 (6)
C4	0.07995 (12)	0.8974 (2)	0.7348 (2)	0.0117 (6)
H4	0.0449	0.8751	0.7123	0.014*
C5	0.09037 (12)	0.9987 (2)	0.7464 (2)	0.0121 (6)
H5	0.0625	1.0455	0.7334	0.015*
C6	0.05363 (13)	0.5813 (2)	0.6616 (2)	0.0144 (7)
H6	0.0230	0.5584	0.6133	0.017*
C7	0.06354 (12)	0.6827 (2)	0.6730 (2)	0.0137 (7)
H7	0.0396	0.7293	0.6329	0.016*
C8	0.10854 (11)	0.7181 (2)	0.7431 (2)	0.0099 (6)
C9	0.14192 (13)	0.6463 (2)	0.8007 (2)	0.0147 (7)
H9	0.1729	0.6671	0.8491	0.018*
C10	0.13017 (13)	0.5451 (2)	0.7879 (3)	0.0168 (7)
H10	0.1528	0.4970	0.8287	0.020*
C11	0.25859 (12)	0.4103 (2)	0.9057 (2)	0.0109 (6)
H11	0.2419	0.4740	0.8964	0.013*
C12	0.31067 (12)	0.4040 (2)	0.9544 (2)	0.0115 (6)
H12	0.3295	0.4633	0.9803	0.014*
C13	0.33621 (12)	0.3117 (2)	0.9664 (2)	0.0099 (6)
C14	0.30682 (11)	0.2278 (2)	0.9260 (2)	0.0111 (6)
H14	0.3232	0.1639	0.9307	0.013*
C15	0.25439 (12)	0.2359 (2)	0.8795 (2)	0.0117 (6)
H15	0.2348	0.1776	0.8536	0.014*
C16	0.47655 (12)	0.3749 (2)	1.0850 (2)	0.0118 (6)
H16	0.4989	0.4314	1.0915	0.014*
C17	0.42538 (12)	0.3837 (2)	1.0310 (2)	0.0115 (6)
H17	0.4126	0.4459	1.0002	0.014*
C18	0.39187 (12)	0.3015 (2)	1.0209 (2)	0.0101 (6)
C19	0.41335 (12)	0.2105 (2)	1.0646 (2)	0.0113 (6)
H19	0.3920	0.1522	1.0570	0.014*
C20	0.46497 (12)	0.2047 (2)	1.1181 (2)	0.0109 (6)
H20	0.4791	0.1426	1.1474	0.013*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00565 (7)	0.00592 (7)	0.00960 (7)	−0.00075 (8)	0.00098 (5)	−0.00046 (8)
O1	0.0140 (12)	0.0039 (10)	0.0155 (11)	−0.0026 (9)	0.0018 (9)	0.0000 (9)
O2	0.0142 (12)	0.0030 (10)	0.0215 (12)	−0.0035 (9)	0.0046 (10)	−0.0026 (9)
O3	0.0036 (10)	0.0125 (11)	0.0143 (11)	0.0003 (9)	−0.0023 (9)	−0.0010 (9)
O4	0.0050 (10)	0.0122 (11)	0.0121 (10)	0.0010 (9)	−0.0009 (8)	−0.0004 (9)
O5	0.0326 (16)	0.0244 (14)	0.0197 (13)	−0.0162 (12)	0.0095 (12)	−0.0016 (11)
O6	0.0301 (16)	0.0144 (12)	0.0295 (14)	0.0025 (11)	0.0136 (12)	0.0065 (11)
O7	0.060 (2)	0.0106 (12)	0.0401 (16)	−0.0062 (12)	0.0397 (16)	0.0002 (12)

O8	0.0165 (13)	0.0297 (14)	0.0104 (11)	0.0076 (11)	0.0032 (10)	0.0031 (10)
O9	0.0118 (11)	0.0138 (12)	0.0155 (11)	0.0024 (9)	0.0028 (9)	0.0025 (9)
O10	0.0190 (13)	0.0168 (12)	0.0236 (13)	0.0047 (10)	0.0115 (11)	−0.0020 (10)
O11	0.0140 (11)	0.0103 (12)	0.0153 (11)	0.0011 (8)	0.0021 (9)	0.0004 (8)
O12	0.0122 (12)	0.0097 (11)	0.0117 (11)	0.0000 (9)	−0.0007 (9)	−0.0002 (9)
O13	0.0160 (13)	0.0240 (13)	0.0159 (12)	−0.0041 (10)	−0.0014 (10)	−0.0109 (10)
N1	0.0105 (14)	0.0081 (13)	0.0081 (12)	−0.0017 (10)	0.0013 (11)	−0.0009 (10)
N2	0.0123 (14)	0.0068 (13)	0.0164 (14)	−0.0004 (11)	0.0064 (12)	−0.0015 (11)
N3	0.0085 (13)	0.0107 (13)	0.0076 (12)	0.0021 (11)	−0.0002 (10)	−0.0008 (10)
N4	0.0082 (12)	0.0122 (13)	0.0074 (11)	0.0004 (11)	0.0017 (10)	−0.0018 (10)
N5	0.040 (2)	0.0092 (14)	0.0285 (17)	−0.0060 (14)	0.0242 (16)	−0.0043 (13)
N6	0.0126 (14)	0.0106 (13)	0.0145 (13)	−0.0015 (11)	0.0042 (11)	−0.0008 (11)
N7	0.0104 (14)	0.0132 (14)	0.0144 (13)	−0.0016 (11)	0.0045 (11)	−0.0036 (11)
C1	0.0098 (16)	0.0119 (16)	0.0146 (15)	−0.0011 (13)	0.0021 (13)	−0.0001 (13)
C2	0.0117 (16)	0.0104 (15)	0.0131 (15)	0.0023 (13)	0.0022 (13)	−0.0014 (12)
C3	0.0124 (16)	0.0084 (15)	0.0081 (14)	0.0005 (13)	0.0023 (12)	0.0018 (12)
C4	0.0089 (16)	0.0103 (15)	0.0138 (15)	−0.0004 (12)	−0.0005 (13)	0.0022 (13)
C5	0.0103 (16)	0.0113 (16)	0.0149 (16)	0.0014 (13)	0.0037 (13)	0.0013 (13)
C6	0.0125 (17)	0.0115 (16)	0.0156 (16)	−0.0009 (13)	−0.0021 (13)	0.0002 (13)
C7	0.0120 (16)	0.0099 (15)	0.0156 (16)	0.0010 (13)	−0.0021 (13)	0.0007 (13)
C8	0.0111 (15)	0.0071 (14)	0.0123 (14)	0.0015 (13)	0.0044 (12)	−0.0008 (13)
C9	0.0114 (16)	0.0114 (16)	0.0186 (17)	0.0010 (13)	−0.0004 (14)	−0.0016 (13)
C10	0.0122 (17)	0.0132 (16)	0.0218 (18)	0.0042 (13)	−0.0007 (14)	−0.0001 (14)
C11	0.0112 (16)	0.0071 (15)	0.0138 (15)	−0.0001 (12)	0.0023 (13)	−0.0019 (12)
C12	0.0090 (16)	0.0102 (15)	0.0145 (15)	−0.0021 (12)	0.0019 (13)	−0.0029 (13)
C13	0.0100 (15)	0.0119 (15)	0.0082 (14)	−0.0005 (12)	0.0032 (12)	−0.0004 (12)
C14	0.0103 (14)	0.0093 (14)	0.0133 (14)	0.0008 (14)	0.0024 (12)	0.0004 (14)
C15	0.0136 (15)	0.0074 (14)	0.0129 (14)	−0.0027 (13)	0.0018 (12)	−0.0020 (13)
C16	0.0114 (16)	0.0095 (15)	0.0148 (15)	−0.0003 (12)	0.0039 (13)	0.0032 (13)
C17	0.0100 (16)	0.0099 (15)	0.0141 (15)	0.0021 (12)	0.0026 (13)	0.0012 (12)
C18	0.0096 (15)	0.0126 (16)	0.0094 (14)	0.0022 (12)	0.0049 (12)	0.0001 (12)
C19	0.0113 (15)	0.0098 (16)	0.0135 (14)	−0.0017 (12)	0.0044 (12)	−0.0007 (12)
C20	0.0135 (16)	0.0085 (16)	0.0113 (14)	−0.0001 (12)	0.0041 (13)	0.0002 (11)

Geometric parameters (Å, º)

Nd1—O4^{i}	2.448 (2)	C1—H1	0.9500
Nd1—O3	2.451 (2)	C2—C3	1.393 (4)
Nd1—O2	2.488 (2)	C2—H2	0.9500
Nd1—O1^{ii}	2.526 (2)	C3—C4	1.396 (4)
Nd1—O5	2.555 (2)	C3—C8	1.482 (4)
Nd1—O8	2.573 (2)	C4—C5	1.376 (4)
Nd1—O11	2.585 (2)	C4—H4	0.9500
Nd1—O12	2.597 (2)	C5—H5	0.9500
Nd1—O9	2.615 (2)	C6—C7	1.377 (4)
Nd1—O6	2.640 (2)	C6—H6	0.9500
O1—N1	1.331 (3)	C7—C8	1.399 (4)
O1—Nd1^{iii}	2.526 (2)	C7—H7	0.9500

O2—N2	1.335 (3)	C8—C9	1.396 (4)
O3—N3	1.328 (3)	C9—C10	1.383 (4)
O4—N4	1.328 (3)	C9—H9	0.9500
O4—Nd1^{iv}	2.448 (2)	C10—H10	0.9500
O5—N5	1.263 (4)	C11—C12	1.371 (4)
O6—N5	1.262 (4)	C11—H11	0.9500
O7—N5	1.238 (3)	C12—C13	1.393 (4)
O8—N6	1.279 (3)	C12—H12	0.9500
O9—N6	1.264 (3)	C13—C14	1.389 (4)
O10—N6	1.227 (3)	C13—C18	1.476 (4)
O11—N7	1.261 (3)	C14—C15	1.375 (4)
O12—N7	1.277 (3)	C14—H14	0.9500
O13—N7	1.237 (3)	C15—H15	0.9500
N1—C5	1.351 (4)	C16—C17	1.370 (4)
N1—C1	1.352 (4)	C16—H16	0.9500
N2—C10	1.347 (4)	C17—C18	1.395 (4)
N2—C6	1.350 (4)	C17—H17	0.9500
N3—C15	1.346 (4)	C18—C19	1.403 (4)
N3—C11	1.358 (4)	C19—C20	1.376 (4)
N4—C16	1.351 (4)	C19—H19	0.9500
N4—C20	1.352 (4)	C20—H20	0.9500
C1—C2	1.375 (4)		

O4^{i}—Nd1—O3	106.54 (7)	O4—N4—C20	120.2 (2)
O4^{i}—Nd1—O2	68.50 (7)	C16—N4—C20	120.6 (3)
O3—Nd1—O2	75.84 (7)	O7—N5—O6	121.4 (3)
O4^{i}—Nd1—O1^{ii}	73.79 (7)	O7—N5—O5	121.2 (3)
O3—Nd1—O1^{ii}	69.19 (7)	O6—N5—O5	117.4 (3)
O2—Nd1—O1^{ii}	117.21 (7)	O7—N5—Nd1	168.5 (2)
O4^{i}—Nd1—O5	153.95 (8)	O6—N5—Nd1	61.29 (16)
O3—Nd1—O5	66.72 (7)	O5—N5—Nd1	57.42 (15)
O2—Nd1—O5	85.50 (8)	O10—N6—O9	122.5 (3)
O1^{ii}—Nd1—O5	122.38 (8)	O10—N6—O8	120.9 (3)
O4^{i}—Nd1—O8	133.41 (7)	O9—N6—O8	116.5 (2)
O3—Nd1—O8	82.44 (7)	O13—N7—O11	121.8 (3)
O2—Nd1—O8	153.59 (7)	O13—N7—O12	120.8 (3)
O1^{ii}—Nd1—O8	67.03 (7)	O11—N7—O12	117.4 (2)
O5—Nd1—O8	72.07 (8)	N1—C1—C2	120.5 (3)
O4^{i}—Nd1—O11	69.68 (7)	N1—C1—H1	119.7
O3—Nd1—O11	166.35 (6)	C2—C1—H1	119.7
O2—Nd1—O11	90.70 (7)	C1—C2—C3	120.8 (3)
O1^{ii}—Nd1—O11	120.39 (6)	C1—C2—H2	119.6
O5—Nd1—O11	110.58 (7)	C3—C2—H2	119.6
O8—Nd1—O11	109.88 (7)	C2—C3—C4	117.0 (3)
O4^{i}—Nd1—O12	70.06 (7)	C2—C3—C8	122.6 (3)
O3—Nd1—O12	142.80 (7)	C4—C3—C8	120.4 (3)
O2—Nd1—O12	130.40 (7)	C5—C4—C3	120.9 (3)
O1^{ii}—Nd1—O12	74.57 (6)	C5—C4—H4	119.6

O5—Nd1—O12	131.16 (7)	C3—C4—H4	119.6
O8—Nd1—O12	75.92 (7)	N1—C5—C4	120.4 (3)
O11—Nd1—O12	49.47 (6)	N1—C5—H5	119.8
O4^{i}—Nd1—O9	130.37 (7)	C4—C5—H5	119.8
O3—Nd1—O9	121.01 (7)	N2—C6—C7	120.6 (3)
O2—Nd1—O9	133.70 (7)	N2—C6—H6	119.7
O1^{ii}—Nd1—O9	109.03 (7)	C7—C6—H6	119.7
O5—Nd1—O9	67.36 (7)	C6—C7—C8	120.7 (3)
O8—Nd1—O9	49.27 (7)	C6—C7—H7	119.7
O11—Nd1—O9	67.02 (7)	C8—C7—H7	119.7
O12—Nd1—O9	63.80 (7)	C9—C8—C7	117.1 (3)
O4^{i}—Nd1—O6	115.92 (7)	C9—C8—C3	121.4 (3)
O3—Nd1—O6	107.00 (7)	C7—C8—C3	121.5 (3)
O2—Nd1—O6	69.17 (7)	C10—C9—C8	120.5 (3)
O1^{ii}—Nd1—O6	170.26 (7)	C10—C9—H9	119.8
O5—Nd1—O6	49.03 (8)	C8—C9—H9	119.8
O8—Nd1—O6	103.89 (7)	N2—C10—C9	120.7 (3)
O11—Nd1—O6	65.12 (7)	N2—C10—H10	119.6
O12—Nd1—O6	107.37 (7)	C9—C10—H10	119.6
O9—Nd1—O6	64.68 (7)	N3—C11—C12	120.4 (3)
O4^{i}—Nd1—N5	139.01 (8)	N3—C11—H11	119.8
O3—Nd1—N5	88.42 (8)	C12—C11—H11	119.8
O2—Nd1—N5	79.15 (7)	C11—C12—C13	120.7 (3)
O1^{ii}—Nd1—N5	146.02 (8)	C11—C12—H12	119.7
O5—Nd1—N5	24.61 (8)	C13—C12—H12	119.7
O8—Nd1—N5	85.48 (8)	C14—C13—C12	117.2 (3)
O11—Nd1—N5	86.77 (8)	C14—C13—C18	120.6 (3)
O12—Nd1—N5	119.07 (7)	C12—C13—C18	122.2 (3)
O9—Nd1—N5	60.38 (7)	C15—C14—C13	121.0 (3)
O6—Nd1—N5	24.79 (8)	C15—C14—H14	119.5
N1—O1—Nd1^{iii}	132.26 (17)	C13—C14—H14	119.5
N2—O2—Nd1	129.77 (17)	N3—C15—C14	120.3 (3)
N3—O3—Nd1	129.30 (16)	N3—C15—H15	119.8
N4—O4—Nd1^{iv}	134.20 (16)	C14—C15—H15	119.8
N5—O5—Nd1	97.97 (19)	N4—C16—C17	120.9 (3)
N5—O6—Nd1	93.92 (19)	N4—C16—H16	119.5
N6—O8—Nd1	97.58 (17)	C17—C16—H16	119.5
N6—O9—Nd1	95.95 (16)	C16—C17—C18	120.3 (3)
N7—O11—Nd1	97.07 (17)	C16—C17—H17	119.8
N7—O12—Nd1	96.06 (16)	C18—C17—H17	119.8
O1—N1—C5	119.2 (2)	C17—C18—C19	117.3 (3)
O1—N1—C1	120.4 (2)	C17—C18—C13	120.5 (3)
C5—N1—C1	120.4 (3)	C19—C18—C13	122.2 (3)
O2—N2—C10	120.1 (3)	C20—C19—C18	120.6 (3)
O2—N2—C6	119.4 (3)	C20—C19—H19	119.7
C10—N2—C6	120.4 (3)	C18—C19—H19	119.7
O3—N3—C15	119.8 (2)	N4—C20—C19	120.2 (3)
O3—N3—C11	119.8 (2)	N4—C20—H20	119.9

C15—N3—C11	120.4 (3)	C19—C20—H20	119.9
O4—N4—C16	119.2 (2)		
Nd1—O3—O4—Nd1^{iv}	4.87 (14)	Nd1—O2—O1—Nd1^{iii}	91.75 (11)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O5^{v}	0.95	2.61	3.353 (4)	135
C4—H4···O13^{vi}	0.95	2.37	3.206 (4)	147
C5—H5···O4^{vii}	0.95	2.37	3.163 (4)	141
C9—H9···O9^{viii}	0.95	2.63	3.216 (4)	121
C9—H9···O10^{v}	0.95	2.58	3.464 (4)	156
C10—H10···O3	0.95	2.30	3.110 (4)	142
C10—H10···O7^{viii}	0.95	2.61	3.289 (4)	129
C11—H11···O10^{v}	0.95	2.50	3.243 (4)	135
C14—H14···O7^{ix}	0.95	2.21	2.998 (4)	139
C15—H15···O1^{ii}	0.95	2.31	3.091 (4)	139
C16—H16···O13^{v}	0.95	2.56	3.159 (4)	121
C17—H17···O12^{v}	0.95	2.37	3.295 (4)	165
C20—H20···O2^{iv}	0.95	2.61	3.294 (4)	130

Symmetry codes: (ii) *x*, *y*−1, *z*; (iv) *x*+1/2, −*y*+1/2, *z*+1/2; (v) −*x*+1/2, *y*+1/2, −*z*+3/2; (vi) −*x*, −*y*+1, −*z*+1; (vii) *x*−1/2, −*y*+3/2, *z*−1/2; (viii) *x*, −*y*+1, *z*+1/2; (ix) −*x*+1/2, *y*−1/2, −*z*+3/2.