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Tris(piperazinediium) bis[tris(pyridine-2,6-dicarboxylato)neodymate(III)] 15.33-hydrate

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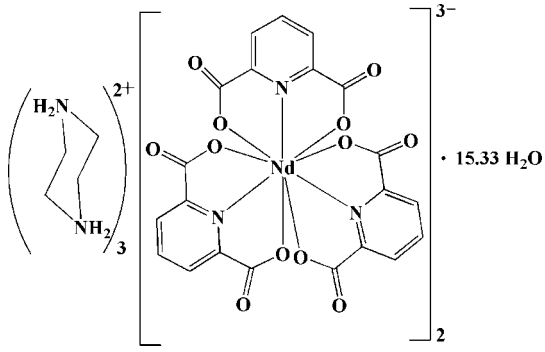
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.064; wR factor = 0.199; data-to-parameter ratio = 17.9.

The title compound, $(C_4H_{12}N_2)_3[Nd(C_7H_3NO_4)_3]_2\cdot 15.33H_2O$ or $(pipzH_2)_3[Nd(pydc)_3]_2\cdot 15.33H_2O$ (in which pipz is piperazine and $pydcH_2$ is pyridine-2,6-dicarboxylic acid), was synthesized by the reaction of $NdCl_3\cdot 6H_2O$ with the proton-transfer compound $(pipzH_2)(pydc)$ in aqueous solution. The nine donor atoms of the three $pydc^{2-}$ ligands form a distorted tricapped trigonal–prismatic arrangement around the Nd^{III} center. Considerable C—O$\cdots\pi$ stacking interactions between CO groups of carboxylate fragments and aromatic rings of $pydc^{2-}$ with distances of 3.135 (5)–3.255 (5) Å are observed. In the crystal structure, a wide range of hydrogen-bonding [of the types O—H$\cdots$O, N—H$\cdots$O and C—H$\cdots$O, with $D\cdots A$ distances ranging from 2.608 (10) to 3.278 (7) Å], ion-pairing and C—O$\cdots\pi$ stacking interactions connect the various components into a supramolecular structure. There is a high degree of solvent disorder in the structure; the occupancies of five water molecules refined to 0.6, 0.5, 0.4, 0.25 and 0.25.

Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki, Ghadermazi *et al.* (2007); Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.* (2007); Aghabozorg, Daneshvar *et al.* (2007). For synthesis, see: Aghabozorg *et al.* (2006).



Experimental

Crystal data

$(C_4H_{12}N_2)_3[Nd(C_7H_3NO_4)_3]_2\cdot 15.33H_2O$
M_r = 915.24
Trigonal, $P\overline{3}$
a = 25.5045 (9) Å
c = 10.0984 (7) Å
V = 5688.7 (5) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 1.46 mm^{-1}
T = 100 (2) K
0.49 × 0.18 × 0.08 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.536, T_{max} = 0.892
64426 measured reflections
9135 independent reflections
7444 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.198
S = 1.02
9135 reflections
509 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 4.81 e Å^{-3}
$\Delta\rho_{min}$ = −2.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O3	2.465 (4)	Nd1—O11	2.487 (4)
Nd1—O7	2.467 (4)	Nd1—N2	2.565 (4)
Nd1—O5	2.483 (4)	Nd1—N1	2.568 (4)
Nd1—O1	2.482 (4)	Nd1—N3	2.575 (4)
Nd1—O9	2.485 (4)		
N2—Nd1—N1	118.22 (12)	N1—Nd1—N3	120.15 (12)
N2—Nd1—N3	121.23 (12)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2*S*—H3$\cdots$O4	0.92	1.97	2.804 (6)	151
N2*S*—H4$\cdots$O6^{i}	0.92	1.92	2.760 (6)	151
N3*S*—H5$\cdots$O10^{ii}	0.92	1.95	2.780 (6)	150
N3*S*—H6$\cdots$O8^{iii}	0.92	1.99	2.836 (6)	153
N1*S*—H1$\cdots$O2^{iv}	0.92	1.92	2.758 (6)	150
N1*S*—H2$\cdots$O12^{v}	0.92	2.03	2.874 (6)	153
O1*W*—H7$\cdots$O9^{ii}	0.85	2.03	2.863 (7)	167
O1*W*—H8$\cdots$O9*W*^{vi}	0.85	2.00	2.838 (17)	166
O2*W*—H9$\cdots$O1^{iv}	0.85	2.43	3.278 (7)	180
O2*W*—H10$\cdots$O1*W*^{ii}	0.85	2.17	3.024 (8)	180
O3*W*—H11$\cdots$O5^{i}	0.85	2.14	2.970 (7)	167
O3*W*—H12$\cdots$O6*W*^{i}	0.85	2.11	2.950 (11)	171
O4*W*—H13$\cdots$O1^{iv}	0.85	2.04	2.878 (7)	166

  doi:10.1107/S1600536807068328

D—H···A	D—H	H···A	D···A	D—H···A
O4W—H14···O8W^{iv}	0.85	2.17	2.985 (14)	162
O5W—H15···O4^{vii}	0.85	1.82	2.674 (6)	180
O5W—H16···O6W^{viii}	0.85	1.95	2.804 (9)	179
O6W—H17···O10W	0.85	2.13	2.972 (10)	174
O6W—H18···O12^{vii}	0.85	2.16	3.011 (10)	180
O7W—H19···O8^{vii}	0.85	1.76	2.608 (10)	179
O7W—H20···O7W^{ix}	0.85	1.95	2.797 (11)	177
O8W—H21···O5W	0.85	1.99	2.787 (12)	156
O8W—H22···O5W^{x}	0.85	1.87	2.723 (11)	180
O9W—H23···O8^{xi}	0.85	2.29	3.136 (18)	179
O9W—H24···O7W	0.85	1.92	2.765 (20)	179
C3S—H3Sc···O10^{ii}	0.99	2.49	3.200 (8)	129
C4S—H4SB···O6^{i}	0.99	2.47	3.179 (8)	128
C4S—H4SB···O7^{iii}	0.99	2.51	3.076 (9)	116
C5S—H5SA···O6^{i}	0.99	2.46	3.180 (8)	129
C6S—H6SB···O3	0.99	2.52	3.092 (8)	116
C6S—H6SB···O10^{ii}	0.99	2.45	3.169 (7)	129
C1S—H1SC···O2^{xii}	0.99	2.43	3.151 (7)	129
C2S—H2SB···O11^{v}	0.99	2.55	3.112 (8)	116
C2S—H2SB···O2^{xii}	0.99	2.49	3.194 (7)	128

Symmetry codes: (i) $x, y, z-1$; (ii) $x-y, x, -z+1$; (iii) $x-y, x, -z$; (iv) $-y, x-y, z$; (v) $-y, x-y, z+1$; (vi) $-x+y+1, -x+1, z-1$; (vii) $-x+1, -y, -z+1$; (viii) $-x+1, -y, -z+2$; (ix) $y+1, -x+y+1, -z+2$; (x) $-y, x-y-1, z$; (xi) $-x+y+1, -x, z+1$; (xii) $y, -x+y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2054).

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supplementary materials

Acta Cryst. (2008). E**64**, m350-m351 [**doi:10.1107/S1600536807068328**]

Tris(piperazinediium) bis[tris(pyridine-2,6-dicarboxylato)neodymate(III)] 15.33-hydrate

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Comment

Recently, we have defined a plan to prepare water soluble proton transfer compounds as novel self assembled systems that can function as suitable ligands in the synthesis of metal complexes. In this regard, we have reported cases in which proton transfers from pyridine-2,6-dicarboxylic acid, $pydcH_2$, and benzene-1,2,4,5-tetracarboxylicacid, $btcH_4$, to propane-1,3-diamine (pn) and 1,10-phenanthroline, (phen), resulted in the formation of novel self-assembled $(pnH_2)(pydc).(pydcH_2)\cdot 2.5H_2O$, $(pnH_2)_2(btc)\cdot 2H_2O$ and $(phenH)_4(btcH_3)_2(btcH_2)$ systems, respectively. The resulting compounds with some remaining sites as electron donors can coordinate to metallic ions (Aghabozorg, Attar Gharamaleki, Ghadermazi *et al.*, 2007; Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.*, 2007; Aghabozorg, Daneshvar *et al.*, 2007, and references therein).

Here, we report on the synthesis and X-ray crystal structure of the title compound. The molecular structure of the title compound (I) is presented in Fig. 1. Selected bond lengths and angles of the structure (I) are presented in Table 1. Hydrogen bond lengths are given separately in Table 2.

In structure (I), Nd^{III} is coordinated by three $(pydc)^{2-}$ groups as tridentate ligands and a nine coordinated complex results. For balancing the anionic complex, protonated piperazine, $(pipzH_2)^{2+}$, exists. The sum of bond angles, N1—Nd1—N2, N1—Nd1—N3 and N2—Nd1—N3 equals to 359.60 (12)° and indicates that Nd1 is located in the center of N1N2N3 plane. The three O atoms O1, O5 and O9 form a triangle and the other three, O3, O7 and O11 form another triangle around the Nd^{III}. So a distorted tricapped prism polyhedron is proposed.

Moreover, there are uncoordinated water molecules which are involved in the formation of hydrogen bonds. These water molecules form six members cyclic rings with acyclic side chains water clusters (Fig. 2).

A noticeable feature of the title compound is the presence of C—O···π stacking interactions between CO group of carboxylates with aromatic rings of $(pydc)^{2-}$ units. The C—O···π distances (measured to the center of phenyl ring) are 3.134 (5) Å for C6—O2···*Cg*1 (1 + *x*, *y*, *z*), 3.245 (5) for C21—O10···*Cg*2 (*x, y, z*) and 3.255 (5) Å for C13—O6···*Cg*3, [*Cg*1, *Cg*2 and *Cg*3 are the centroids of N1/C1—C5, N2/C8—C12 and N3/C15—C19 rings, respectively] (Fig. 3).

In the crystal structure, a wide range of non-covalent interactions consisting of hydrogen bonding (of the type O—H···O, N—H···O and C—H···O with D···A ranging from 2.608 (10) to 3.278 (7) Å, ion pairing and C—O···π stacking connect the various components into a supramolecular structure (Table 2, Fig. 4).

Experimental

The proton transfer compound of $(pipzH_2)(pydc)$ was prepared according to our reported procedure (Aghabozorg *et al.*, 2006). A solution of $NdCl_3\cdot 6H_2O$ (320 mg, 1 mmol) in water (15 ml) was added to a solution of a solution of proton transfer

compound ($pipzH_2$)(pydc) (500 mg, 2 mmol) in water (10 ml) in a 1:2 molar ratio. Colorless crystals of (I) suitable for X-ray characterization were obtained after a few days at room temperature.

Refinement

There is a high positive residual density of 4.81 e $Å^{-3}$ at 0.63 Å near the Nd1 center due to considerable absorption effects which could not be completely corrected.

There is a high solvent disorder in the structure. Occupancies of water molecules O7W, O8W, O9W, O10W and O11W were found out by refinement of occupation factors for this molecules as free variables and are equal to 0.6, 1/2, 0.4, 0.25 and 1/4, respectively.

The hydrogen atoms positions on carbon atoms were found geometrically. The hydrogen atoms on ordered water molecules and nitrogen atoms were found from difference Fourier maps, and for disordered water molecules were not located. All hydrogen atoms were treated in riding model with the U_{iso}(H) parameters equal to 1.2 U_{eq}(C), 1.2 U_{eq}(N) and 1.5 U_{eq}(O) where U_{eq}(C), U_{eq}(N) and U_{eq}(O) are the equivalent thermal parameters of the atoms to which corresponding H atoms are bonded.

Figures

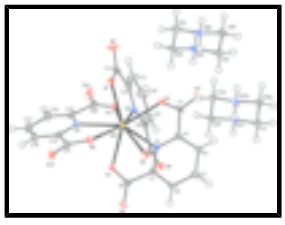


Fig. 1. The molecular structure of (I), displacement ellipsoids are drawn at the 50% probability level. Water molecules are omitted for clarity.

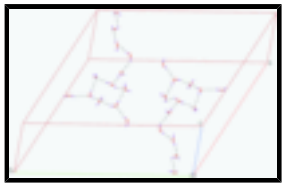


Fig. 2. C—O···π stacking interactions between CO groups of carboxylates with aromatic rings of $(pydc)^{2-}$ units. The C—O···π distances (measured to the center of phenyl ring) are 3.134 (5) Å for C6—O2···*Cg*1 (1 + *x*, *y*, *z*), 3.245 (5) Å for C21—O10···*Cg*2 (*x*, *y*, *z*) and 3.255 (5) Å for C13—O6···*Cg*3, [*Cg*1, *Cg*2 and *Cg*3 are the centroids of N1/C1—C5, N2/C8—C12 and N3/C15—C19 rings, respectively].

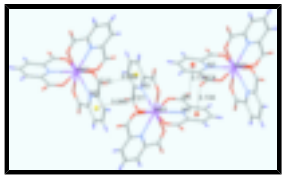


Fig. 3. Six membrane cyclic rings with acyclic side chains water clusters in the compound (I).

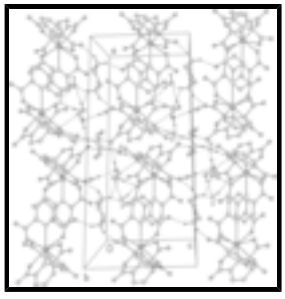


Fig. 4. The crystal packing of the compound (I), hydrogen bonds are shown as dashed lines.

Tris(piperazinediium) bis[tris(pyridine-2,6-dicarboxylato)neodymiumate(III)] 15.33-hydrate

Crystal data

$(C_4H_{12}N_2)_3[Nd(C_7H_3NO_4)_3]_2{\cdot}15.33H_2O$	$Z = 6$
$M_r = 915.24$	$F_{000} = 2798$
Trigonal, $P\bar{3}$	$D_x = 1.603$ Mg m^{-3}
Hall symbol: -P 3	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 25.5045$ (9) Å	Cell parameters from 9656 reflections
$b = 25.5045$ (9) Å	$\theta = 2.6$–31.5º
$c = 10.0984$ (7) Å	$\mu = 1.46$ mm^{-1}
$\alpha = 90$º	$T = 100$ (2) K
$\beta = 90$º	Prism, pink
$\gamma = 120$º	0.49 × 0.18 × 0.08 mm
$V = 5688.7$ (5) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	9135 independent reflections
Radiation source: fine-focus sealed tube	7444 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.055$
$T = 100$(2) K	$\theta_{max} = 28.0$º
ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -33\rightarrow33$
$T_{min} = 0.536$, $T_{max} = 0.892$	$k = -33\rightarrow33$
64426 measured reflections	$l = -13\rightarrow13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.063$	H-atom parameters constrained
$wR(F^2) = 0.198$	$w = 1/[\sigma^2(F_o^2) + (0.12P)^2 + 36P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
9135 reflections	$\Delta\rho_{max} = 4.81$ e Å^{-3}
509 parameters	$\Delta\rho_{min} = -2.19$ e Å^{-3}
18 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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Nd1	0.331570 (11)	−0.005899 (11)	0.42662 (3)	0.01072 (12)	
O1	0.38216 (18)	−0.03403 (16)	0.5997 (4)	0.0180 (8)	
O2	0.46277 (18)	−0.01274 (17)	0.7241 (4)	0.0169 (8)	
O3	0.38330 (17)	0.07347 (16)	0.2577 (4)	0.0148 (7)	
O4	0.46472 (18)	0.14173 (18)	0.1487 (4)	0.0186 (8)	
O5	0.36067 (18)	0.07296 (17)	0.5999 (4)	0.0172 (8)	
O6	0.3421 (2)	0.13558 (18)	0.7208 (4)	0.0222 (9)	
O7	0.25222 (18)	−0.03294 (16)	0.2577 (4)	0.0165 (8)	
O8	0.1863 (2)	−0.0172 (2)	0.1468 (4)	0.0303 (11)	
O9	0.25092 (18)	−0.05731 (17)	0.5959 (4)	0.0178 (8)	
O10	0.1930 (2)	−0.13711 (18)	0.7233 (4)	0.0234 (9)	
O11	0.36004 (17)	−0.05794 (17)	0.2571 (4)	0.0162 (7)	
O12	0.3501 (2)	−0.13946 (19)	0.1546 (4)	0.0297 (10)	
N1	0.4476 (2)	0.05714 (18)	0.4369 (4)	0.0114 (8)	
N2	0.2714 (2)	0.05001 (18)	0.4347 (4)	0.0133 (8)	
N3	0.27787 (19)	−0.12230 (19)	0.4359 (4)	0.0126 (8)	
C1	0.4768 (2)	0.0497 (2)	0.5382 (5)	0.0132 (9)	
C2	0.5381 (2)	0.0882 (2)	0.5601 (5)	0.0158 (10)	
H2A	0.5577	0.0822	0.6338	0.019*	
C3	0.5706 (3)	0.1360 (3)	0.4715 (6)	0.0195 (11)	
H3A	0.6125	0.1633	0.4843	0.023*	
C4	0.5401 (2)	0.1427 (2)	0.3642 (5)	0.0170 (10)	
H4A	0.5610	0.1741	0.3013	0.020*	
C5	0.4785 (2)	0.1026 (2)	0.3516 (5)	0.0126 (9)	
C6	0.4374 (3)	−0.0035 (2)	0.6287 (5)	0.0144 (10)	
C7	0.4391 (2)	0.1062 (2)	0.2437 (5)	0.0126 (9)	
C8	0.2805 (3)	0.0888 (2)	0.5331 (5)	0.0159 (10)	
C9	0.2451 (3)	0.1149 (3)	0.5509 (6)	0.0232 (12)	
H9A	0.2520	0.1415	0.6229	0.028*	
C10	0.1985 (3)	0.1010 (3)	0.4598 (6)	0.0268 (13)	
H10A	0.1731	0.1181	0.4688	0.032*	
C11	0.1901 (3)	0.0619 (3)	0.3566 (6)	0.0242 (12)	
H11A	0.1592	0.0523	0.2928	0.029*	

C12	0.2269 (3)	0.0370 (2)	0.3475 (5)	0.0164 (10)
C13	0.3317 (3)	0.1005 (2)	0.6274 (5)	0.0160 (10)
C14	0.2214 (3)	−0.0082 (2)	0.2421 (5)	0.0185 (11)
C15	0.2920 (2)	−0.1530 (2)	0.3489 (5)	0.0150 (10)
C16	0.2680 (3)	−0.2154 (2)	0.3588 (6)	0.0207 (11)
H16A	0.2778	−0.2366	0.2954	0.025*
C17	0.2292 (3)	−0.2458 (2)	0.4636 (6)	0.0241 (12)
H17A	0.2127	−0.2882	0.4736	0.029*
C18	0.2145 (3)	−0.2137 (2)	0.5542 (6)	0.0208 (11)
H18A	0.1881	−0.2335	0.6265	0.025*
C19	0.2398 (2)	−0.1517 (2)	0.5348 (5)	0.0145 (10)
C20	0.3377 (2)	−0.1140 (2)	0.2444 (5)	0.0169 (10)
C21	0.2260 (2)	−0.1127 (2)	0.6265 (5)	0.0144 (10)
N2S	0.3770 (2)	0.1421 (2)	−0.0182 (5)	0.0184 (9)
H3	0.4037	0.1313	0.0164	0.022*
H4	0.3743	0.1348	−0.1079	0.022*
N3S	0.2955 (2)	0.1879 (2)	0.0138 (5)	0.0201 (10)
H5	0.2980	0.1953	0.1034	0.024*
H6	0.2688	0.1984	−0.0215	0.024*
C3S	0.4008 (3)	0.2077 (2)	0.0051 (6)	0.0184 (11)
H3SB	0.4404	0.2315	−0.0397	0.022*
H3SC	0.4071	0.2163	0.1012	0.022*
C4S	0.3567 (3)	0.2264 (3)	−0.0477 (6)	0.0191 (11)
H4SA	0.3718	0.2695	−0.0268	0.023*
H4SB	0.3536	0.2216	−0.1451	0.023*
C5S	0.2722 (3)	0.1220 (3)	−0.0092 (6)	0.0228 (12)
H5SA	0.2662	0.1133	−0.1053	0.027*
H5SB	0.2326	0.0980	0.0353	0.027*
C6S	0.3159 (3)	0.1037 (2)	0.0434 (5)	0.0190 (11)
H6SA	0.3008	0.0605	0.0229	0.023*
H6SB	0.3190	0.1086	0.1408	0.023*
N1S	0.0447 (2)	0.4816 (2)	0.9869 (4)	0.0171 (9)
H1	0.0448	0.4761	0.8969	0.020*
H2	0.0726	0.4732	1.0242	0.020*
C1S	0.0629 (2)	0.5463 (2)	1.0145 (5)	0.0172 (10)
H1SB	0.1030	0.5733	0.9741	0.021*
H1SC	0.0666	0.5534	1.1113	0.021*
C2S	−0.0168 (3)	0.4387 (2)	1.0410 (5)	0.0176 (11)
H2SB	−0.0161	0.4417	1.1388	0.021*
H2SC	−0.0283	0.3967	1.0169	0.021*
O1W	0.2187 (3)	0.2131 (3)	0.1999 (5)	0.0417 (13)
H7	0.2406	0.2202	0.2684	0.063*
H8	0.1816	0.1861	0.2057	0.063*
O2W	0.0045 (2)	0.3336 (2)	0.8678 (6)	0.0386 (14)
H9	0.0120	0.3551	0.7985	0.058*
H10	0.0048	0.3013	0.8491	0.058*
O3W	0.4578 (3)	0.1242 (3)	−0.1969 (5)	0.0473 (15)
H11	0.4346	0.1133	−0.2640	0.071*
H12	0.4951	0.1500	−0.2075	0.071*

O4W	0.1237 (3)	0.4570 (4)	0.8062 (5)	0.0565 (18)	
H13	0.1017	0.4500	0.7380	0.085*	
H14	0.1567	0.4893	0.7897	0.085*	
O5W	0.4304 (2)	−0.2332 (2)	0.9394 (5)	0.0404 (12)	
H15	0.4638	−0.2041	0.9117	0.061*	
H16	0.4247	−0.2273	1.0197	0.061*	
O6W	0.5887 (4)	0.2126 (4)	0.7969 (7)	0.085 (2)	
H17	0.6117	0.2483	0.7682	0.127*	
H18	0.6059	0.1919	0.8106	0.127*	
O7W	0.8981 (4)	−0.0019 (4)	0.9461 (11)	0.058 (3)	0.60
H19	0.8703	0.0043	0.9172	0.086*	0.60
H20	0.9281	0.0284	0.9818	0.086*	0.60
O8W	0.3286 (5)	−0.2430 (5)	0.8135 (10)	0.046 (3)	0.50
H21	0.3628	−0.2401	0.8281	0.069*	0.50
H22	0.2989	−0.2723	0.8528	0.069*	0.50
O9W	0.8626 (7)	−0.0465 (7)	1.1997 (15)	0.056 (4)	0.40
H23	0.8442	−0.0845	1.1867	0.084*	0.40
H24	0.8733	−0.0333	1.1214	0.084*	0.40
O10W	0.6667	0.3333	0.6747 (12)	0.058 (4)	0.75
O11W	0.0224 (9)	−0.0463 (9)	0.403 (2)	0.041 (5)	0.25

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.01785 (17)	0.00708 (15)	0.00477 (18)	0.00439 (11)	−0.00048 (8)	0.00019 (8)
O1	0.026 (2)	0.0124 (17)	0.0108 (18)	0.0059 (15)	−0.0037 (15)	0.0012 (13)
O2	0.025 (2)	0.0203 (19)	0.0088 (17)	0.0144 (16)	−0.0007 (14)	0.0038 (14)
O3	0.0186 (18)	0.0156 (17)	0.0116 (18)	0.0095 (15)	−0.0020 (14)	0.0033 (14)
O4	0.025 (2)	0.0221 (19)	0.0144 (19)	0.0157 (17)	0.0053 (15)	0.0114 (15)
O5	0.024 (2)	0.0142 (17)	0.0122 (18)	0.0089 (16)	−0.0010 (14)	−0.0033 (14)
O6	0.039 (2)	0.0194 (19)	0.0120 (19)	0.0179 (19)	−0.0076 (17)	−0.0075 (15)
O7	0.025 (2)	0.0135 (17)	0.0108 (18)	0.0096 (15)	−0.0037 (14)	−0.0049 (14)
O8	0.054 (3)	0.027 (2)	0.020 (2)	0.028 (2)	−0.024 (2)	−0.0138 (17)
O9	0.025 (2)	0.0139 (18)	0.0133 (18)	0.0089 (16)	0.0024 (15)	0.0012 (14)
O10	0.032 (2)	0.0157 (19)	0.0132 (19)	0.0046 (17)	0.0092 (16)	−0.0001 (15)
O11	0.0204 (18)	0.0142 (17)	0.0110 (18)	0.0064 (15)	0.0037 (14)	0.0014 (13)
O12	0.032 (2)	0.018 (2)	0.024 (2)	0.0018 (18)	0.0131 (18)	−0.0075 (17)
N1	0.019 (2)	0.0097 (18)	0.0068 (19)	0.0084 (16)	0.0011 (15)	0.0001 (15)
N2	0.022 (2)	0.0080 (18)	0.009 (2)	0.0064 (17)	−0.0020 (16)	−0.0013 (15)
N3	0.016 (2)	0.0105 (19)	0.008 (2)	0.0038 (16)	−0.0018 (15)	−0.0013 (15)
C1	0.024 (3)	0.013 (2)	0.005 (2)	0.011 (2)	0.0002 (18)	−0.0009 (17)
C2	0.019 (2)	0.019 (2)	0.009 (2)	0.010 (2)	−0.0007 (19)	0.0010 (19)
C3	0.018 (3)	0.023 (3)	0.015 (3)	0.008 (2)	−0.001 (2)	0.004 (2)
C4	0.021 (3)	0.016 (2)	0.015 (3)	0.010 (2)	0.001 (2)	0.0059 (19)
C5	0.022 (3)	0.011 (2)	0.009 (2)	0.011 (2)	0.0009 (18)	0.0000 (17)
C6	0.025 (3)	0.012 (2)	0.006 (2)	0.009 (2)	0.0001 (19)	0.0001 (17)
C7	0.027 (3)	0.015 (2)	0.003 (2)	0.016 (2)	0.0022 (18)	0.0025 (17)
C8	0.027 (3)	0.011 (2)	0.007 (2)	0.007 (2)	−0.0030 (19)	−0.0007 (18)

C9	0.035 (3)	0.027 (3)	0.014 (3)	0.020 (3)	−0.003 (2)	−0.009 (2)
C10	0.035 (3)	0.031 (3)	0.021 (3)	0.022 (3)	−0.006 (2)	−0.009 (2)
C11	0.029 (3)	0.026 (3)	0.022 (3)	0.017 (3)	−0.010 (2)	−0.008 (2)
C12	0.026 (3)	0.011 (2)	0.010 (2)	0.008 (2)	−0.001 (2)	−0.0009 (18)
C13	0.029 (3)	0.008 (2)	0.009 (2)	0.008 (2)	−0.002 (2)	−0.0015 (17)
C14	0.035 (3)	0.012 (2)	0.007 (2)	0.010 (2)	−0.005 (2)	−0.0012 (18)
C15	0.013 (2)	0.014 (2)	0.013 (2)	0.0029 (19)	−0.0017 (18)	−0.0048 (18)
C16	0.023 (3)	0.012 (2)	0.021 (3)	0.004 (2)	0.003 (2)	−0.006 (2)
C17	0.029 (3)	0.009 (2)	0.025 (3)	0.003 (2)	0.002 (2)	−0.003 (2)
C18	0.024 (3)	0.012 (2)	0.015 (3)	0.000 (2)	0.005 (2)	0.0006 (19)
C19	0.016 (2)	0.011 (2)	0.010 (2)	0.0024 (19)	−0.0008 (18)	−0.0023 (18)
C20	0.017 (2)	0.015 (2)	0.009 (2)	0.002 (2)	−0.0007 (19)	−0.0041 (19)
C21	0.019 (2)	0.014 (2)	0.006 (2)	0.005 (2)	0.0010 (18)	−0.0004 (18)
N2S	0.031 (3)	0.023 (2)	0.012 (2)	0.022 (2)	−0.0039 (18)	−0.0012 (17)
N3S	0.029 (3)	0.029 (3)	0.013 (2)	0.023 (2)	−0.0060 (18)	0.0002 (18)
C3S	0.024 (3)	0.021 (3)	0.015 (3)	0.015 (2)	−0.004 (2)	0.000 (2)
C4S	0.028 (3)	0.023 (3)	0.015 (3)	0.019 (2)	−0.005 (2)	0.000 (2)
C5S	0.027 (3)	0.028 (3)	0.015 (3)	0.015 (3)	−0.007 (2)	0.001 (2)
C6S	0.032 (3)	0.017 (3)	0.011 (2)	0.015 (2)	−0.005 (2)	0.0008 (19)
N1S	0.021 (2)	0.021 (2)	0.010 (2)	0.0104 (19)	−0.0030 (17)	0.0002 (17)
C1S	0.021 (3)	0.014 (2)	0.012 (2)	0.005 (2)	−0.0055 (19)	−0.0031 (18)
C2S	0.025 (3)	0.015 (2)	0.011 (2)	0.008 (2)	−0.003 (2)	−0.0010 (19)
O1W	0.050 (3)	0.074 (4)	0.023 (2)	0.047 (3)	0.001 (2)	0.008 (2)
O2W	0.055 (3)	0.063 (4)	0.015 (3)	0.042 (3)	0.0003 (19)	0.0022 (19)
O3W	0.071 (4)	0.084 (4)	0.018 (2)	0.063 (4)	0.000 (2)	0.002 (3)
O4W	0.064 (4)	0.115 (6)	0.027 (3)	0.072 (4)	−0.004 (3)	−0.002 (3)
O5W	0.039 (3)	0.031 (3)	0.042 (3)	0.011 (2)	0.017 (2)	0.009 (2)
O6W	0.103 (6)	0.109 (7)	0.049 (4)	0.058 (5)	0.001 (4)	−0.016 (4)
O7W	0.042 (5)	0.038 (5)	0.091 (8)	0.020 (4)	−0.022 (5)	0.005 (5)
O8W	0.030 (4)	0.049 (4)	0.043 (4)	0.007 (3)	−0.001 (3)	0.021 (3)
O9W	0.064 (6)	0.063 (6)	0.045 (5)	0.034 (4)	−0.014 (4)	0.003 (4)
O10W	0.076 (6)	0.076 (6)	0.022 (6)	0.038 (3)	0.000	0.000
O11W	0.041 (6)	0.041 (6)	0.042 (6)	0.023 (5)	0.001 (4)	−0.002 (4)

Geometric parameters (Å, °)

Nd1—O3	2.465 (4)	C17—H17A	0.9500
Nd1—O7	2.467 (4)	C18—C19	1.390 (7)
Nd1—O5	2.483 (4)	C18—H18A	0.9500
Nd1—O1	2.482 (4)	C19—C21	1.524 (7)
Nd1—O9	2.485 (4)	N2S—C3S	1.487 (7)
Nd1—O11	2.487 (4)	N2S—C6S	1.501 (8)
Nd1—N2	2.565 (4)	N2S—H3	0.9200
Nd1—N1	2.568 (4)	N2S—H4	0.9200
Nd1—N3	2.575 (4)	N3S—C5S	1.495 (8)
O1—C6	1.258 (7)	N3S—C4S	1.501 (8)
O2—C6	1.246 (6)	N3S—H5	0.9200
O3—C7	1.247 (7)	N3S—H6	0.9200
O4—C7	1.255 (6)	C3S—C4S	1.521 (7)

O5—C13	1.278 (7)	C3S—H3SB	0.9900
O6—C13	1.235 (6)	C3S—H3SC	0.9900
O7—C14	1.240 (7)	C4S—H4SA	0.9900
O8—C14	1.254 (7)	C4S—H4SB	0.9900
O9—C21	1.263 (6)	C5S—C6S	1.503 (8)
O10—C21	1.236 (6)	C5S—H5SA	0.9900
O11—C20	1.254 (6)	C5S—H5SB	0.9900
O12—C20	1.245 (7)	C6S—H6SA	0.9900
N1—C1	1.333 (6)	C6S—H6SB	0.9900
N1—C5	1.340 (6)	N1S—C2S	1.497 (7)
N2—C8	1.338 (6)	N1S—C1S	1.499 (7)
N2—C12	1.341 (7)	N1S—H1	0.9200
N3—C19	1.332 (7)	N1S—H2	0.9200
N3—C15	1.340 (7)	C1S—C2S^{i}	1.515 (8)
C1—C2	1.386 (7)	C1S—H1SB	0.9900
C1—C6	1.524 (7)	C1S—H1SC	0.9900
C2—C3	1.401 (7)	C2S—C1S^{i}	1.515 (8)
C2—H2A	0.9500	C2S—H2SB	0.9900
C3—C4	1.393 (7)	C2S—H2SC	0.9900
C3—H3A	0.9500	O1W—H7	0.8499
C4—C5	1.386 (7)	O1W—H8	0.8500
C4—H4A	0.9500	O2W—H9	0.8501
C5—C7	1.516 (7)	O2W—H10	0.8498
C7—O4	1.255 (6)	O3W—H11	0.8500
C8—C9	1.375 (8)	O3W—H12	0.8501
C8—C13	1.521 (7)	O4W—H13	0.8500
C9—C10	1.401 (8)	O4W—H14	0.8498
C9—H9A	0.9500	O5W—H15	0.8500
C10—C11	1.383 (8)	O5W—H16	0.8502
C10—H10A	0.9500	O6W—H17	0.8499
C11—C12	1.374 (8)	O6W—H18	0.8500
C11—H11A	0.9500	O7W—H19	0.8503
C12—C14	1.523 (7)	O7W—H20	0.8494
C15—C16	1.393 (7)	O8W—H21	0.8501
C15—C20	1.517 (7)	O8W—H22	0.8500
C16—C17	1.390 (8)	O9W—H23	0.8500
C16—H16A	0.9500	O9W—H24	0.8499
C17—C18	1.398 (8)		
O3—Nd1—O7	77.20 (13)	O6—C13—C8	118.2 (5)
O3—Nd1—O5	90.11 (12)	O5—C13—C8	115.6 (4)
O7—Nd1—O5	125.79 (12)	O7—C14—O8	125.4 (5)
O3—Nd1—O1	125.64 (12)	O7—C14—C12	117.1 (5)
O7—Nd1—O1	151.47 (12)	O8—C14—C12	117.6 (5)
O5—Nd1—O1	75.51 (13)	N3—C15—C16	121.8 (5)
O3—Nd1—O9	150.59 (12)	N3—C15—C20	114.5 (4)
O7—Nd1—O9	88.93 (13)	C16—C15—C20	123.6 (5)
O5—Nd1—O9	77.05 (13)	C17—C16—C15	118.3 (5)
O1—Nd1—O9	77.04 (13)	C17—C16—H16A	120.8

O3—Nd1—O11	77.45 (12)	C15—C16—H16A	120.8
O7—Nd1—O11	78.02 (13)	C16—C17—C18	119.8 (5)
O5—Nd1—O11	150.31 (13)	C16—C17—H17A	120.1
O1—Nd1—O11	89.88 (13)	C18—C17—H17A	120.1
O9—Nd1—O11	125.28 (12)	C19—C18—C17	117.8 (5)
O3—Nd1—N2	77.80 (13)	C19—C18—H18A	121.1
O7—Nd1—N2	62.76 (13)	C17—C18—H18A	121.1
O5—Nd1—N2	63.06 (13)	N3—C19—C18	122.6 (5)
O1—Nd1—N2	132.85 (13)	N3—C19—C21	115.4 (4)
O9—Nd1—N2	72.79 (13)	C18—C19—C21	122.0 (5)
O11—Nd1—N2	137.21 (13)	O12—C20—O11	125.4 (5)
O3—Nd1—N1	62.48 (12)	O12—C20—C15	118.5 (5)
O7—Nd1—N1	136.93 (13)	O11—C20—C15	116.0 (5)
O5—Nd1—N1	71.35 (13)	O10—C21—O9	126.3 (5)
O1—Nd1—N1	63.23 (13)	O10—C21—C19	118.2 (5)
O9—Nd1—N1	133.88 (13)	O9—C21—C19	115.5 (4)
O11—Nd1—N1	79.02 (13)	C3S—N2S—C6S	112.1 (4)
N2—Nd1—N1	118.22 (12)	C3S—N2S—H3	109.2
O3—Nd1—N3	136.85 (13)	C6S—N2S—H3	109.2
O7—Nd1—N3	79.27 (13)	C3S—N2S—H4	109.2
O5—Nd1—N3	132.81 (13)	C6S—N2S—H4	109.2
O1—Nd1—N3	72.23 (13)	H3—N2S—H4	107.9
O9—Nd1—N3	62.87 (13)	C5S—N3S—C4S	111.7 (4)
O11—Nd1—N3	62.53 (13)	C5S—N3S—H5	109.3
N2—Nd1—N3	121.23 (12)	C4S—N3S—H5	109.3
N1—Nd1—N3	120.15 (12)	C5S—N3S—H6	109.3
C6—O1—Nd1	124.6 (3)	C4S—N3S—H6	109.3
C7—O3—Nd1	126.3 (3)	H5—N3S—H6	107.9
C13—O5—Nd1	125.3 (3)	N2S—C3S—C4S	110.3 (4)
C14—O7—Nd1	125.8 (3)	N2S—C3S—H3SB	109.6
C21—O9—Nd1	125.4 (3)	C4S—C3S—H3SB	109.6
C20—O11—Nd1	126.3 (3)	N2S—C3S—H3SC	109.6
C1—N1—C5	119.2 (5)	C4S—C3S—H3SC	109.6
C1—N1—Nd1	119.5 (3)	H3SB—C3S—H3SC	108.1
C5—N1—Nd1	120.7 (3)	N3S—C4S—C3S	109.9 (4)
C8—N2—C12	118.8 (5)	N3S—C4S—H4SA	109.7
C8—N2—Nd1	120.3 (3)	C3S—C4S—H4SA	109.7
C12—N2—Nd1	120.7 (3)	N3S—C4S—H4SB	109.7
C19—N3—C15	119.7 (4)	C3S—C4S—H4SB	109.7
C19—N3—Nd1	119.6 (3)	H4SA—C4S—H4SB	108.2
C15—N3—Nd1	120.4 (3)	N3S—C5S—C6S	110.8 (5)
N1—C1—C2	122.3 (5)	N3S—C5S—H5SA	109.5
N1—C1—C6	114.9 (5)	C6S—C5S—H5SA	109.5
C2—C1—C6	122.8 (5)	N3S—C5S—H5SB	109.5
C1—C2—C3	118.7 (5)	C6S—C5S—H5SB	109.5
C1—C2—H2A	120.6	H5SA—C5S—H5SB	108.1
C3—C2—H2A	120.6	C5S—C6S—N2S	109.9 (4)
C4—C3—C2	118.7 (5)	C5S—C6S—H6SA	109.7
C4—C3—H3A	120.6	N2S—C6S—H6SA	109.7

C2—C3—H3A	120.6	C5S—C6S—H6SB	109.7
C5—C4—C3	118.5 (5)	N2S—C6S—H6SB	109.7
C5—C4—H4A	120.8	H6SA—C6S—H6SB	108.2
C3—C4—H4A	120.8	C2S—N1S—C1S	111.8 (4)
N1—C5—C4	122.6 (5)	C2S—N1S—H1	109.3
N1—C5—C7	113.2 (4)	C1S—N1S—H1	109.3
C4—C5—C7	124.2 (5)	C2S—N1S—H2	109.3
O2—C6—O1	126.1 (5)	C1S—N1S—H2	109.3
O2—C6—C1	117.3 (5)	H1—N1S—H2	107.9
O1—C6—C1	116.6 (4)	N1S—C1S—C2S^{i}	110.9 (4)
O3—C7—O4	125.3 (5)	N1S—C1S—H1SB	109.5
O3—C7—O4	125.3 (5)	C2S^{i}—C1S—H1SB	109.5
O3—C7—C5	116.6 (4)	N1S—C1S—H1SC	109.5
O4—C7—C5	118.1 (5)	C2S^{i}—C1S—H1SC	109.5
O4—C7—C5	118.1 (5)	H1SB—C1S—H1SC	108.0
N2—C8—C9	122.9 (5)	N1S—C2S—C1S^{i}	110.0 (4)
N2—C8—C13	115.0 (5)	N1S—C2S—H2SB	109.7
C9—C8—C13	122.1 (5)	C1S^{i}—C2S—H2SB	109.7
C8—C9—C10	118.1 (5)	N1S—C2S—H2SC	109.7
C8—C9—H9A	120.9	C1S^{i}—C2S—H2SC	109.7
C10—C9—H9A	120.9	H2SB—C2S—H2SC	108.2
C11—C10—C9	118.8 (6)	H7—O1W—H8	117.6
C11—C10—H10A	120.6	H9—O2W—H10	109.6
C9—C10—H10A	120.6	H11—O3W—H12	118.7
C12—C11—C10	119.2 (5)	H13—O4W—H14	105.9
C12—C11—H11A	120.4	H15—O5W—H16	110.1
C10—C11—H11A	120.4	H17—O6W—H18	115.1
N2—C12—C11	122.1 (5)	H19—O7W—H20	115.6
N2—C12—C14	113.1 (5)	H21—O8W—H22	114.8
C11—C12—C14	124.8 (5)	H23—O9W—H24	101.1
O6—C13—O5	126.2 (5)		
O3—Nd1—O1—C6	12.5 (5)	N2—Nd1—N3—C15	132.0 (4)
O7—Nd1—O1—C6	150.9 (4)	N1—Nd1—N3—C15	−55.3 (4)
O5—Nd1—O1—C6	−66.9 (4)	C5—N1—C1—C2	1.3 (7)
O9—Nd1—O1—C6	−146.7 (4)	Nd1—N1—C1—C2	−170.3 (4)
O11—Nd1—O1—C6	86.9 (4)	C5—N1—C1—C6	−179.7 (4)
N2—Nd1—O1—C6	−95.5 (4)	Nd1—N1—C1—C6	8.7 (5)
N1—Nd1—O1—C6	9.2 (4)	N1—C1—C2—C3	−1.0 (8)
N3—Nd1—O1—C6	148.0 (4)	C6—C1—C2—C3	−179.8 (5)
O7—Nd1—O3—C7	−160.7 (4)	C1—C2—C3—C4	−0.5 (8)
O5—Nd1—O3—C7	72.5 (4)	C2—C3—C4—C5	1.5 (8)
O1—Nd1—O3—C7	0.4 (5)	C1—N1—C5—C4	−0.2 (7)
O9—Nd1—O3—C7	135.6 (4)	Nd1—N1—C5—C4	171.3 (4)
O11—Nd1—O3—C7	−80.3 (4)	C1—N1—C5—C7	−178.7 (4)
N2—Nd1—O3—C7	134.9 (4)	Nd1—N1—C5—C7	−7.3 (5)
N1—Nd1—O3—C7	3.7 (4)	C3—C4—C5—N1	−1.2 (8)
N3—Nd1—O3—C7	−102.1 (4)	C3—C4—C5—C7	177.2 (5)

O3—Nd1—O5—C13	84.2 (4)	Nd1—O1—C6—O2	171.7 (4)
O7—Nd1—O5—C13	9.9 (5)	Nd1—O1—C6—C1	−8.4 (6)
O1—Nd1—O5—C13	−148.9 (4)	N1—C1—C6—O2	179.2 (4)
O9—Nd1—O5—C13	−69.1 (4)	C2—C1—C6—O2	−1.8 (7)
O11—Nd1—O5—C13	148.4 (4)	N1—C1—C6—O1	−0.7 (7)
N2—Nd1—O5—C13	7.9 (4)	C2—C1—C6—O1	178.3 (5)
N1—Nd1—O5—C13	144.9 (4)	Nd1—O3—C7—O4	171.8 (4)
N3—Nd1—O5—C13	−100.8 (4)	Nd1—O3—C7—O4	171.8 (4)
O3—Nd1—O7—C14	−78.3 (5)	Nd1—O3—C7—C5	−8.8 (6)
O5—Nd1—O7—C14	2.5 (5)	O4—O4—C7—O3	0.00 (15)
O1—Nd1—O7—C14	135.3 (4)	O4—O4—C7—C5	0.0 (3)
O9—Nd1—O7—C14	75.6 (4)	N1—C5—C7—O3	10.1 (6)
O11—Nd1—O7—C14	−157.9 (5)	C4—C5—C7—O3	−168.4 (5)
N2—Nd1—O7—C14	4.5 (4)	N1—C5—C7—O4	−170.4 (4)
N1—Nd1—O7—C14	−98.7 (5)	C4—C5—C7—O4	11.1 (7)
N3—Nd1—O7—C14	138.2 (5)	N1—C5—C7—O4	−170.4 (4)
O3—Nd1—O9—C21	149.9 (4)	C4—C5—C7—O4	11.1 (7)
O7—Nd1—O9—C21	88.9 (4)	C12—N2—C8—C9	1.7 (8)
O5—Nd1—O9—C21	−143.9 (4)	Nd1—N2—C8—C9	−172.5 (4)
O1—Nd1—O9—C21	−66.1 (4)	C12—N2—C8—C13	179.7 (5)
O11—Nd1—O9—C21	14.4 (5)	Nd1—N2—C8—C13	5.4 (6)
N2—Nd1—O9—C21	150.6 (4)	N2—C8—C9—C10	−1.5 (9)
N1—Nd1—O9—C21	−96.5 (4)	C13—C8—C9—C10	−179.3 (5)
N3—Nd1—O9—C21	10.4 (4)	C8—C9—C10—C11	0.1 (10)
O3—Nd1—O11—C20	−161.4 (5)	C9—C10—C11—C12	1.0 (10)
O7—Nd1—O11—C20	−82.1 (5)	C8—N2—C12—C11	−0.6 (8)
O5—Nd1—O11—C20	131.3 (4)	Nd1—N2—C12—C11	173.7 (4)
O1—Nd1—O11—C20	71.9 (4)	C8—N2—C12—C14	−179.4 (5)
O9—Nd1—O11—C20	−2.1 (5)	Nd1—N2—C12—C14	−5.1 (6)
N2—Nd1—O11—C20	−105.4 (4)	C10—C11—C12—N2	−0.8 (9)
N1—Nd1—O11—C20	134.6 (4)	C10—C11—C12—C14	177.8 (6)
N3—Nd1—O11—C20	1.9 (4)	Nd1—O5—C13—O6	172.8 (4)
O3—Nd1—N1—C1	174.1 (4)	Nd1—O5—C13—C8	−8.2 (6)
O7—Nd1—N1—C1	−163.3 (3)	N2—C8—C13—O6	−179.5 (5)
O5—Nd1—N1—C1	73.8 (4)	C9—C8—C13—O6	−1.5 (8)
O1—Nd1—N1—C1	−9.0 (3)	N2—C8—C13—O5	1.4 (7)
O9—Nd1—N1—C1	24.6 (4)	C9—C8—C13—O5	179.4 (5)
O11—Nd1—N1—C1	−104.4 (4)	Nd1—O7—C14—O8	171.0 (5)
N2—Nd1—N1—C1	117.5 (3)	Nd1—O7—C14—C12	−8.7 (7)
N3—Nd1—N1—C1	−55.5 (4)	N2—C12—C14—O7	8.7 (7)
O3—Nd1—N1—C5	2.7 (3)	C11—C12—C14—O7	−170.1 (6)
O7—Nd1—N1—C5	25.3 (4)	N2—C12—C14—O8	−171.1 (5)
O5—Nd1—N1—C5	−97.6 (4)	C11—C12—C14—O8	10.1 (9)
O1—Nd1—N1—C5	179.6 (4)	C19—N3—C15—C16	−0.1 (8)
O9—Nd1—N1—C5	−146.8 (3)	Nd1—N3—C15—C16	173.9 (4)
O11—Nd1—N1—C5	84.1 (4)	C19—N3—C15—C20	−177.7 (5)
N2—Nd1—N1—C5	−53.9 (4)	Nd1—N3—C15—C20	−3.6 (6)
N3—Nd1—N1—C5	133.1 (3)	N3—C15—C16—C17	−1.1 (9)
O3—Nd1—N2—C8	−103.0 (4)	C20—C15—C16—C17	176.2 (5)

O7—Nd1—N2—C8	175.3 (4)	C15—C16—C17—C18	1.1 (9)
O5—Nd1—N2—C8	−6.5 (4)	C16—C17—C18—C19	0.0 (9)
O1—Nd1—N2—C8	24.8 (5)	C15—N3—C19—C18	1.4 (8)
O9—Nd1—N2—C8	77.4 (4)	Nd1—N3—C19—C18	−172.7 (4)
O11—Nd1—N2—C8	−158.9 (3)	C15—N3—C19—C21	−179.0 (5)
N1—Nd1—N2—C8	−53.7 (4)	Nd1—N3—C19—C21	6.9 (6)
N3—Nd1—N2—C8	119.1 (4)	C17—C18—C19—N3	−1.3 (9)
O3—Nd1—N2—C12	82.9 (4)	C17—C18—C19—C21	179.1 (5)
O7—Nd1—N2—C12	1.1 (4)	Nd1—O11—C20—O12	175.9 (4)
O5—Nd1—N2—C12	179.3 (4)	Nd1—O11—C20—C15	−4.4 (7)
O1—Nd1—N2—C12	−149.4 (4)	N3—C15—C20—O12	−175.2 (5)
O9—Nd1—N2—C12	−96.8 (4)	C16—C15—C20—O12	7.3 (8)
O11—Nd1—N2—C12	27.0 (5)	N3—C15—C20—O11	5.1 (7)
N1—Nd1—N2—C12	132.1 (4)	C16—C15—C20—O11	−172.4 (5)
N3—Nd1—N2—C12	−55.0 (4)	Nd1—O9—C21—O10	168.0 (4)
O3—Nd1—N3—C19	−160.6 (3)	Nd1—O9—C21—C19	−10.9 (6)
O7—Nd1—N3—C19	−102.7 (4)	N3—C19—C21—O10	−177.0 (5)
O5—Nd1—N3—C19	26.8 (5)	C18—C19—C21—O10	2.7 (8)
O1—Nd1—N3—C19	75.9 (4)	N3—C19—C21—O9	2.0 (7)
O9—Nd1—N3—C19	−8.4 (4)	C18—C19—C21—O9	−178.4 (5)
O11—Nd1—N3—C19	175.3 (4)	C6S—N2S—C3S—C4S	−57.2 (6)
N2—Nd1—N3—C19	−54.0 (4)	C5S—N3S—C4S—C3S	−56.4 (6)
N1—Nd1—N3—C19	118.7 (4)	N2S—C3S—C4S—N3S	55.9 (6)
O3—Nd1—N3—C15	25.4 (5)	C4S—N3S—C5S—C6S	57.1 (6)
O7—Nd1—N3—C15	83.2 (4)	N3S—C5S—C6S—N2S	−56.2 (6)
O5—Nd1—N3—C15	−147.3 (4)	C3S—N2S—C6S—C5S	57.2 (6)
O1—Nd1—N3—C15	−98.2 (4)	C2S—N1S—C1S—C2S^{i}	−56.8 (6)
O9—Nd1—N3—C15	177.6 (4)	C1S—N1S—C2S—C1S^{i}	56.3 (6)
O11—Nd1—N3—C15	1.3 (4)		

Symmetry codes: (i) −*x*, −*y*+1, −*z*+2.

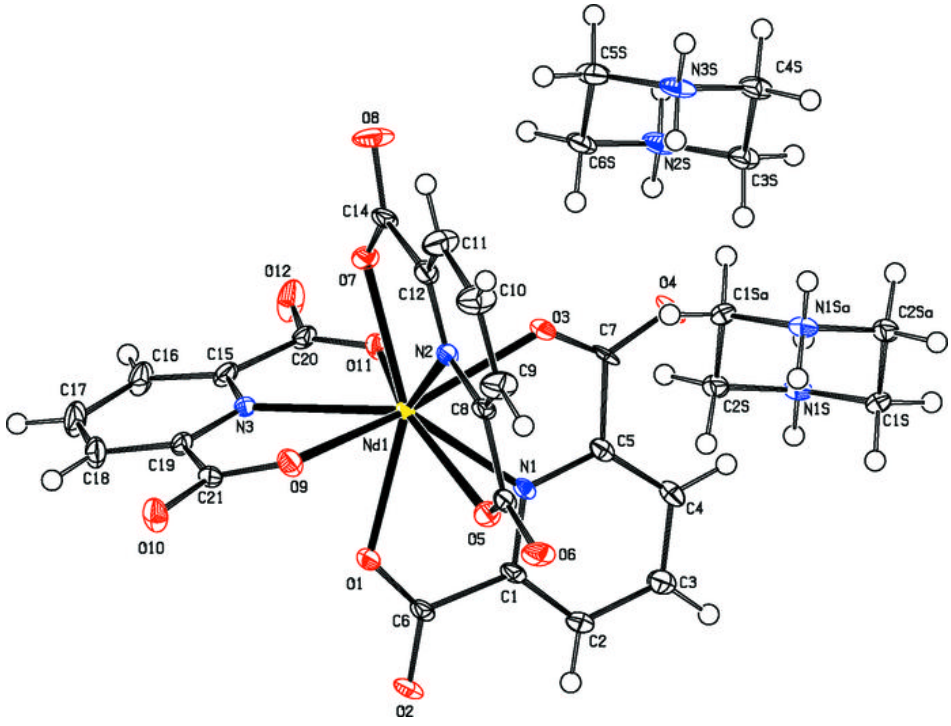
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2S—H3···O4	0.92	1.97	2.804 (6)	151
N2S—H4···O6^{ii}	0.92	1.92	2.760 (6)	151
N3S—H5···O10^{iii}	0.92	1.95	2.780 (6)	150
N3S—H6···O8^{iv}	0.92	1.99	2.836 (6)	153
N1S—H1···O2^{v}	0.92	1.92	2.758 (6)	150
N1S—H2···O12^{vi}	0.92	2.03	2.874 (6)	153
O1W—H7···O9^{iii}	0.85	2.03	2.863 (7)	167
O1W—H8···O9W^{vii}	0.85	2.01	2.838 (17)	167
O2W—H9···O1^{v}	0.85	2.43	3.278 (7)	180
O2W—H10···O1W^{iii}	0.85	2.17	3.024 (8)	180
O3W—H11···O5^{ii}	0.85	2.14	2.970 (7)	167
O3W—H12···O6W^{ii}	0.85	2.11	2.950 (11)	171

O4W—H13···O1^{v}	0.85	2.05	2.878 (7)	166
O4W—H14···O8W^{v}	0.85	2.17	2.985 (14)	162
O5W—H15···O4^{viii}	0.85	1.82	2.674 (6)	180
O5W—H16···O6W^{ix}	0.85	1.95	2.804 (9)	179
O6W—H17···O10W	0.85	2.13	2.972 (10)	174
O6W—H18···O12^{viii}	0.85	2.16	3.011 (10)	180
O7W—H19···O8^{viii}	0.85	1.76	2.608 (10)	179
O7W—H20···O7W^{x}	0.85	1.95	2.797 (11)	177
O8W—H21···O5W	0.85	1.99	2.787 (12)	156
O8W—H22···O5W^{xi}	0.85	1.87	2.723 (11)	180
O9W—H23···O8^{xii}	0.85	2.29	3.136 (18)	179
O9W—H24···O7W	0.85	1.92	2.765 (20)	179
C3S—H3Sc···O10^{iii}	0.99	2.49	3.200 (8)	129
C4S—H4SB···O6^{ii}	0.99	2.47	3.179 (8)	128
C4S—H4SB···O7^{iv}	0.99	2.51	3.076 (9)	116
C5S—H5SA···O6^{ii}	0.99	2.46	3.180 (8)	129
C6S—H6SB···O3	0.99	2.52	3.092 (8)	116
C6S—H6SB···O10^{iii}	0.99	2.45	3.169 (7)	129
C1S—H1SC···O2^{xiii}	0.99	2.43	3.151 (7)	129
C2S—H2SB···O11^{vi}	0.99	2.55	3.112 (8)	116
C2S—H2SB···O2^{xiii}	0.99	2.49	3.194 (7)	128

Symmetry codes: (ii) *x*, *y*, *z*−1; (iii) *x*−*y*, *x*, −*z*+1; (iv) *x*−*y*, *x*, −*z*; (v) −*y*, *x*−*y*, *z*; (vi) −*y*, *x*−*y*, *z*+1; (vii) −*x*+*y*+1, −*x*+1, *z*−1; (viii) −*x*+1, −*y*, −*z*+1; (ix) −*x*+1, −*y*, −*z*+2; (x) *y*+1, −*x*+*y*+1, −*z*+2; (xi) −*y*, *x*−*y*−1, *z*; (xii) −*x*+*y*+1, −*x*, *z*+1; (xiii) *y*, −*x*+*y*+1, −*z*+2.

Fig. 1


C5S
N3S
C4S
C6S
N2S
C3S
O8
C14
C11
O12
O7
C12
C10
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N1Sa
C2Sa
O3
C7
C16
C15
C20
O11
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C9
C17
C8
C2S
N1S
C1S
N3
Nd1
C5
C19
C18
N1
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O6
O1
C3
C1
C6
C2
O2

Fig. 2

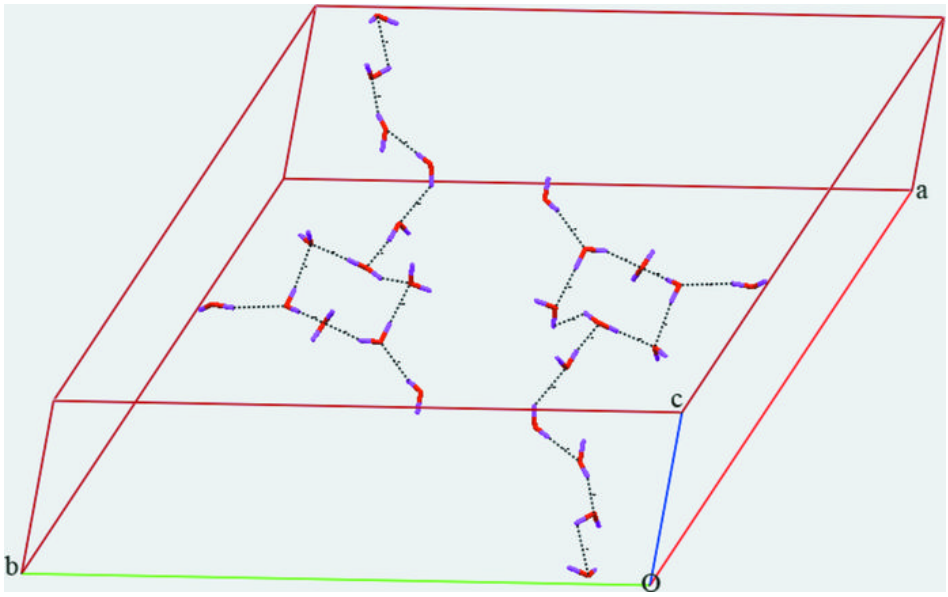

Fig. 3

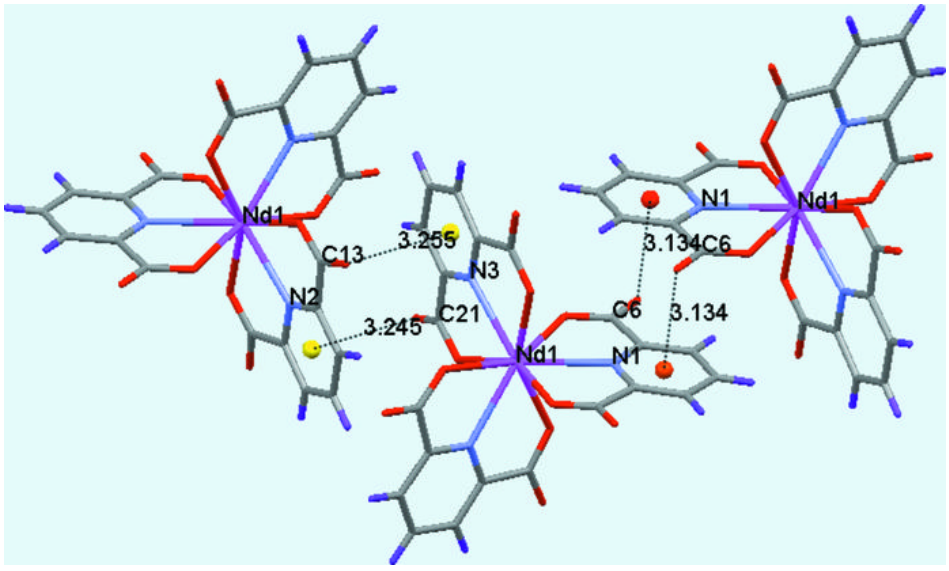

Fig. 4