

Poly[diaqua(μ_2 -oxalato- $\kappa^4 O^1, O^2, O^1', O^2'$)(μ_2 -pyrazine-2-carboxylato- $\kappa^4 N^1, O:O, O'$)neodymium(III)]

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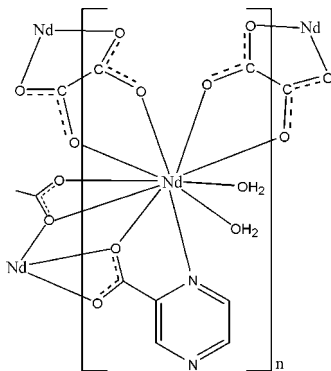
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.011$ Å; R factor = 0.051; wR factor = 0.132; data-to-parameter ratio = 10.4.

In the title complex, $[Nd(C_5H_3N_2O_2)(C_2O_4)(H_2O)_2]_n$, the Nd^{III} atom is ten-coordinated by one N atom and three O atoms from two pyrazine-2-carboxylate ligands, four O atoms from two oxalate ligands and two water molecules in a distorted bicapped square-antiprismatic geometry. The two crystallographically independent oxalate ligands, each lying on an inversion center, act as bridging ligands, linking Nd atoms into an extended zigzag chain. Neighboring chains are linked by the pyrazine-2-carboxylate ligands into a two-dimensional layerlike network in the $(10\bar{1})$ plane. The layers are further connected by $O-H\cdots O$ and $O-H\cdots N$ hydrogen bonds, forming a three-dimensional supramolecular network.

Related literature

For general background to lanthanide coordination frameworks, see: Han *et al.* (2009); Li *et al.* (2006); Wang *et al.* (2006); Zhou *et al.* (2006).



Experimental

Crystal data

$[Nd(C_5H_3N_2O_2)(C_2O_4)(H_2O)_2]$	$\gamma = 96.306 (3)^\circ$
$M_r = 391.39$	$V = 517.0 (2) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.948 (3) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.6512 (18) \text{ \AA}$	$\mu = 5.06 \text{ mm}^{-1}$
$c = 8.7425 (18) \text{ \AA}$	$T = 296 \text{ K}$
$\alpha = 115.525 (2)^\circ$	$0.23 \times 0.19 \times 0.17 \text{ mm}$
$\beta = 101.970 (3)^\circ$	

Data collection

Bruker APEXII CCD diffractometer	2533 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1824 independent reflections
$T_{\min} = 0.320, T_{\max} = 0.420$	1756 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.065$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.132$	$\Delta\rho_{\text{max}} = 1.95 \text{ e \AA}^{-3}$
$S = 1.08$	$\Delta\rho_{\text{min}} = -2.98 \text{ e \AA}^{-3}$
1824 reflections	
175 parameters	
6 restraints	

Table 1

Selected bond lengths (Å).

Nd1—O2W	2.467 (5)	Nd1—O1W	2.549 (6)
Nd1—O3	2.474 (5)	Nd1—O2 ⁱⁱⁱ	2.557 (5)
Nd1—O6 ⁱ	2.490 (5)	Nd1—O2	2.573 (5)
Nd1—O4 ⁱⁱ	2.508 (5)	Nd1—N1 ⁱⁱⁱ	2.765 (6)
Nd1—O5	2.512 (5)	Nd1—O1	2.885 (6)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O1 ^{iv}	0.84 (9)	2.02 (6)	2.707 (8)	139 (7)
O1W—H2W \cdots O6 ^v	0.85 (8)	2.07 (4)	2.838 (8)	152 (6)
O2W—H3W \cdots N2 ^{vi}	0.84 (5)	2.50 (5)	3.229 (9)	145 (6)
O2W—H4W \cdots O4 ^{vii}	0.84 (8)	2.13 (4)	2.872 (8)	147 (7)

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 1999); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2217).

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supplementary materials

Acta Cryst. (2009). E65, m1065-m1066 [doi:10.1107/S1600536809031250]

Poly[*diaqua*(μ_2 -oxalato- $\kappa^4 O^1, O^2:O^{1'}, O^{2'}$)(μ_2 -pyrazine-2-carboxylato- $\kappa^4 N^1, O:O, O'$)neodymium(III)]

K.-C. Chen, H.-M. Luo, Q.-H. Meng, Y.-F. Luo and R.-H. Zeng

Comment

In recent years, many research groups have devoted their work to the design and synthesis of lanthanide coordination frameworks with bridging multifunctional organic ligands, not only because of their fascinating topological networks, but also due to their potential applications in ion exchange, gas storage, catalysis and luminescence (Wang *et al.*, 2006; Zhou *et al.*, 2006). As a building block, pyrazine-2-carboxylic acid and oxalic acid are good ligands with multifunctional coordination sites providing a high likelihood for the generation of structures with high dimensions (Han *et al.*, 2009; Li *et al.*, 2006). Recently, we obtained the title coordination polymer under hydrothermal conditions.

In the title compound, the Nd^{III} atom is coordinated by seven O atoms and one N atom from two pyrazine-2-carboxylate ligands and two oxalate ligands, and by two water molecules in a distorted bicapped square-antiprismatic geometry (Fig. 1). The Nd^{III} atoms are linked by the oxalate ligands, forming an extended zigzag chain. These chains are linked by the pyrazine-2-carboxylate ligands into a two-dimensional layerlike network (Fig. 2). The Nd—O and Nd—N bond lengths range from 2.467 (4) to 2.885 (6) Å (Table 1). O—H \cdots O and O—H \cdots N hydrogen bonds (Table 2) involving the pyrazine-2-carboxylate ligands, coordinated water molecules and oxalate ligands assemble neighboring layers into a three-dimensional supramolecular network.

Experimental

A mixture of Nd₂O₃ (0.245 g, 0.75 mmol), pyrazine-2-carboxylic acid (0.186 g, 1.5 mmol), oxalic acid (0.135 g, 1.5 mmol), water (10 ml) in the presence of HNO₃ (0.024 g, 0.385 mmol) was stirred vigorously for 20 min and then sealed in a Teflon-lined stainless-steel autoclave (20 ml capacity). The autoclave was heated and maintained at 433 K for 3 d, and then cooled to room temperature at 5 K h⁻¹. Colorless block crystals of the title compound were obtained.

Refinement

Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O—H = 0.84 (1) and H \cdots H = 1.34 (1) Å, and with a fixed $U_{iso}(H)$. C-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms, with C—H = 0.93 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual electron density was found 0.96 Å from Nd1 and the deepest hole 0.87 Å from Nd1.

Figures

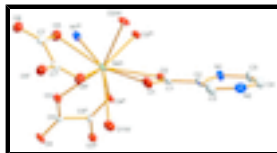


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) 1-x, 1-y, 1-z; (ii) 2-x, 2-y, 2-z; (iii) 2-x, 1-y, 2-z.]

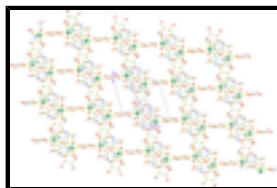


Fig. 2. View of the layered network in the title compound.

Poly[*diaqua*(μ_2 -oxalato- $\kappa^4 O^1, O^2:O^1, O^2$)(μ_2 -pyrazine-2-carboxylato- $\kappa^4 N^1, O:O, O'$)neodymium(III)]

Crystal data

[Nd(C₅H₃N₂O₂)(C₂O₄)(H₂O)₂]

$M_r = 391.39$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.948$ (3) Å

$b = 8.6512$ (18) Å

$c = 8.7425$ (18) Å

$\alpha = 115.525$ (2)°

$\beta = 101.970$ (3)°

$\gamma = 96.306$ (3)°

$V = 517.0$ (2) Å³

$Z = 2$

$F_{000} = 374$

$D_x = 2.514$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2522 reflections

$\theta = 2.7$ – 28.3 °

$\mu = 5.06$ mm⁻¹

$T = 296$ K

Block, colorless

$0.23 \times 0.19 \times 0.17$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ K

φ and ω scans

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

$T_{\min} = 0.320$, $T_{\max} = 0.420$

2533 measured reflections

1824 independent reflections

1756 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.065$

$\theta_{\text{max}} = 25.2$ °

$\theta_{\text{min}} = 2.7$ °

$h = -8 \rightarrow 9$

$k = -8 \rightarrow 10$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$$R[F^2 > 2\sigma(F^2)] = 0.051$$

$$wR(F^2) = 0.132$$

$$S = 1.08$$

1824 reflections

175 parameters

6 restraints

Primary atom site location: structure-invariant direct methods

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.0313P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 1.95 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -2.98 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.1008 (9)	0.3421 (10)	0.7510 (9)	0.0146 (15)
C2	1.2220 (10)	0.2213 (10)	0.7476 (10)	0.0175 (15)
C3	1.2449 (13)	0.0959 (12)	0.5928 (12)	0.0246 (19)
H3	1.1882	0.0920	0.4865	0.030*
C4	1.4345 (11)	0.0053 (11)	0.7489 (11)	0.0227 (17)
H4	1.5126	-0.0660	0.7543	0.027*
C5	1.4166 (11)	0.1312 (11)	0.9049 (11)	0.0235 (17)
H5	1.4818	0.1415	1.0116	0.028*
C6	0.9283 (8)	1.0062 (9)	0.9289 (9)	0.0114 (14)
C7	0.4413 (9)	0.5252 (9)	0.5645 (9)	0.0156 (15)
H1W	1.058 (11)	0.745 (10)	0.649 (9)	0.023*
H2W	1.143 (10)	0.630 (10)	0.676 (10)	0.023*
H3W	0.599 (5)	0.229 (10)	0.680 (9)	0.023*
H4W	0.731 (9)	0.226 (9)	0.802 (10)	0.023*
N1	1.3077 (9)	0.2389 (9)	0.9065 (8)	0.0175 (13)
N2	1.3439 (9)	-0.0191 (9)	0.5892 (9)	0.0240 (15)
Nd1	0.83941 (4)	0.58653 (4)	0.82456 (4)	0.0124 (2)
O1	1.0011 (8)	0.3228 (8)	0.6106 (7)	0.0244 (13)
O2	1.1050 (7)	0.4616 (7)	0.9021 (7)	0.0182 (11)
O3	0.8094 (7)	0.8693 (7)	0.8272 (7)	0.0185 (11)
O4	0.9419 (7)	1.1485 (7)	0.9251 (7)	0.0192 (11)
O5	0.5149 (7)	0.5678 (8)	0.7214 (7)	0.0230 (12)
O6	0.2843 (7)	0.5193 (8)	0.4984 (6)	0.0210 (11)
O1W	1.0754 (9)	0.6971 (9)	0.7148 (8)	0.0240 (13)
O2W	0.7008 (7)	0.2834 (7)	0.7480 (7)	0.0204 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.019 (4)	0.013 (4)	0.016 (4)	0.002 (3)	0.009 (3)	0.009 (3)
C2	0.024 (4)	0.013 (4)	0.016 (4)	0.001 (3)	0.005 (3)	0.007 (3)
C3	0.034 (5)	0.016 (5)	0.020 (4)	0.005 (4)	0.007 (4)	0.006 (4)
C4	0.028 (4)	0.016 (4)	0.028 (4)	0.010 (3)	0.016 (4)	0.010 (4)
C5	0.025 (4)	0.024 (4)	0.030 (4)	0.011 (3)	0.009 (3)	0.018 (4)

supplementary materials

C6	0.008 (3)	0.006 (3)	0.014 (3)	-0.001 (2)	-0.001 (3)	0.001 (3)
C7	0.018 (4)	0.006 (4)	0.016 (4)	0.000 (3)	0.007 (3)	-0.001 (3)
N1	0.023 (3)	0.015 (3)	0.018 (3)	0.008 (3)	0.007 (3)	0.009 (3)
N2	0.029 (4)	0.013 (3)	0.027 (4)	0.003 (3)	0.014 (3)	0.004 (3)
Nd1	0.0159 (3)	0.0065 (3)	0.0146 (3)	0.00016 (19)	0.0035 (2)	0.0058 (2)
O1	0.032 (3)	0.027 (3)	0.021 (3)	0.010 (3)	0.009 (2)	0.016 (3)
O2	0.022 (3)	0.014 (3)	0.024 (3)	0.006 (2)	0.011 (2)	0.012 (2)
O3	0.016 (3)	0.013 (3)	0.024 (3)	0.000 (2)	0.000 (2)	0.010 (2)
O4	0.025 (3)	0.010 (3)	0.024 (3)	0.002 (2)	0.003 (2)	0.011 (2)
O5	0.022 (3)	0.033 (3)	0.019 (3)	0.009 (2)	0.008 (2)	0.014 (3)
O6	0.019 (3)	0.024 (3)	0.015 (3)	0.004 (2)	0.003 (2)	0.006 (2)
O1W	0.033 (3)	0.022 (3)	0.022 (3)	0.008 (3)	0.013 (3)	0.012 (3)
O2W	0.029 (3)	0.007 (3)	0.022 (3)	-0.003 (2)	0.006 (2)	0.006 (2)

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

C1—O1	1.246 (9)	Nd1—O2W	2.467 (5)
C1—O2	1.270 (9)	Nd1—O3	2.474 (5)
C1—C2	1.492 (10)	Nd1—O6 ⁱⁱ	2.490 (5)
C2—N1	1.350 (10)	Nd1—O4 ⁱ	2.508 (5)
C2—C3	1.386 (11)	Nd1—O5	2.512 (5)
C3—N2	1.328 (11)	Nd1—O1W	2.549 (6)
C3—H3	0.9300	Nd1—O2 ⁱⁱⁱ	2.557 (5)
C4—N2	1.345 (11)	Nd1—O2	2.573 (5)
C4—C5	1.379 (11)	Nd1—N1 ⁱⁱⁱ	2.765 (6)
C4—H4	0.9300	Nd1—O1	2.885 (6)
C5—N1	1.337 (10)	O2—Nd1 ⁱⁱⁱ	2.557 (5)
C5—H5	0.9300	O4—Nd1 ⁱ	2.508 (5)
C6—O4	1.239 (9)	O6—Nd1 ⁱⁱ	2.490 (5)
C6—O3	1.259 (9)	O1W—H1W	0.84 (9)
C6—C6 ⁱ	1.553 (13)	O1W—H2W	0.85 (8)
C7—O5	1.243 (9)	O2W—H3W	0.84 (5)
C7—O6	1.247 (9)	O2W—H4W	0.84 (8)
C7—C7 ⁱⁱ	1.560 (13)		
O1—C1—O2	123.1 (7)	O6 ⁱⁱ —Nd1—O2 ⁱⁱⁱ	151.94 (19)
O1—C1—C2	120.3 (6)	O4 ⁱ —Nd1—O2 ⁱⁱⁱ	72.00 (17)
O2—C1—C2	116.6 (6)	O5—Nd1—O2 ⁱⁱⁱ	107.89 (16)
N1—C2—C3	121.0 (7)	O1W—Nd1—O2 ⁱⁱⁱ	125.89 (18)
N1—C2—C1	115.7 (6)	O2W—Nd1—O2	76.93 (18)
C3—C2—C1	123.3 (7)	O3—Nd1—O2	133.80 (17)
N2—C3—C2	123.2 (8)	O6 ⁱⁱ —Nd1—O2	113.72 (16)
N2—C3—H3	118.4	O4 ⁱ —Nd1—O2	76.60 (17)
C2—C3—H3	118.4	O5—Nd1—O2	153.11 (18)
N2—C4—C5	122.9 (7)	O1W—Nd1—O2	74.92 (18)
N2—C4—H4	118.6	O2 ⁱⁱⁱ —Nd1—O2	60.11 (19)

C5—C4—H4	118.6	O2W—Nd1—N1 ⁱⁱⁱ	97.86 (19)
N1—C5—C4	121.6 (7)	O3—Nd1—N1 ⁱⁱⁱ	72.90 (18)
N1—C5—H5	119.2	O6 ⁱⁱ —Nd1—N1 ⁱⁱⁱ	128.29 (18)
C4—C5—H5	119.2	O4 ⁱ —Nd1—N1 ⁱⁱⁱ	68.70 (19)
O4—C6—O3	126.2 (6)	O5—Nd1—N1 ⁱⁱⁱ	65.79 (18)
O4—C6—C6 ⁱ	117.3 (8)	O1W—Nd1—N1 ⁱⁱⁱ	131.7 (2)
O3—C6—C6 ⁱ	116.4 (8)	O2 ⁱⁱⁱ —Nd1—N1 ⁱⁱⁱ	59.62 (17)
O5—C7—O6	127.3 (6)	O2—Nd1—N1 ⁱⁱⁱ	116.80 (17)
O5—C7—C7 ⁱⁱ	116.5 (8)	O2W—Nd1—O1	66.01 (18)
O6—C7—C7 ⁱⁱ	116.2 (8)	O3—Nd1—O1	128.48 (16)
C5—N1—C2	116.2 (7)	O6 ⁱⁱ —Nd1—O1	66.65 (16)
C5—N1—Nd1 ⁱⁱⁱ	126.3 (5)	O4 ⁱ —Nd1—O1	113.54 (17)
C2—N1—Nd1 ⁱⁱⁱ	114.6 (5)	O5—Nd1—O1	120.34 (17)
C3—N2—C4	114.9 (7)	O1W—Nd1—O1	64.46 (19)
O2W—Nd1—O3	149.08 (18)	O2 ⁱⁱⁱ —Nd1—O1	99.62 (15)
O2W—Nd1—O6 ⁱⁱ	83.06 (18)	O2—Nd1—O1	47.38 (16)
O3—Nd1—O6 ⁱⁱ	80.47 (18)	N1 ⁱⁱⁱ —Nd1—O1	158.20 (17)
O2W—Nd1—O4 ⁱ	139.97 (17)	C1—O1—Nd1	87.4 (4)
O3—Nd1—O4 ⁱ	65.15 (16)	C1—O2—Nd1 ⁱⁱⁱ	122.1 (4)
O6 ⁱⁱ —Nd1—O4 ⁱ	135.42 (18)	C1—O2—Nd1	101.6 (4)
O2W—Nd1—O5	76.22 (19)	Nd1 ⁱⁱⁱ —O2—Nd1	119.89 (19)
O3—Nd1—O5	73.09 (18)	C6—O3—Nd1	120.1 (4)
O6 ⁱⁱ —Nd1—O5	64.36 (16)	C6—O4—Nd1 ⁱ	119.1 (4)
O4 ⁱ —Nd1—O5	124.93 (17)	C7—O5—Nd1	121.0 (4)
O2W—Nd1—O1W	130.01 (19)	C7—O6—Nd1 ⁱⁱ	121.8 (4)
O3—Nd1—O1W	68.27 (19)	Nd1—O1W—H1W	125 (5)
O6 ⁱⁱ —Nd1—O1W	71.92 (19)	Nd1—O1W—H2W	117 (6)
O4 ⁱ —Nd1—O1W	69.52 (19)	H1W—O1W—H2W	105 (8)
O5—Nd1—O1W	125.09 (18)	Nd1—O2W—H3W	124 (5)
O2W—Nd1—O2 ⁱⁱⁱ	68.90 (17)	Nd1—O2W—H4W	128 (5)
O3—Nd1—O2 ⁱⁱⁱ	124.64 (16)	H3W—O2W—H4W	106 (8)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—H1W \cdots O1 ^{iv}	0.84 (9)	2.02 (6)	2.707 (8)	139 (7)
O1W—H2W \cdots O6 ^v	0.85 (8)	2.07 (4)	2.838 (8)	152 (6)
O2W—H3W \cdots N2 ^{vi}	0.84 (5)	2.50 (5)	3.229 (9)	145 (6)
O2W—H4W \cdots O4 ^{vii}	0.84 (8)	2.13 (4)	2.872 (8)	147 (7)

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

Fig. 1

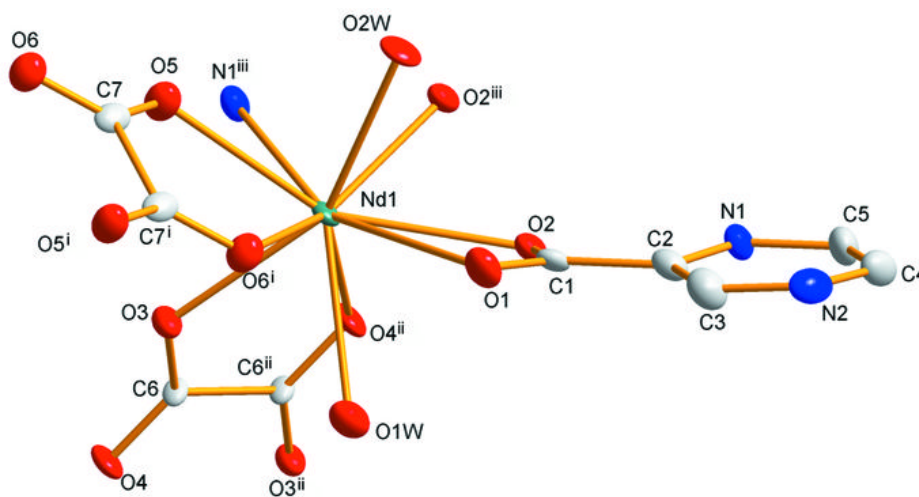


Fig. 2

