Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[(μ_4-iminiodiacetato)bis(μ_3-iminodiacetato)lanthanum(III)nickel(II)] monohydrate]

Xiang-Yang Hu,[a] Yan-Ping Ren[a] and Seik Weng Ng[b]*

[a]Key Laboratory of Analytical Sciences of the Ministry of Education, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

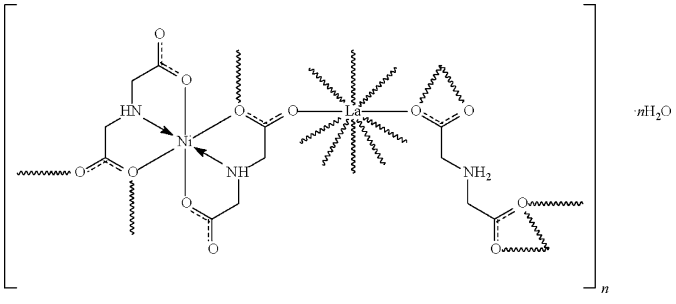
Received 11 June 2007; accepted 5 July 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.024; wR factor = 0.062; data-to-parameter ratio = 14.4.

The Ni^{II} atom in the title compound, $\{[LaNi(C_4H_5NO_4)_2(C_4H_6NO_4)]\cdot H_2O\}_n$ is O,N,O'-chelated by two iminodiacetate dianions and it occupies a special position of site symmetry $\overline{1}$; the $[Ni(C_4H_5NO_4)_2]$ unit functions as a μ_2-bridge that links the $[La(C_4H_6NO_4)]$ units into a layer structure. The iminiodiacetate monoanion in the $O,O'_{carboxyl}$-chelated $[La(C_4H_6NO_4)]$ unit lies about a special position of site symmetry 2; one of the two O atoms is also coordinated to another La atom. The rare-earth atom lies in a bicapped square-antiprismatic environment in the layer coordination polymer.

Related literature

Heterometallic derivatives of iminodiacetic acid are exemplified by diaquabis(iminodiacetato)calciumcobalt tetrahydrate (Kuz'menko *et al.*, 1992) and diaquabis(iminodiacetato)-cadmiumcobalt (Long *et al.*, 2003). For a lanthanum/zinc complex, see: Xu *et al.* (2004). For lanthanum/copper complexes, see: Ren *et al.* (2003*a*,*b*); Liu *et al.* (2003). For lanthanum/nickel complexes, see: Kong *et al.* (2007). For diaqua(iminodiacetato)nickel, see: Wu *et al.* (2003). For other lanthanum derivatives, see: Albertsson & Oskarsson (1968, 1974); Bombieri *et al.* (1974); Li *et al.* (1997, 1999).



Experimental

Crystal data

$[LaNi(C_4H_5NO_4)_2(C_4H_6NO_4)]\cdot H_2O$
M_r = 609.91
Monoclinic, $C2/c$
a = 9.7390 (4) Å
b = 23.859 (1) Å
c = 8.5312 (4) Å
β = 114.732 (1)°
V = 1800.5 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.47 mm^{-1}
T = 173 (2) K
0.29 × 0.12 × 0.12 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.531, T_{max} = 0.681
7464 measured reflections
2049 independent reflections
2046 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.062
S = 1.25
2049 reflections
142 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected bond lengths (Å).

La1—O1^{i}	2.558 (2)	La1—O5^{v}	2.673 (2)
La1—O1^{ii}	2.558 (2)	La1—O6^{iv}	2.773 (2)
La1—O2	2.585 (2)	La1—O6^{v}	2.773 (2)
La1—O2^{iii}	2.585 (2)	Ni1—O2	2.048 (2)
La1—O5	2.438 (2)	Ni1—O3	2.038 (2)
La1—O5^{iii}	2.438 (2)	Ni1—N1	2.093 (3)
La1—O5^{iv}	2.673 (2)		

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

The authors thank Xiamen University and the University of Malaya for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HJ3046).

References

Albertsson, J. & Oskarsson, A. (1968). *Acta Chem. Scand.* **22**, 1700–1702.
Albertsson, J. & Oskarsson, A. (1974). *Acta Chem. Scand.* **28**, 347–355.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bombieri, G., Forsellini, E., Tomat, G., Magon, L. & Graziani, R. (1974). *Acta Cryst.* B**30**, 2659–2663.
Bruker (2002). *SAINT* (Version 6.28A) and *SMART* (Version 6.28A). Bruker AXS Inc., Madison, Wisconsin, USA.
Kong, X.-J., Ren, Y.-P., Long, L.-S., Zheng, Z.-P., Huang, R.-B. & Zheng, L.-S. (2007). *J. Am. Chem. Soc.* **129**, 7106–7107.
Kuz'menko, I. V., Polynova, T. N., Porai-Koshits, M. A. & Poznyak, A. L. (1992). *Koord. Khim.* **18**, 620–626.
Li, J.-R., Wang, Z.-M., Yan, C.-H., Zhou, L.-P. & Jin, T.-Z. (1999). *Acta Cryst.* C**55**, 2073–2075.
Li, J.-R., Zhou, L.-P. & Jin, T. Z. (1997). *Chem. J. Chin. Univ.* **18**, 1255–1258.

  doi:10.1107/S1600536807032904

Liu, Q.-D., Li, J.-R., Gao, S., Ma, B.-Q., Kou, H. Z., Ouyang, L., Huang, R.-L., Zhang, X.-X. & Yu, K.-B. (2003). *Eur. J. Inorg. Chem.* pp. 731–736.
Long, L.-S., Ren, Y.-P., Huang, R.-B., Zheng, L.-S. & Ng, S. W. (2003). *Appl. Organomet. Chem.* **17**, 741–742.
Ren, Y.-P., Long, L.-S., Mao, B.-W., Yuan, Y.-Z., Huang, R.-B. & Zheng, L.-S. (2003*a*). *Angew. Chem. Int. Ed.* **42**, 532–535.
Ren, Y.-P., Long, L.-S., Mao, B.-W., Yuan, Y.-Z., Huang, R.-B. & Zheng, L.-S. (2003*b*). *Angew. Chem. Int. Ed.* **42**, 2108.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Westrip, S. P. (2007). *publCIF*. In preparation.
Wu, Y.-R., Long, L.-S., Huang, R.-B., Zheng, L.-S. & Ng, S. W. (2003). *Acta Cryst.* E**59**, m390–m392.
Xu, H.-B., Zhao, Y.-H., Su, Z.-M., Li, G.-H., Ma, Y., Shao, K.-S., Zhu, D.-X., Zhang, H.-J. & Yue, S.-M. (2004). *Chem. Lett.* **33**, 446–447.

supplementary materials

Acta Cryst. (2007). E**63**, m2124-m2125 [**doi:10.1107/S1600536807032904**]

Poly[[(μ_4-iminiodiacetato)bis(μ_3-iminodiacetato)lanthanum(III)nickel(II)] monohydrate]

X.-Y. Hu, Y.-P. Ren and S. W. Ng

Comment

The iminodiacetate [$^{-}$O(O)CCH$_2$NHCH$_2$C(O)O^{-}] dianion forms a large number of crystalline metal derivatives in which it *O*,*N*,*O*'-chelates to the metal. These studies have largely addressed compounds having one type of metal only; diaquadi(iminodiacetato)calciumcobalt tetrahydrate (Kuz'menko *et al.*, 1992) and diaquadi(iminodiacetato)cadmiumcobalt (Long *et al.*, 2003) represent unusual examples of heterometallic systems. The two compound adopt layer structures. A series of lanthanum/copper complexes is known that exhibit porosity; the three-dimensional network is also thermally stable when lattice molecules are removed (Ren *et al.*, 2003*a*,b). Another series of lanthanum/copper complexes, [LnCu$_6$(OH)$_3$(C$_4$H$_6$NO$_4$)$_2$(C$_4$H$_5$NO$_4$)$_4$]·(ClO$_4$)$_2$·25H$_2$O, features antiferromagnetic Ln–Cu interactions as the rare earth atom is surrounded by six copper atoms at a distance of approximately 3.5 Å (Liu *et al.*, 2003).

The present study extends an earlier study on a metal derivative of iminodiacetic acid that features both *d*- and *f*-block elements within the same framework. The hydrothermal reaction of lanthanum nitrate, nickel nitrate and iminodiacetic acid gave a gigantic metal cluster consisting of 20 lanthanum and 30 nickel atoms in the formula unit, [La$_{20}$Ni$_{30}$(C$_4$H$_5$NO$_4$)$_{30}$(CO$_3$)$_6$(NO$_3$)$_6$(OH)$_{30}$(H$_2$O)$_{12}$](CO$_3$)$_6$·72H$_2$O (Kong *et al.*, 2007). Changing the lanthanum nitrate reactant to lanthanum chloride yielded the title compound, which has only one of each metal atom in formula unit. In [(C$_4$H$_5$NO$_4$)$_2$(C$_4$H$_6$NO$_4$)LaNi·H$_2$O]$_n$ (Fig. 1), two deprotonated iminodiacetate dianions each chelate to the nickel atom, the three chelating atoms occupying *fac* positions of the octahedral geometry of nickel, a feature that is also found in diaqua(iminodiacetato)nickel (Wu *et al.*, 2003). Meanwhile, the iminodiacetate monoanion, which lies about a twofold rotation axis, *O*,*O*'-chelates to the water-coordinated lanthanum atom. One of the two oxygen atoms is additionally involved in bridging to another lanthanum atom, so that the geometry of the *f*-block metal is a ten-coordinate bicapped square antiprism (Fig. 2) in the layer structure. Hydrogen bonds link the layers into a three-dimensional network motif.

The somewhat uncommon iminodiacetate monoanion has also been found in other rare-earth complexes such as the neodymium (Albertsson & Oskarsson, 1968) praseodymium (Albertsson & Oskarsson, 1974; Li *et al.*, 1999), uranium (Bombieri *et al.*, 1974), yttrium (Li *et al.*, 1997) and lanthanum complexes. The lanthanum complex is also a heterometallic compound having lanthanum and zinc bridged into a linear chain (Xu *et al.*, 2004).

Experimental

Iminodiacetic acid (0.399 g, 3.0 mmol), nickel nitrate hexahydrate (0.436 g, 1.50 mmol) and lanthanum trichloride monohydrate (0.407 g, 1.0 mmol) were dissolved in water (15 ml). Aqueous sodium hydroxide (1 *M*) was added to the solution to a pH of approximately 5.5. The mixtue was placed din a 25-ml, Teflon-lined, stainless-steel Parr bomb. The bomb was heated to 453 K for 8 h. It was cooled to 373 K at 20 K h^{-1} and then kept at this temperature of 3 h before being allowed to cool to room temperate at 3 K h^{-1}. Blue needle-shaped crystals were obtained in 70% yield (based on iminodiacetic acid. CH&N elemental analysis. Calc. for C$_{12}$H$_{18}$LaN$_3$NiO$_{13}$: Found: C 23.63, N 6.89, H, 2.97%. Found: C 23.45, N, 6.82, H 3.10%.

Refinement

The water molecule was allowed to refine off the twofold rotation axis, and its anisotropic temperature factors were restrained to be nearly isotropic. An examination of hydrogen bonding interactions suggested that one of its H-atoms occupies the symmetry-related site of the water O-atom and would then not hydrogen bond to an acceptor. The other should be linked to an acceptor. The positions of the two were then set manually. The two H-atoms were not refined.

Carbon- and nitrogen-bound H-atoms were positioned geometrically (C–H 0.93 and 0.97 Å; N–H 0.88 Å), and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

The final difference Fourier map had a large peak at 0.85 Å from La1 but was otherwise featureless.

Figures

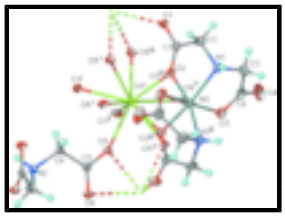


Fig. 1. **Figure 1**. Thermal ellipsoid plot of a portion of the polymeric structure of $[(C_4H_5NO_4)_2(C_4H_6NO_4)LaNi{\cdot}H_2O]_n$; displacement ellipsoids are drawn at the 70% probability level, and hydrogen atoms as spheres of arbitrary radius. The water molecule is not shown. Symmetry codes: (i)1 − *x*, 1 − *y*, 2 − *z*; (ii) *x*, 1 − *y*, *z* − 1/2; (iii) 1 - *x* *y*, 3/2 − *z*; (iv) 1 − *x*, 1 − *y*, 1 − *z*; (v) *x*, 1 − *y*, 1/2 + *z*.

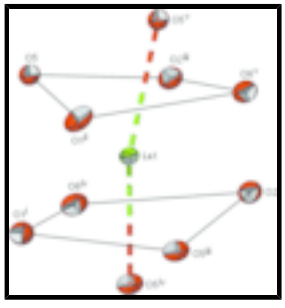


Fig. 2. **Figure 2**. Bicapped square-antiprismatic geometry of lanthanum.

Poly[[(μ4-iminiodiacetato)bis(μ3-iminodiacetato)lanthanum(III)nickel(II)] monohydrate]

Crystal data

$[LaNi(C_4H_5NO_4)_2(C_4H_6NO_4)]{\cdot}H_2O$	F_{000} = 1200
M_r = 609.91	D_x = 2.250 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 6635 reflections
a = 9.7390 (4) Å	θ = 2.5–28.3º
b = 23.859 (1) Å	μ = 3.47 mm^{-1}
c = 8.5312 (4) Å	*T* = 173 (2) K
β = 114.732 (1)º	Column, blue
V = 1800.5 (1) Å^3	0.29 × 0.12 × 0.12 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	2049 independent reflections
Radiation source: fine-focus sealed tube	2046 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 173(2)$ K	$\theta_{max} = 27.5^{o}$
φ and ω scans	$\theta_{min} = 1.7^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.531$, $T_{max} = 0.681$	$k = -30 \rightarrow 30$
7464 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.024$	H-atom parameters constrained
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.025P)^2 + 7.2608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.25$	$(\Delta/\sigma)_{max} = 0.001$
2049 reflections	$\Delta\rho_{max} = 1.07$ e Å^{-3}
142 parameters	$\Delta\rho_{min} = -0.59$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
La1	0.5000	0.506465 (9)	0.7500	0.01011 (8)	
Ni1	0.5000	0.66141 (2)	0.7500	0.01438 (12)	
O1	0.3730 (3)	0.58240 (9)	1.0855 (3)	0.0192 (5)	
O2	0.4288 (2)	0.59806 (9)	0.8602 (3)	0.0160 (4)	
O3	0.2951 (3)	0.66506 (9)	0.5435 (3)	0.0201 (5)	
O4	0.0546 (3)	0.68604 (11)	0.4774 (4)	0.0313 (6)	
O5	0.6443 (2)	0.47668 (9)	0.5902 (3)	0.0148 (4)	
O6	0.7921 (2)	0.45955 (9)	0.4593 (3)	0.0175 (4)	
O1w	0.958 (3)	0.4153 (7)	0.255 (4)	0.175 (8)	0.50
H1w1	0.9572	0.4361	0.3381	0.262*	0.50
H1w2	1.0410	0.4162	0.2436	0.262*	0.50
N1	0.3913 (3)	0.71032 (10)	0.8677 (3)	0.0166 (5)	
H1n	0.4419	0.7416	0.9068	0.020*	
N2	1.0000	0.40180 (15)	0.7500	0.0144 (7)	
H2n1	0.9617	0.3800	0.6587	0.017*	0.50
H2n2	1.0383	0.3800	0.8413	0.017*	0.50

C1	0.3964 (3)	0.61346 (12)	0.9834 (4)	0.0151 (5)
C2	0.3938 (4)	0.67636 (13)	1.0123 (4)	0.0224 (7)
H2A	0.3035	0.6855	1.0327	0.027*
H2B	0.4842	0.6866	1.1176	0.027*
C3	0.2385 (4)	0.72313 (14)	0.7375 (4)	0.0217 (6)
H3A	0.2335	0.7633	0.7064	0.026*
H3B	0.1652	0.7167	0.7883	0.026*
C4	0.1924 (4)	0.68802 (13)	0.5741 (4)	0.0200 (6)
C5	0.7663 (3)	0.45831 (12)	0.5895 (4)	0.0137 (5)
C6	0.8756 (3)	0.43440 (13)	0.7608 (4)	0.0169 (6)
H6A	0.9192	0.4656	0.8434	0.020*
H6B	0.8191	0.4100	0.8070	0.020*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.01116 (12)	0.01078 (12)	0.00888 (12)	0.000	0.00465 (9)	0.000
Ni1	0.0187 (3)	0.0133 (3)	0.0114 (2)	0.000	0.0065 (2)	0.000
O1	0.0244 (12)	0.0185 (11)	0.0194 (11)	0.0046 (8)	0.0137 (10)	0.0052 (8)
O2	0.0205 (10)	0.0138 (10)	0.0156 (10)	0.0006 (8)	0.0096 (9)	0.0005 (8)
O3	0.0241 (11)	0.0190 (11)	0.0139 (10)	0.0018 (9)	0.0048 (9)	−0.0010 (8)
O4	0.0216 (12)	0.0256 (13)	0.0340 (14)	0.0035 (10)	−0.0008 (11)	−0.0099 (11)
O5	0.0124 (9)	0.0201 (10)	0.0121 (9)	0.0036 (8)	0.0052 (8)	0.0011 (8)
O6	0.0168 (10)	0.0225 (11)	0.0148 (10)	0.0021 (8)	0.0082 (8)	0.0010 (8)
O1w	0.169 (12)	0.198 (11)	0.168 (10)	0.028 (8)	0.082 (9)	−0.011 (8)
N1	0.0220 (13)	0.0115 (11)	0.0160 (12)	−0.0005 (9)	0.0077 (11)	−0.0004 (9)
N2	0.0115 (16)	0.0148 (16)	0.0150 (16)	0.000	0.0038 (13)	0.000
C1	0.0139 (13)	0.0169 (14)	0.0119 (13)	0.0022 (10)	0.0029 (11)	0.0008 (10)
C2	0.0375 (19)	0.0163 (15)	0.0182 (15)	0.0020 (13)	0.0165 (14)	−0.0005 (12)
C3	0.0230 (16)	0.0201 (15)	0.0204 (15)	0.0057 (12)	0.0075 (13)	−0.0019 (12)
C4	0.0248 (16)	0.0136 (14)	0.0177 (15)	0.0015 (12)	0.0052 (13)	0.0012 (11)
C5	0.0130 (13)	0.0129 (13)	0.0145 (13)	−0.0007 (10)	0.0052 (11)	−0.0004 (10)
C6	0.0119 (13)	0.0242 (15)	0.0154 (14)	0.0047 (11)	0.0065 (11)	0.0040 (11)

Geometric parameters (Å, °)

La1—O1^{i}	2.558 (2)	O5—La1^{iv}	2.673 (2)
La1—O1^{ii}	2.558 (2)	O6—C5	1.238 (4)
La1—O2	2.585 (2)	O6—La1^{iv}	2.773 (2)
La1—O2^{iii}	2.585 (2)	O1w—H1w1	0.87
La1—O5	2.438 (2)	O1w—H1w2	0.856
La1—O5^{iii}	2.438 (2)	N1—C2	1.468 (4)
La1—O5^{iv}	2.673 (2)	N1—C3	1.469 (4)
La1—O5^{v}	2.673 (2)	N1—H1n	0.8800
La1—O6^{iv}	2.773 (2)	N2—C6	1.475 (3)
La1—O6^{v}	2.773 (2)	N2—C6^{vi}	1.475 (3)
Ni1—O2	2.048 (2)	N2—H2n1	0.8800

Ni1—O2^{iii}	2.048 (2)	N2—H2n2	0.8800
Ni1—O3	2.038 (2)	C1—C2	1.523 (4)
Ni1—O3^{iii}	2.038 (2)	C2—H2A	0.9900
Ni1—N1	2.093 (3)	C2—H2B	0.9900
Ni1—N1^{iii}	2.093 (3)	C3—C4	1.524 (4)
O1—C1	1.235 (4)	C3—H3A	0.9900
O1—La1^{i}	2.558 (2)	C3—H3B	0.9900
O2—C1	1.272 (4)	C5—C6	1.514 (4)
O3—C4	1.260 (4)	C6—H6A	0.9900
O4—C4	1.248 (4)	C6—H6B	0.9900
O5—C5	1.269 (3)		
O5^{iii}—La1—O5	146.10 (10)	O3—Ni1—N1^{iii}	94.06 (10)
O5^{iii}—La1—O1^{ii}	78.79 (7)	O3^{iii}—Ni1—N1^{iii}	83.21 (10)
O5—La1—O1^{ii}	73.20 (7)	O2^{iii}—Ni1—N1^{iii}	81.68 (9)
O5^{iii}—La1—O1^{i}	73.20 (7)	O2—Ni1—N1^{iii}	165.47 (9)
O5—La1—O1^{i}	78.79 (7)	N1—Ni1—N1^{iii}	112.22 (14)
O1^{ii}—La1—O1^{i}	68.03 (11)	C1—O1—La1^{i}	134.0 (2)
O5^{iii}—La1—O2	74.83 (7)	C1—O2—Ni1	114.52 (19)
O5—La1—O2	138.99 (7)	C1—O2—La1	137.87 (19)
O1^{ii}—La1—O2	139.33 (7)	Ni1—O2—La1	105.28 (8)
O1^{i}—La1—O2	130.01 (7)	C4—O3—Ni1	114.5 (2)
O5^{iii}—La1—O2^{iii}	138.99 (7)	C5—O5—La1	149.69 (19)
O5—La1—O2^{iii}	74.83 (7)	C5—O5—La1^{iv}	96.62 (17)
O1^{ii}—La1—O2^{iii}	130.01 (7)	La1—O5—La1^{iv}	113.52 (8)
O1^{i}—La1—O2^{iii}	139.33 (7)	C5—O6—La1^{iv}	92.63 (17)
O2—La1—O2^{iii}	64.59 (9)	H1w1—O1w—H1w2	114
O5^{iii}—La1—O5^{iv}	119.13 (8)	C2—N1—C3	113.9 (3)
O5—La1—O5^{iv}	66.48 (8)	C2—N1—Ni1	105.16 (18)
O1^{ii}—La1—O5^{iv}	67.37 (7)	C3—N1—Ni1	108.01 (19)
O1^{i}—La1—O5^{iv}	129.37 (7)	C2—N1—H1n	109.9
O2—La1—O5^{iv}	99.69 (6)	C3—N1—H1n	109.9
O2^{iii}—La1—O5^{iv}	65.00 (7)	Ni1—N1—H1n	109.9
O5^{iii}—La1—O5^{v}	66.48 (8)	C6—N2—C6^{vi}	116.3 (3)
O5—La1—O5^{v}	119.13 (8)	C6—N2—H2n1	108.2
O1^{ii}—La1—O5^{v}	129.37 (7)	C6^{vi}—N2—H2n1	108.2
O1^{i}—La1—O5^{v}	67.37 (7)	C6—N2—H2n2	108.2
O2—La1—O5^{v}	65.00 (7)	C6^{vi}—N2—H2n2	108.2
O2^{iii}—La1—O5^{v}	99.69 (7)	H2n1—N2—H2n2	107.4
O5^{iv}—La1—O5^{v}	162.69 (9)	O1—C1—O2	126.3 (3)
O5^{iii}—La1—O6^{v}	113.67 (6)	O1—C1—C2	117.2 (3)
O5—La1—O6^{v}	76.65 (7)	O2—C1—C2	116.4 (3)
O1^{ii}—La1—O6^{v}	136.56 (7)	N1—C2—C1	113.8 (3)

O1^{i}—La1—O6^{v}	76.04 (7)	N1—C2—H2A	108.8
O2—La1—O6^{v}	82.97 (7)	C1—C2—H2A	108.8
O2^{iii}—La1—O6^{v}	68.16 (7)	N1—C2—H2B	108.8
O5^{iv}—La1—O6^{v}	125.93 (6)	C1—C2—H2B	108.8
O5^{v}—La1—O6^{v}	47.57 (6)	H2A—C2—H2B	107.7
O5^{iii}—La1—O6^{iv}	76.65 (7)	N1—C3—C4	113.3 (3)
O5—La1—O6^{iv}	113.67 (6)	N1—C3—H3A	108.9
O1^{ii}—La1—O6^{iv}	76.04 (7)	C4—C3—H3A	108.9
O1^{i}—La1—O6^{iv}	136.56 (7)	N1—C3—H3B	108.9
O2—La1—O6^{iv}	68.16 (7)	C4—C3—H3B	108.9
O2^{iii}—La1—O6^{iv}	82.97 (7)	H3A—C3—H3B	107.7
O5^{iv}—La1—O6^{iv}	47.57 (6)	O4—C4—O3	125.0 (3)
O5^{v}—La1—O6^{iv}	125.93 (6)	O4—C4—C3	116.7 (3)
O6^{v}—La1—O6^{iv}	145.99 (9)	O3—C4—C3	118.2 (3)
O3—Ni1—O3^{iii}	175.11 (13)	O6—C5—O5	122.5 (3)
O3—Ni1—O2^{iii}	91.83 (9)	O6—C5—C6	123.4 (3)
O3^{iii}—Ni1—O2^{iii}	91.78 (9)	O5—C5—C6	114.1 (2)
O3—Ni1—O2	91.78 (9)	N2—C6—C5	113.8 (2)
O3^{iii}—Ni1—O2	91.83 (9)	N2—C6—H6A	108.8
O2^{iii}—Ni1—O2	84.85 (12)	C5—C6—H6A	108.8
O3—Ni1—N1	83.21 (10)	N2—C6—H6B	108.8
O3^{iii}—Ni1—N1	94.06 (10)	C5—C6—H6B	108.8
O2^{iii}—Ni1—N1	165.47 (10)	H6A—C6—H6B	107.7
O2—Ni1—N1	81.68 (9)		
O3—Ni1—O2—C1	−102.5 (2)	O1^{ii}—La1—O5—La1^{iv}	72.12 (9)
O3^{iii}—Ni1—O2—C1	74.2 (2)	O1^{i}—La1—O5—La1^{iv}	142.32 (10)
O2^{iii}—Ni1—O2—C1	165.8 (2)	O2—La1—O5—La1^{iv}	−77.24 (12)
N1—Ni1—O2—C1	−19.6 (2)	O2^{iii}—La1—O5—La1^{iv}	−68.93 (8)
N1^{iii}—Ni1—O2—C1	143.8 (3)	O5^{iv}—La1—O5—La1^{iv}	0.0
O3—Ni1—O2—La1	91.68 (9)	O5^{v}—La1—O5—La1^{iv}	−161.70 (9)
O3^{iii}—Ni1—O2—La1	−91.62 (9)	O6^{v}—La1—O5—La1^{iv}	−139.55 (9)
O2^{iii}—Ni1—O2—La1	0.0	O6^{iv}—La1—O5—La1^{iv}	6.16 (11)
N1—Ni1—O2—La1	174.55 (10)	O3—Ni1—N1—C2	117.8 (2)
N1^{iii}—Ni1—O2—La1	−22.0 (4)	O3^{iii}—Ni1—N1—C2	−66.3 (2)
O5^{iii}—La1—O2—C1	25.4 (3)	O2^{iii}—Ni1—N1—C2	47.2 (5)
O5—La1—O2—C1	−151.7 (3)	O2—Ni1—N1—C2	25.0 (2)
O1^{ii}—La1—O2—C1	76.8 (3)	N1^{iii}—Ni1—N1—C2	−150.6 (2)
O1^{i}—La1—O2—C1	−26.4 (3)	O3—Ni1—N1—C3	−4.2 (2)
O2^{iii}—La1—O2—C1	−160.6 (3)	O3^{iii}—Ni1—N1—C3	171.7 (2)
O5^{iv}—La1—O2—C1	143.2 (3)	O2^{iii}—Ni1—N1—C3	−74.9 (4)
O5^{v}—La1—O2—C1	−45.3 (3)	O2—Ni1—N1—C3	−97.0 (2)

O6^{v}—La1—O2—C1	−91.5 (3)	N1^{iii}—Ni1—N1—C3	87.4 (2)
O6^{iv}—La1—O2—C1	106.9 (3)	La1^{i}—O1—C1—O2	42.4 (5)
O5^{iii}—La1—O2—Ni1	−173.97 (10)	La1^{i}—O1—C1—C2	−134.4 (3)
O5—La1—O2—Ni1	8.89 (15)	Ni1—O2—C1—O1	−168.5 (2)
O1^{ii}—La1—O2—Ni1	−122.63 (10)	La1—O2—C1—O1	−9.1 (5)
O1^{i}—La1—O2—Ni1	134.23 (9)	Ni1—O2—C1—C2	8.3 (3)
O2^{iii}—La1—O2—Ni1	0.0	La1—O2—C1—C2	167.7 (2)
O5^{iv}—La1—O2—Ni1	−56.24 (9)	C3—N1—C2—C1	89.9 (3)
O5^{v}—La1—O2—Ni1	115.28 (10)	Ni1—N1—C2—C1	−28.2 (3)
O6^{v}—La1—O2—Ni1	69.12 (9)	O1—C1—C2—N1	−168.1 (3)
O6^{iv}—La1—O2—Ni1	−92.54 (9)	O2—C1—C2—N1	14.7 (4)
O2^{iii}—Ni1—O3—C4	159.8 (2)	C2—N1—C3—C4	−103.8 (3)
O2—Ni1—O3—C4	74.9 (2)	Ni1—N1—C3—C4	12.7 (3)
N1—Ni1—O3—C4	−6.5 (2)	Ni1—O3—C4—O4	−166.8 (3)
N1^{iii}—Ni1—O3—C4	−118.5 (2)	Ni1—O3—C4—C3	16.0 (4)
O5^{iii}—La1—O5—C5	−78.8 (4)	N1—C3—C4—O4	162.7 (3)
O1^{ii}—La1—O5—C5	−114.4 (4)	N1—C3—C4—O3	−19.9 (4)
O1^{i}—La1—O5—C5	−44.2 (4)	La1^{iv}—O6—C5—O5	−8.2 (3)
O2—La1—O5—C5	96.2 (4)	La1^{iv}—O6—C5—C6	171.1 (3)
O2^{iii}—La1—O5—C5	104.6 (4)	La1—O5—C5—O6	−165.4 (3)
O5^{iv}—La1—O5—C5	173.5 (4)	La1^{iv}—O5—C5—O6	8.6 (3)
O5^{v}—La1—O5—C5	11.8 (4)	La1—O5—C5—C6	15.2 (5)
O6^{v}—La1—O5—C5	33.9 (4)	La1^{iv}—O5—C5—C6	−170.8 (2)
O6^{iv}—La1—O5—C5	179.6 (4)	C6^{vi}—N2—C6—C5	77.8 (2)
C5^{v}—La1—O5—C5	25.2 (4)	O6—C5—C6—N2	−12.6 (4)
C5^{iv}—La1—O5—C5	174.8 (3)	O5—C5—C6—N2	166.8 (3)
O5^{iii}—La1—O5—La1^{iv}	107.71 (8)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1n···O4^{vii}	0.88	2.00	2.877 (4)	176
N2—H2n1···O4^{iv}	0.88	1.92	2.752 (4)	156
N2—H2n2···O4^{viii}	0.88	1.92	2.752 (4)	156
O1w—H1w1···O6	0.87	2.31	3.01 (2)	138

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

Fig. 1

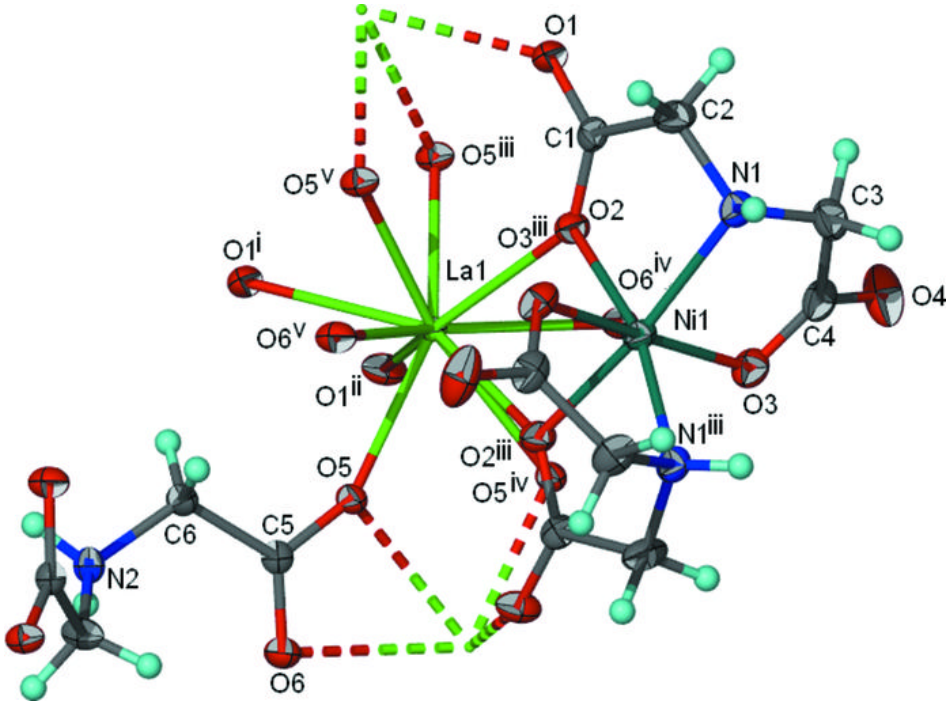

O1
C2
C1
O5iii
O5v
N1
C3
O2
O3iii
O1i
La1
O6iv
O4
Ni1
O6v
C4
O1ii
O3
N1iii
O2iii
O5
O5iv
C6
C5
N2
O6

Fig. 2