Diaquabis(biuretato-$\kappa^2 O,O'$)nickel(II) dichloride

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.004 Å
R factor = 0.047
wR factor = 0.101
Data-to-parameter ratio = 23.5

For details of how these key indicators were
automatically derived from the article, see
http://journals.iucr.org/e.

The title compound, [Ni(C$_2$H$_5$N$_3$O$_2$)$_2$(H$_2$O)$_2$]Cl$_2$, contains
Ni^{2+} cations octahedrally coordinated by two bidentate biuret
molecules in an O,O'-bidentate coordination mode and two
water molecules, the latter in a *trans* configuration. Two
chloride anions provide charge compensation. Numerous N—
H$\cdots$O (mean H$\cdots$O = 2.17 Å, mean N—H$\cdots$O = 164° and
mean N$\cdots$O = 2.991 Å), N—H$\cdots$Cl (mean H$\cdots$Cl = 2.46 Å,
mean N—H$\cdots$Cl = 162° and mean N$\cdots$Cl = 3.278 Å) and O—
H$\cdots$Cl (mean H$\cdots$Cl = 2.19 Å, mean O—H$\cdots$Cl = 159° and
mean O$\cdots$Cl = 3.068 Å) hydrogen bonds help to stabilize the
crystal packing.

Comment

Biuret, H$_2$N—CO—NH—CO—NH$_2$ (or C$_2$H$_5$N$_3$O$_2$), has long
been recognized as a ligand in coordination chemistry
(Wiedemann, 1848). In low-pH or neutral conditions, biuret
commonly shows O,O'-bidentate coordination to metal
cations [*e.g.* with zinc (Nardelli *et al.*, 1963), copper (Freeman
& Smith, 1966) or samarium (Haddad, 1987)]. When biuret is
deprotonated in basic conditions, N,N'-bidentate coordination
can arise [*e.g.* with copper (Pajunen & Pajunen, 1982)].

(I)
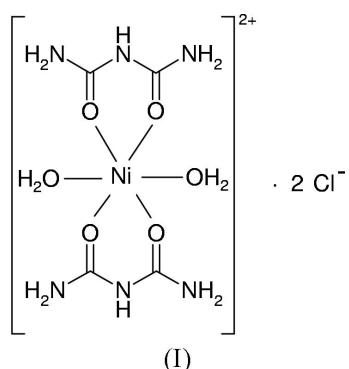
In the present paper, we report the synthesis and structure
of a nickel(II) complex of biuret, *viz.* [Ni(C$_2$H$_5$N$_3$O$_2$)$_2$-
(H$_2$O)$_2$]Cl$_2$, (I) (Fig. 1). Compound (I) contains Ni^{2+} cations
coordinated by two distinct biuret molecules, in O,O'-biden-
tate mode (thus forming six-membered chelate rings), and two
trans water molecules. The structure is completed by two
uncoordinated chloride ions, which provide charge balance
and participate in an extensive hydrogen-bond network (see
below). The resulting NiO$_6$ moiety of the [Ni(C$_2$H$_5$-
N$_3$O$_2$)$_2$(H$_2$O)$_2$]$^{2+}$ grouping (Table 1) is close to being an
undistorted octahedron [Ni—O = 2.014 (2)–2.083 (2) Å, mean
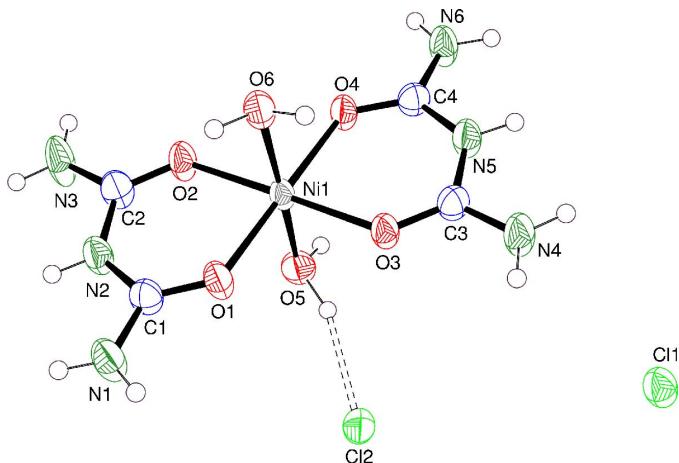
Figure 1
Asymmetric unit of (I), showing 50% probability displacement ellipsoids. H atoms are drawn as small spheres of arbitrary radii and the hydrogen bond is indicated by dashed lines.
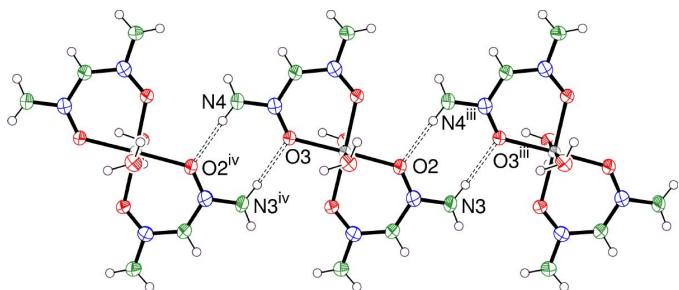
Figure 2
Detail of (I), showing how the N3—H4···O3^{iii} and N4—H6···O2^{iv} hydrogen bonds (dashed lines; see Table 2 for symmetry codes) link the [Ni(C$_2$H$_5$N$_3$O$_2$)$_2$(H$_2$O)$_2$]$^{2+}$ groupings into an infinite chain propagating along [100].

Ni—O = 2.041 (3) Å; *cis* and *trans* O—Ni—O = 87.47 (9)–93.51 (8)° and 176.14 (9)–178.94 (8)°, respectively], indicating that the nickel(II) cation is a good 'fit' for the biuret O,O′ bite angle. The two biuret molecules in (I) can be broken down into two H$_2$N—CO—NH fragments, fused *via* the central HN group [*i.e. via* atoms N2 and N5 in (I)]. For the non-H atoms, the four H$_2$N—CO—NH fragments are all essentially planar (for C1/O1/N1/N2, r.m.s. deviation from the least-squares plane = 0.0021 Å; for C2/O2/N2/N3, 0.0017 Å; for C3/O3/N4/N5, 0.0023 Å; for C4/O4/N5/N6, 0.0032 Å). The dihedral angle between the C1- and C2-containing fragments is 4.8 (3)°, with a corresponding value of 3.19 (3)° for the C3 and C4 fragments. This configuration can be compared with a twist angle between the fused H$_2$N—CO—NH fragments of 6.35° in [Cu(C$_2$H$_5$N$_3$O$_2$)$_2$]Cl$_2$ (Freeman & Smith, 1966). The dihedral angle between mean planes of the two biuret ligand molecules in (I) is 1.90 (13)°.

The Ni atom in (I) is slightly displaced from the least-squares plane of the approximate square of biuret O atoms (O1–O4) coordinating to it, by 0.0086 (13) Å. The biuret O$_4$ square itself is slightly folded, with deviations from the O1–O4 mean plane of −0.0121 (12), 0.0119 (12), 0.0121 (12) and

−0.0119 (12) Å for atoms O1, O2, O3 and O4, respectively. In the copper analogue (Freeman & Smith, 1966), the CuO$_4$ square is constrained by space-group symmetry to be perfectly flat. Overall, the [Ni(C$_2$H$_5$N$_3$O$_2$)$_2$]$^{2+}$ grouping in (I) is close to planar [r.m.s. deviation from the mean plane = 0.030 Å; maximum deviation = 0.076 (3) Å for N2], whereas the [Cu(C$_2$H$_5$N$_3$O$_2$)$_2$]$^{2+}$ grouping in [Cu(C$_2$H$_5$N$_3$O$_2$)$_2$]Cl$_2$ is distinctly puckered (Freeman & Smith, 1966) about the O···O′ axes (bite lines) of the biuret molecules. As well as electrostatic and van der Waals forces, numerous hydrogen bonds (Table 2) help to define the crystal packing in (I). These include N—H···O bonds (mean H···O = 2.17 Å, mean N—H···O = 164° and mean N···O = 2.991 Å) to O acceptors from both the biuret and the water ligands, N—H···Cl interactions (mean H···Cl = 2.46 Å, mean N—H···Cl = 162° and mean N···Cl = 3.278 Å) and O—H···Cl interactions (mean H···Cl = 2.19 Å, mean O—H···Cl = 159° and mean O···Cl = 3.068 Å).

Perhaps the most interesting hydrogen bonds are N3—H4···O3^{iii} and N4—H6···O2^{iv} (see Fig. 2 and Table 2 for symmetry information), which link the [Ni(C$_2$H$_5$N$_3$O$_2$)$_2$(H$_2$O)$_2$]$^{2+}$ groupings into a chain propagating along [100]. The supramolecular (Bernstein *et al.*, 1995) motif is an R_2^2(8) ring. The remaining H bonds serve to crosslink the [100] chains into a three-dimensional network (Fig. 3) *via* the chloride ions. Overall, Cl1 and Cl2 accept five hydrogen bonds each.

Figure 3
Projection on to (100) of (I), showing the hydrogen-bond cross-linking (dashed lines) between the chains shown in Fig. 2.

Experimental

Aqueous solutions of $NiCl_2$ and biuret (both 0.1 M) were mixed in a 1:1 ratio at room temperature, resulting in a green solution. Small block-like green crystals of (I) grew over the course of a few days as the water slowly evaporated and were harvested by vacuum filtration and washing with acetone.

Crystal data

$[Ni(C_2H_5N_3O_2)_2(H_2O)_2]Cl_2$	$D_x = 1.780$ Mg m^{-3}
$M_r = 371.82$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3015
$a = 7.3872$ (4) Å	reflections
$b = 27.5675$ (16) Å	$\theta = 3.0–29.5°$
$c = 7.6687$ (4) Å	$\mu = 1.82$ mm^{-1}
$\beta = 117.344$ (1)°	$T = 293$ (2) K
$V = 1387.21$ (13) Å^3	Block, green
$Z = 4$	$0.15 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART 1000 CCD diffractometer	4037 independent reflections
ω scans	2416 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan ($SADABS$; Bruker, 1999)	$R_{int} = 0.053$
$T_{min} = 0.773$, $T_{max} = 0.839$	$\theta_{max} = 30.0°$
14042 measured reflections	$h = -10 \rightarrow 8$
	$k = -38 \rightarrow 38$
	$l = -9 \rightarrow 10$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2]$
$wR(F^2) = 0.101$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{max} < 0.001$
4037 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
172 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O3	2.014 (2)	Ni1—O1	2.024 (2)
Ni1—O2	2.018 (2)	Ni1—O6	2.080 (2)
Ni1—O4	2.024 (2)	Ni1—O5	2.083 (2)
O1—C1—N2—C2	−5.1 (6)	O4—C4—N5—C3	4.3 (6)
O2—C2—N2—C1	6.7 (6)	O3—C3—N5—C4	−3.3 (6)

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N1—H1$\cdots$Cl2^i	0.86	2.49	3.340 (3)	173
N1—H2$\cdots$O5^{ii}	0.86	2.33	3.089 (4)	147
N2—H3$\cdots$Cl2^{ii}	0.86	2.45	3.266 (3)	158
N3—H4$\cdots$O3^{iii}	0.86	2.10	2.943 (4)	168
N3—H5$\cdots$Cl2^{ii}	0.86	2.43	3.239 (3)	158
N4—H6$\cdots$O2^{iv}	0.86	2.06	2.910 (4)	168
N4—H7$\cdots$Cl1^v	0.86	2.45	3.252 (3)	155
N5—H8$\cdots$Cl1^v	0.86	2.51	3.310 (3)	156
N6—H9$\cdots$Cl1^{vi}	0.86	2.41	3.259 (3)	169
N6—H10$\cdots$O6^{vii}	0.86	2.17	3.023 (3)	173
O5—H11$\cdots$Cl2	0.94	2.16	3.068 (2)	161
O5—H12$\cdots$Cl1^{iii}	0.91	2.21	3.115 (2)	171
O6—H13$\cdots$Cl2^{viii}	0.98	2.18	3.060 (2)	149
O6—H14$\cdots$Cl1^{viii}	0.88	2.20	3.027 (2)	155

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

The water H atoms were found in difference maps and were refined as riding on their carrier atoms in their as-found relative positions. The N-bound H atoms were placed in calculated positions assuming sp^2 hybridization for the N atoms and refined as riding on their carrier atoms. The constraint $U_{iso}(H) = 1.2U_{eq}$(carrier atom) was applied in all cases.

Data collection: $SMART$ (Bruker, 1999); cell refinement: $SAINT$-$Plus$ (Bruker, 1999); data reduction: $SAINT$-$Plus$; program(s) used to solve structure: $SHELXS97$ (Sheldrick, 1997); program(s) used to refine structure: $SHELXL97$ (Sheldrick, 1997); molecular graphics: $ORTEP$-3 (Farrugia, 1997); software used to prepare material for publication: $SHELXL97$.

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supporting information

Diaquabis(biuretato-*κ²O,O′*)nickel(II) dichloride

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Diaquabis(biuretato-*κ²O,O′*)nickel(II) dichloride

Crystal data
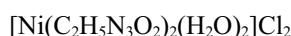
$[Ni(C_2H_5N_3O_2)_2(H_2O)_2]Cl_2$	$F(000) = 760$
$M_r = 371.82$	$D_x = 1.780$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *Kα* radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3015 reflections
$a = 7.3872$ (4) Å	$\theta = 3.0$–$29.5°$
$b = 27.5675$ (16) Å	$\mu = 1.82$ mm^{-1}
$c = 7.6687$ (4) Å	$T = 293$ K
$\beta = 117.344$ (1)°	Block, green
$V = 1387.21$ (13) Å^3	$0.15 \times 0.12 \times 0.10$ mm
$Z = 4$	

Data collection

Bruker SMART 1000 CCD diffractometer	14042 measured reflections
Radiation source: fine-focus sealed tube	4037 independent reflections
Graphite monochromator	2416 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.053$
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$\theta_{max} = 30.0°$, $\theta_{min} = 3.0°$
	$h = -10 \rightarrow 8$
	$k = -38 \rightarrow 38$
$T_{min} = 0.773$, $T_{max} = 0.839$	$l = -9 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.101$	
$S = 0.96$	H-atom parameters constrained
4037 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2]$
172 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.76$ e Å^{-3}
	$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	$U_{iso}*/U_{eq}$
Ni1	0.80268 (6)	0.125527 (13)	0.32664 (6)	0.03046 (12)
C1	0.8121 (5)	0.02016 (11)	0.2587 (5)	0.0363 (8)
C2	1.1095 (5)	0.06564 (11)	0.2773 (5)	0.0406 (8)
N1	0.7399 (4)	−0.02492 (10)	0.2330 (5)	0.0531 (9)
H1	0.6234	−0.0305	0.2287	0.064*
H2	0.8099	−0.0484	0.2208	0.064*
N2	1.0015 (4)	0.02374 (10)	0.2650 (4)	0.0419 (7)
H3	1.0587	−0.0031	0.2607	0.050*
N3	1.2783 (5)	0.05885 (11)	0.2623 (6)	0.0654 (11)
H4	1.3544	0.0832	0.2697	0.078*
H5	1.3123	0.0301	0.2451	0.078*
O1	0.7160 (3)	0.05514 (7)	0.2769 (4)	0.0407 (6)
O2	1.0539 (3)	0.10651 (8)	0.3023 (4)	0.0434 (6)
C3	0.4936 (5)	0.18368 (11)	0.3785 (5)	0.0365 (7)
C4	0.7877 (5)	0.23070 (11)	0.3984 (5)	0.0345 (7)
N4	0.3254 (5)	0.18961 (11)	0.3945 (5)	0.0589 (9)
H6	0.2503	0.1650	0.3861	0.071*
H7	0.2904	0.2181	0.4135	0.071*
N5	0.6018 (4)	0.22604 (9)	0.3972 (4)	0.0414 (7)
H8	0.5465	0.2524	0.4095	0.050*
N6	0.8615 (5)	0.27574 (9)	0.4285 (5)	0.0494 (8)
H9	0.9761	0.2816	0.4292	0.059*
H10	0.7944	0.2989	0.4473	0.059*
O3	0.5507 (3)	0.14320 (7)	0.3511 (3)	0.0367 (5)
O4	0.8813 (3)	0.19646 (7)	0.3708 (3)	0.0367 (5)
O5	0.9625 (3)	0.11171 (8)	0.6268 (3)	0.0414 (6)
H11	0.8746	0.1024	0.6790	0.050*
H12	1.0370	0.1374	0.6995	0.050*
O6	0.6618 (3)	0.14025 (7)	0.0272 (3)	0.0385 (5)
H13	0.6310	0.1096	−0.0452	0.046*
H14	0.5429	0.1508	0.0129	0.046*
Cl1	0.25969 (13)	0.19350 (3)	0.87623 (14)	0.0473 (2)
Cl2	0.70170 (15)	0.05765 (3)	0.78053 (15)	0.0485 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0271 (2)	0.02096 (17)	0.0516 (3)	−0.00128 (16)	0.02523 (18)	−0.00374 (17)
C1	0.0340 (18)	0.0300 (15)	0.046 (2)	−0.0049 (13)	0.0197 (17)	−0.0057 (13)
C2	0.0303 (17)	0.0339 (17)	0.059 (2)	−0.0039 (14)	0.0220 (17)	−0.0066 (15)

N1	0.0429 (18)	0.0282 (14)	0.101 (3)	−0.0037 (12)	0.0440 (19)	−0.0091 (15)
N2	0.0354 (16)	0.0285 (14)	0.070 (2)	0.0013 (11)	0.0310 (16)	−0.0050 (13)
N3	0.0457 (18)	0.0348 (16)	0.140 (3)	−0.0083 (14)	0.063 (2)	−0.0249 (18)
O1	0.0345 (12)	0.0243 (11)	0.0723 (16)	−0.0021 (9)	0.0322 (12)	−0.0070 (10)
O2	0.0354 (12)	0.0303 (11)	0.0780 (18)	−0.0031 (10)	0.0377 (13)	−0.0103 (11)
C3	0.0331 (18)	0.0339 (16)	0.049 (2)	−0.0029 (14)	0.0242 (16)	−0.0034 (14)
C4	0.0314 (17)	0.0336 (16)	0.0414 (19)	−0.0041 (13)	0.0191 (16)	−0.0028 (14)
N4	0.0500 (19)	0.0343 (16)	0.120 (3)	−0.0020 (14)	0.062 (2)	−0.0050 (17)
N5	0.0369 (16)	0.0295 (14)	0.069 (2)	−0.0034 (12)	0.0344 (16)	−0.0088 (13)
N6	0.0484 (18)	0.0267 (14)	0.092 (3)	−0.0073 (13)	0.0484 (19)	−0.0138 (14)
O3	0.0318 (12)	0.0256 (10)	0.0634 (16)	−0.0018 (9)	0.0309 (12)	−0.0046 (10)
O4	0.0349 (12)	0.0255 (10)	0.0611 (15)	−0.0037 (9)	0.0320 (12)	−0.0080 (10)
O5	0.0379 (13)	0.0349 (12)	0.0555 (15)	−0.0046 (10)	0.0251 (12)	−0.0016 (10)
O6	0.0378 (13)	0.0303 (11)	0.0530 (14)	0.0005 (9)	0.0257 (12)	−0.0044 (10)
Cl1	0.0364 (4)	0.0373 (4)	0.0693 (6)	0.0004 (4)	0.0253 (5)	−0.0030 (4)
Cl2	0.0576 (6)	0.0355 (4)	0.0704 (6)	−0.0030 (4)	0.0449 (5)	−0.0062 (4)

Geometric parameters (Å, º)

Ni1—O3	2.014 (2)	N3—H5	0.8600
Ni1—O2	2.018 (2)	C3—O3	1.245 (4)
Ni1—O4	2.024 (2)	C3—N4	1.314 (4)
Ni1—O1	2.024 (2)	C3—N5	1.385 (4)
Ni1—O6	2.080 (2)	C4—O4	1.244 (4)
Ni1—O5	2.083 (2)	C4—N6	1.333 (4)
C1—O1	1.243 (4)	C4—N5	1.375 (4)
C1—N1	1.331 (4)	N4—H6	0.8600
C1—N2	1.382 (4)	N4—H7	0.8600
C2—O2	1.244 (4)	N5—H8	0.8600
C2—N3	1.317 (4)	N6—H9	0.8600
C2—N2	1.382 (4)	N6—H10	0.8600
N1—H1	0.8600	O5—H11	0.9419
N1—H2	0.8600	O5—H12	0.9121
N2—H3	0.8600	O6—H13	0.9778
N3—H4	0.8600	O6—H14	0.8833
O3—Ni1—O2	178.94 (8)	C2—N3—H5	120.0
O3—Ni1—O4	87.54 (8)	H4—N3—H5	120.0
O2—Ni1—O4	93.51 (8)	C1—O1—Ni1	128.1 (2)
O3—Ni1—O1	91.35 (9)	C2—O2—Ni1	129.2 (2)
O2—Ni1—O1	87.61 (9)	O3—C3—N4	122.4 (3)
O4—Ni1—O1	178.38 (9)	O3—C3—N5	123.3 (3)
O3—Ni1—O6	92.32 (9)	N4—C3—N5	114.3 (3)
O2—Ni1—O6	87.91 (10)	O4—C4—N6	121.4 (3)
O4—Ni1—O6	87.47 (9)	O4—C4—N5	124.0 (3)
O1—Ni1—O6	91.41 (9)	N6—C4—N5	114.6 (3)
O3—Ni1—O5	91.17 (9)	C3—N4—H6	120.0
O2—Ni1—O5	88.63 (10)	C3—N4—H7	120.0

O4—Ni1—O5	91.04 (9)	H6—N4—H7	120.0
O1—Ni1—O5	90.15 (9)	C4—N5—C3	127.3 (3)
O6—Ni1—O5	176.14 (9)	C4—N5—H8	116.3
O1—C1—N1	122.1 (3)	C3—N5—H8	116.3
O1—C1—N2	124.2 (3)	C4—N6—H9	120.0
N1—C1—N2	113.7 (3)	C4—N6—H10	120.0
O2—C2—N3	122.4 (3)	H9—N6—H10	120.0
O2—C2—N2	123.1 (3)	C3—O3—Ni1	129.2 (2)
N3—C2—N2	114.5 (3)	C4—O4—Ni1	128.5 (2)
C1—N1—H1	120.0	Ni1—O5—H11	111.6
C1—N1—H2	120.0	Ni1—O5—H12	114.2
H1—N1—H2	120.0	H11—O5—H12	107.0
C1—N2—C2	127.3 (3)	Ni1—O6—H13	109.0
C1—N2—H3	116.4	Ni1—O6—H14	99.6
C2—N2—H3	116.4	H13—O6—H14	104.8
C2—N3—H4	120.0		
O1—C1—N2—C2	−5.1 (6)	O4—C4—N5—C3	4.3 (6)
N1—C1—N2—C2	175.6 (3)	N6—C4—N5—C3	−176.8 (3)
O2—C2—N2—C1	6.7 (6)	O3—C3—N5—C4	−3.3 (6)
N3—C2—N2—C1	−173.9 (3)	N4—C3—N5—C4	176.0 (3)
N1—C1—O1—Ni1	177.6 (3)	N4—C3—O3—Ni1	−178.9 (3)
N2—C1—O1—Ni1	−1.7 (5)	N5—C3—O3—Ni1	0.3 (5)
O3—Ni1—O1—C1	−175.2 (3)	O4—Ni1—O3—C3	1.1 (3)
O2—Ni1—O1—C1	4.6 (3)	O1—Ni1—O3—C3	−177.7 (3)
O6—Ni1—O1—C1	92.5 (3)	O6—Ni1—O3—C3	−86.3 (3)
O5—Ni1—O1—C1	−84.0 (3)	O5—Ni1—O3—C3	92.1 (3)
N3—C2—O2—Ni1	179.4 (3)	N6—C4—O4—Ni1	178.9 (2)
N2—C2—O2—Ni1	−1.3 (5)	N5—C4—O4—Ni1	−2.2 (5)
O4—Ni1—O2—C2	178.0 (3)	O3—Ni1—O4—C4	−0.1 (3)
O1—Ni1—O2—C2	−3.2 (3)	O2—Ni1—O4—C4	−179.9 (3)
O6—Ni1—O2—C2	−94.7 (3)	O6—Ni1—O4—C4	92.3 (3)
O5—Ni1—O2—C2	87.0 (3)	O5—Ni1—O4—C4	−91.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl2[i]	0.86	2.49	3.340 (3)	173
N1—H2···O5[ii]	0.86	2.33	3.089 (4)	147
N2—H3···Cl2[ii]	0.86	2.45	3.266 (3)	158
N3—H4···O3[iii]	0.86	2.10	2.943 (4)	168
N3—H5···Cl2[ii]	0.86	2.43	3.239 (3)	158
N4—H6···O2[iv]	0.86	2.06	2.910 (4)	168
N4—H7···Cl1[v]	0.86	2.45	3.252 (3)	155
N5—H8···Cl1[v]	0.86	2.51	3.310 (3)	156
N6—H9···Cl1[vi]	0.86	2.41	3.259 (3)	169
N6—H10···O6[vii]	0.86	2.17	3.023 (3)	173
O5—H11···Cl2	0.94	2.16	3.068 (2)	161

O5—H12···Cl1[iii]	0.91	2.21	3.115 (2)	171
O6—H13···Cl2[viii]	0.98	2.18	3.060 (2)	149
O6—H14···Cl1[viii]	0.88	2.20	3.027 (2)	155

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