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Bis[*N*-ethyl-*N*′-(pyridin-2-ylmethylene)-ethane-1,2-diamine]nickel(II) bis(perchlorate)

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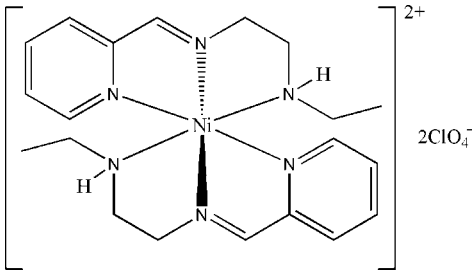
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.059; wR factor = 0.189; data-to-parameter ratio = 18.2.

The asymmetric unit of the title compound, $[Ni(C_{10}H_{15}N_3)_2](ClO_4)_2$, consists of 1.5 mononuclear nickel(II) complex cations, two perchlorate anions and two half-perchlorate anions. One of the complex cations and two of the perchlorate anions possess crystallographic twofold rotation symmetry. The Ni atom is coordinated by six N atoms from two *N*-ethyl-*N*′-(pyridin-2-ylmethylene)ethane-1,2-diamine ligands in a slightly distorted octahedral geometry. All chemically equivalent bond lengths and angles in the two complex molecules are comparable with each other. Each ligand adopts an approximately planar geometry, except for the terminal ethyl groups. The crystal structure involves intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Li *et al.* (2005, 2007); Zhou *et al.* (2004).



Experimental

Crystal data

$[Ni(C_{10}H_{15}N_3)_2](ClO_4)_2$
M_r = 612.11
Monoclinic, $P2/c$
a = 21.1172 (18) Å
b = 16.8787 (14) Å
c = 12.0819 (10) Å
β = 105.531 (1)°
V = 4149.1 (6) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 298 (2) K
0.37 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.721, T_{max} = 0.751
23631 measured reflections
9187 independent reflections
5711 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.189
S = 0.99
9187 reflections
505 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O4^{i}	0.91	2.39	3.300 (6)	173
N6—H6A···O3^{i}	0.91	2.51	3.359 (6)	156
N6—H6A···O4^{i}	0.91	2.62	3.443 (6)	150
N9—H9C···O12^{ii}	0.91	2.27	3.141 (9)	160

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2138).

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  doi:10.1107/S160053680703108X

supplementary materials

Acta Cryst. (2007). E**63**, m2026 [**doi:10.1107/S160053680703108X**]

Bis[*N*-ethyl-*N*'-(pyridin-2-ylmethylene)ethane-1,2-diamine]nickel(II) bis(perchlorate)

Z. Hong

Comment

The title complex is a mononuclear nickel(II) compound (Fig. 1). The structure consists of two mononuclear nickel(II) molecules, one with twofold symmetry, and four perchlorate anions, two with twofold symmetry. The Ni atom is six-coordinated by two Schiff base ligands. Each Schiff base ligand acts as a tridentate ligand, and ligates to the nickel atom through the imine N, amine N, and pyridine N atoms. The bond lengths related to the metal centres are comparable to the values in other similar nickel(II) complexes (Zhou *et al.*, 2004; Li *et al.*, 2005; Li *et al.*, 2007).

Experimental

All the reagents used were of commercial grade and used without further purification. *N*-Ethylethane-1,2-diamine (1.0 mmol, 88.2 mg) and pyridine-2-carbaldehyde (1.0 mmol, 107.1 mg) were mixed in a methanol solution (10 ml). The mixture was stirred for 1 h at room temperature. To the mixture was added with stirring a methanol solution (10 ml) of $Ni(ClO_4)_2·7H_2O$ (0.5 mmol, 192.0 mg). After keeping the filtrate in air for a week, green block-shaped crystals were formed.

Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.97 Å, N–H distances of 0.91 Å, and with U_{iso}(H) set at 1.2U_{eq}(C,*N*) and 1.5U_{eq}(methyl C). The structure contains solvent accessible voids of 65 $Å^3$, which might accommodate a disordered methanol molecule.

Figures

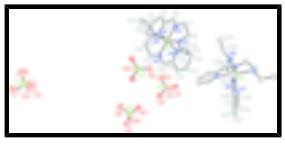


Fig. 1. The structure of compound (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Bis[*N*-ethyl-*N*'-(pyridin-2-ylmethylene)ethane-1,2-diamine]nickel(II) bis(perchlorate)

Crystal data

$[Ni(C_{10}H_{15}N_3)_2](ClO_4)_2$	F_{000} = 1908
M_r = 612.11	D_x = 1.470 Mg m^{-3}
Monoclinic, *P*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yc	Cell parameters from 5221 reflections
a = 21.1172 (18) Å	θ = 2.3–24.9º

b = 16.8787 (14) Å	μ = 0.95 mm^{-1}
c = 12.0819 (10) Å	T = 298 (2) K
β = 105.5310 (10)º	Block, green
V = 4149.1 (6) Å^3	0.37 × 0.35 × 0.32 mm
Z = 6	

Data collection

Bruker SMART CCD area-detector diffractometer	9187 independent reflections
Radiation source: fine-focus sealed tube	5711 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −27→23
T_{min} = 0.721, T_{max} = 0.751	k = −20→21
23631 measured reflections	l = −8→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.189	$w = 1/[\sigma^2(F_o^2) + (0.1156P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max} < 0.001$
9187 reflections	$\Delta\rho_{max}$ = 1.86 e Å^{-3}
505 parameters	$\Delta\rho_{min}$ = −0.47 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}
Ni1	0.31911 (2)	0.27828 (3)	0.42248 (4)	0.04209 (16)
Ni2	0.0000	0.19438 (4)	0.7500	0.04130 (19)
Cl1	0.20287 (5)	0.59652 (6)	0.53647 (9)	0.0550 (3)
Cl2	0.30375 (6)	0.93789 (9)	0.53709 (11)	0.0734 (3)
Cl3	0.5000	0.44214 (9)	0.7500	0.0589 (4)
Cl4	1.0000	0.88866 (11)	0.7500	0.0808 (5)
O1	0.1344 (2)	0.5861 (3)	0.4961 (4)	0.0975 (13)
O2	0.2341 (3)	0.5720 (3)	0.4539 (4)	0.1139 (15)
O3	0.2268 (2)	0.5531 (3)	0.6417 (3)	0.0907 (12)
O4	0.2134 (2)	0.6791 (2)	0.5604 (4)	0.1028 (14)
O5	0.2732 (3)	0.8631 (3)	0.5367 (4)	0.1117 (15)
O6	0.3564 (3)	0.9301 (4)	0.4928 (6)	0.139 (2)
O7	0.3176 (4)	0.9736 (5)	0.6419 (7)	0.178 (3)
O8	0.2592 (3)	0.9910 (4)	0.4709 (7)	0.165 (3)
O9	0.44959 (18)	0.3930 (2)	0.7721 (4)	0.0946 (13)
O10	0.4710 (2)	0.4896 (3)	0.6554 (4)	0.0968 (13)
O11	0.9805 (6)	0.8420 (7)	0.8234 (9)	0.247 (4)
O12	0.9476 (4)	0.9348 (5)	0.6847 (8)	0.202 (4)
N1	0.41192 (17)	0.22489 (19)	0.4957 (3)	0.0490 (8)
N2	0.30283 (18)	0.1667 (2)	0.3666 (3)	0.0523 (8)
N3	0.21667 (17)	0.2880 (2)	0.3311 (3)	0.0538 (8)
H3A	0.2157	0.3014	0.2577	0.065*
N4	0.30009 (16)	0.26354 (19)	0.5868 (3)	0.0479 (7)
N5	0.33348 (16)	0.38789 (17)	0.4875 (3)	0.0467 (7)
N6	0.35160 (17)	0.3331 (2)	0.2886 (3)	0.0511 (8)
H6A	0.3149	0.3499	0.2352	0.061*
N7	−0.04676 (17)	0.28965 (19)	0.8184 (3)	0.0489 (8)
N8	0.05468 (16)	0.1998 (2)	0.9136 (3)	0.0485 (8)
N9	0.07312 (17)	0.1091 (2)	0.7407 (3)	0.0560 (9)
H9C	0.0571	0.0602	0.7501	0.067*
C1	0.4097 (2)	0.1459 (3)	0.4762 (4)	0.0590 (11)
C2	0.4615 (3)	0.0978 (3)	0.5292 (6)	0.0881 (17)
H2	0.4581	0.0432	0.5181	0.106*
C3	0.5184 (3)	0.1296 (4)	0.5984 (6)	0.0884 (17)
H3	0.5544	0.0980	0.6328	0.106*
C4	0.5198 (3)	0.2089 (3)	0.6140 (5)	0.0769 (14)
H4	0.5577	0.2327	0.6589	0.092*
C5	0.4661 (2)	0.2545 (3)	0.5646 (4)	0.0585 (10)
H5	0.4679	0.3085	0.5802	0.070*
C6	0.3490 (3)	0.1178 (3)	0.3993 (4)	0.0638 (12)
H6	0.3442	0.0653	0.3748	0.077*
C7	0.2369 (3)	0.1508 (3)	0.2934 (5)	0.0712 (13)
H7A	0.2243	0.0967	0.3042	0.085*
H7B	0.2360	0.1577	0.2133	0.085*
C8	0.1907 (2)	0.2069 (3)	0.3253 (4)	0.0679 (13)

H8A	0.1483	0.2044	0.2688	0.081*
H8B	0.1845	0.1921	0.3993	0.081*
C9	0.1764 (2)	0.3482 (4)	0.3703 (4)	0.0725 (14)
H9A	0.1997	0.3983	0.3798	0.087*
H9B	0.1719	0.3325	0.4451	0.087*
C10	0.1076 (2)	0.3609 (4)	0.2898 (5)	0.0830 (16)
H10A	0.1111	0.3723	0.2138	0.125*
H10B	0.0868	0.4045	0.3170	0.125*
H10C	0.0819	0.3138	0.2881	0.125*
C11	0.30700 (18)	0.3322 (2)	0.6458 (3)	0.0481 (9)
C12	0.2992 (2)	0.3359 (3)	0.7559 (4)	0.0640 (12)
H12	0.3018	0.3843	0.7936	0.077*
C13	0.2877 (3)	0.2682 (4)	0.8086 (4)	0.0748 (15)
H13	0.2828	0.2698	0.8828	0.090*
C14	0.2833 (2)	0.1975 (3)	0.7507 (4)	0.0704 (13)
H14	0.2764	0.1504	0.7858	0.084*
C15	0.2892 (2)	0.1974 (3)	0.6397 (4)	0.0559 (10)
H15	0.2855	0.1496	0.6003	0.067*
C16	0.3246 (2)	0.3997 (2)	0.5852 (4)	0.0522 (10)
H16	0.3291	0.4501	0.6176	0.063*
C17	0.3510 (2)	0.4467 (2)	0.4132 (4)	0.0590 (11)
H17A	0.3785	0.4874	0.4588	0.071*
H17B	0.3118	0.4716	0.3654	0.071*
C18	0.3879 (2)	0.4048 (3)	0.3391 (4)	0.0601 (11)
H18A	0.3928	0.4399	0.2784	0.072*
H18B	0.4314	0.3902	0.3852	0.072*
C19	0.3889 (3)	0.2821 (3)	0.2270 (5)	0.0704 (13)
H19A	0.3634	0.2346	0.2013	0.084*
H19B	0.4296	0.2659	0.2813	0.084*
C20	0.4055 (3)	0.3198 (4)	0.1240 (5)	0.0900 (17)
H20A	0.3679	0.3481	0.0791	0.135*
H20B	0.4175	0.2793	0.0777	0.135*
H20C	0.4416	0.3559	0.1501	0.135*
C21	−0.0118 (2)	0.3087 (3)	0.9265 (3)	0.0511 (9)
C22	−0.0265 (3)	0.3722 (3)	0.9825 (5)	0.0741 (14)
H22	−0.0016	0.3839	1.0565	0.089*
C23	−0.0789 (3)	0.4198 (4)	0.9291 (6)	0.0844 (16)
H23	−0.0898	0.4639	0.9664	0.101*
C24	−0.1139 (3)	0.4012 (3)	0.8219 (5)	0.0749 (14)
H24	−0.1496	0.4321	0.7843	0.090*
C25	−0.0962 (2)	0.3357 (3)	0.7682 (4)	0.0604 (11)
H25	−0.1203	0.3238	0.6937	0.073*
C26	0.0431 (2)	0.2535 (3)	0.9762 (3)	0.0551 (10)
H26	0.0681	0.2587	1.0519	0.066*
C27	0.1063 (2)	0.1424 (3)	0.9449 (4)	0.0666 (12)
H27A	0.0902	0.0944	0.9723	0.080*
H27B	0.1423	0.1630	1.0057	0.080*
C28	0.1292 (2)	0.1247 (3)	0.8407 (5)	0.0752 (14)
H28A	0.1541	0.1694	0.8243	0.090*

H28B	0.1580	0.0789	0.8553	0.090*
C29	0.0924 (3)	0.1083 (4)	0.6315 (5)	0.0818 (15)
H29A	0.1110	0.1595	0.6214	0.098*
H29B	0.0534	0.1009	0.5684	0.098*
C30	0.1424 (3)	0.0436 (4)	0.6256 (6)	0.099 (2)
H30A	0.1861	0.0643	0.6537	0.148*
H30B	0.1355	0.0267	0.5474	0.148*
H30C	0.1368	−0.0006	0.6720	0.148*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0470 (3)	0.0382 (3)	0.0413 (3)	−0.00535 (19)	0.0122 (2)	−0.00498 (18)
Ni2	0.0396 (4)	0.0423 (4)	0.0393 (4)	0.000	0.0057 (3)	0.000
Cl1	0.0577 (6)	0.0561 (6)	0.0508 (6)	−0.0040 (4)	0.0138 (4)	0.0025 (4)
Cl2	0.0608 (7)	0.0933 (9)	0.0646 (7)	−0.0078 (6)	0.0145 (5)	0.0098 (6)
Cl3	0.0446 (7)	0.0530 (8)	0.0717 (10)	0.000	0.0025 (6)	0.000
Cl4	0.0786 (12)	0.0614 (10)	0.1100 (15)	0.000	0.0386 (11)	0.000
O1	0.069 (2)	0.109 (3)	0.103 (3)	−0.017 (2)	0.004 (2)	0.024 (2)
O2	0.125 (4)	0.137 (4)	0.098 (3)	0.015 (3)	0.060 (3)	−0.013 (3)
O3	0.092 (3)	0.106 (3)	0.067 (2)	0.017 (2)	0.0094 (19)	0.024 (2)
O4	0.124 (4)	0.065 (2)	0.115 (3)	−0.012 (2)	0.025 (3)	−0.008 (2)
O5	0.117 (4)	0.105 (3)	0.115 (4)	−0.020 (3)	0.036 (3)	0.025 (3)
O6	0.109 (4)	0.147 (5)	0.185 (6)	−0.011 (4)	0.081 (4)	−0.002 (4)
O7	0.194 (6)	0.183 (6)	0.161 (5)	−0.028 (5)	0.056 (5)	−0.063 (5)
O8	0.091 (4)	0.160 (6)	0.225 (7)	−0.011 (4)	0.009 (4)	0.086 (5)
O9	0.060 (2)	0.092 (3)	0.125 (3)	−0.0135 (19)	0.013 (2)	0.030 (2)
O10	0.084 (3)	0.101 (3)	0.093 (3)	0.012 (2)	0.003 (2)	0.031 (2)
O11	0.267 (8)	0.254 (8)	0.222 (7)	−0.082 (7)	0.068 (6)	0.066 (6)
O12	0.204 (6)	0.178 (6)	0.202 (7)	0.069 (5)	0.016 (5)	−0.012 (5)
N1	0.0518 (19)	0.0443 (18)	0.0517 (19)	−0.0033 (14)	0.0153 (15)	−0.0045 (14)
N2	0.063 (2)	0.0439 (18)	0.0500 (19)	−0.0118 (16)	0.0160 (16)	−0.0104 (15)
N3	0.0504 (19)	0.066 (2)	0.0447 (18)	−0.0030 (16)	0.0120 (15)	−0.0045 (15)
N4	0.0466 (18)	0.0494 (19)	0.0480 (18)	−0.0039 (14)	0.0129 (14)	−0.0027 (14)
N5	0.0462 (18)	0.0368 (16)	0.053 (2)	−0.0003 (13)	0.0055 (14)	−0.0031 (14)
N6	0.0492 (18)	0.0555 (19)	0.0481 (18)	−0.0056 (15)	0.0120 (14)	0.0019 (15)
N7	0.0494 (18)	0.0518 (19)	0.0448 (18)	0.0034 (14)	0.0116 (14)	0.0036 (14)
N8	0.0454 (18)	0.0546 (19)	0.0403 (17)	0.0012 (14)	0.0025 (13)	0.0028 (14)
N9	0.051 (2)	0.0526 (19)	0.064 (2)	0.0048 (15)	0.0147 (16)	−0.0063 (16)
C1	0.067 (3)	0.046 (2)	0.070 (3)	0.008 (2)	0.029 (2)	−0.004 (2)
C2	0.095 (4)	0.062 (3)	0.111 (5)	0.022 (3)	0.032 (4)	−0.008 (3)
C3	0.074 (4)	0.087 (4)	0.100 (4)	0.029 (3)	0.016 (3)	0.000 (3)
C4	0.061 (3)	0.085 (4)	0.082 (4)	0.004 (3)	0.015 (3)	−0.005 (3)
C5	0.058 (3)	0.061 (3)	0.058 (3)	0.004 (2)	0.017 (2)	−0.003 (2)
C6	0.084 (3)	0.038 (2)	0.073 (3)	−0.005 (2)	0.026 (2)	−0.014 (2)
C7	0.077 (3)	0.064 (3)	0.070 (3)	−0.027 (2)	0.015 (2)	−0.017 (2)
C8	0.063 (3)	0.079 (3)	0.060 (3)	−0.024 (2)	0.014 (2)	−0.011 (2)
C9	0.055 (3)	0.105 (4)	0.055 (3)	0.008 (3)	0.009 (2)	−0.012 (3)

C10	0.055 (3)	0.115 (4)	0.080 (4)	0.011 (3)	0.019 (2)	−0.003 (3)
C11	0.0379 (19)	0.059 (2)	0.045 (2)	−0.0020 (16)	0.0080 (15)	−0.0121 (18)
C12	0.058 (3)	0.085 (3)	0.051 (2)	−0.012 (2)	0.018 (2)	−0.023 (2)
C13	0.069 (3)	0.113 (4)	0.046 (2)	−0.023 (3)	0.022 (2)	−0.014 (3)
C14	0.065 (3)	0.088 (3)	0.060 (3)	−0.017 (3)	0.019 (2)	0.015 (3)
C15	0.060 (3)	0.056 (2)	0.055 (2)	−0.0085 (19)	0.0208 (19)	−0.0024 (19)
C16	0.055 (2)	0.042 (2)	0.054 (2)	0.0034 (17)	0.0044 (18)	−0.0133 (17)
C17	0.074 (3)	0.040 (2)	0.059 (3)	−0.0061 (19)	0.009 (2)	0.0025 (18)
C18	0.060 (3)	0.055 (2)	0.065 (3)	−0.009 (2)	0.016 (2)	0.013 (2)
C19	0.080 (3)	0.069 (3)	0.070 (3)	−0.010 (2)	0.035 (3)	−0.009 (2)
C20	0.094 (4)	0.117 (5)	0.071 (3)	−0.004 (4)	0.043 (3)	−0.005 (3)
C21	0.055 (2)	0.055 (2)	0.045 (2)	−0.0008 (18)	0.0146 (17)	−0.0033 (18)
C22	0.073 (3)	0.087 (4)	0.063 (3)	0.003 (3)	0.019 (2)	−0.023 (3)
C23	0.080 (4)	0.073 (3)	0.109 (5)	0.017 (3)	0.040 (3)	−0.014 (3)
C24	0.075 (3)	0.066 (3)	0.085 (4)	0.026 (2)	0.024 (3)	0.009 (3)
C25	0.063 (3)	0.061 (3)	0.055 (2)	0.018 (2)	0.012 (2)	0.008 (2)
C26	0.054 (2)	0.069 (3)	0.039 (2)	0.000 (2)	0.0057 (17)	−0.0001 (19)
C27	0.068 (3)	0.069 (3)	0.053 (3)	0.019 (2)	−0.002 (2)	0.007 (2)
C28	0.049 (3)	0.079 (3)	0.090 (4)	0.017 (2)	0.006 (2)	0.002 (3)
C29	0.075 (4)	0.082 (4)	0.095 (4)	0.003 (3)	0.035 (3)	−0.008 (3)
C30	0.089 (4)	0.091 (4)	0.125 (6)	0.012 (3)	0.044 (4)	−0.032 (4)

Geometric parameters (Å, °)

Ni1—N2	1.999 (3)	C4—H4	0.9300
Ni1—N5	2.001 (3)	C5—H5	0.9300
Ni1—N1	2.123 (3)	C6—H6	0.9300
Ni1—N6	2.130 (3)	C7—C8	1.483 (7)
Ni1—N4	2.143 (3)	C7—H7A	0.9700
Ni1—N3	2.156 (3)	C7—H7B	0.9700
Ni2—N8^{i}	2.007 (3)	C8—H8A	0.9700
Ni2—N8	2.007 (3)	C8—H8B	0.9700
Ni2—N9^{i}	2.136 (3)	C9—C10	1.531 (7)
Ni2—N9	2.136 (3)	C9—H9A	0.9700
Ni2—N7	2.164 (3)	C9—H9B	0.9700
Ni2—N7^{i}	2.164 (3)	C10—H10A	0.9600
Cl1—O2	1.398 (4)	C10—H10B	0.9600
Cl1—O1	1.407 (4)	C10—H10C	0.9600
Cl1—O4	1.429 (4)	C11—C12	1.385 (6)
Cl1—O3	1.437 (4)	C11—C16	1.456 (6)
Cl2—O7	1.361 (7)	C12—C13	1.361 (7)
Cl2—O6	1.363 (5)	C12—H12	0.9300
Cl2—O8	1.388 (6)	C13—C14	1.374 (8)
Cl2—O5	1.418 (5)	C13—H13	0.9300
Cl3—O10^{ii}	1.396 (4)	C14—C15	1.379 (7)
Cl3—O10	1.396 (4)	C14—H14	0.9300
Cl3—O9^{ii}	1.430 (4)	C15—H15	0.9300
Cl3—O9	1.430 (4)	C16—H16	0.9300

Cl4—O11^{iii}	1.331 (9)	C17—C18	1.510 (7)
Cl4—O11	1.331 (9)	C17—H17A	0.9700
Cl4—O12^{iii}	1.409 (7)	C17—H17B	0.9700
Cl4—O12	1.409 (7)	C18—H18A	0.9700
N1—C5	1.320 (6)	C18—H18B	0.9700
N1—C1	1.353 (5)	C19—C20	1.520 (8)
N2—C6	1.257 (6)	C19—H19A	0.9700
N2—C7	1.461 (6)	C19—H19B	0.9700
N3—C8	1.469 (6)	C20—H20A	0.9600
N3—C9	1.482 (6)	C20—H20B	0.9600
N3—H3A	0.9100	C20—H20C	0.9600
N4—C15	1.337 (6)	C21—C22	1.348 (7)
N4—C11	1.348 (5)	C21—C26	1.482 (6)
N5—C16	1.260 (5)	C22—C23	1.380 (8)
N5—C17	1.452 (5)	C22—H22	0.9300
N6—C18	1.473 (5)	C23—C24	1.345 (8)
N6—C19	1.493 (6)	C23—H23	0.9300
N6—H6A	0.9100	C24—C25	1.382 (7)
N7—C25	1.313 (5)	C24—H24	0.9300
N7—C21	1.355 (5)	C25—H25	0.9300
N8—C26	1.245 (6)	C26—H26	0.9300
N8—C27	1.432 (5)	C27—C28	1.495 (8)
N9—C28	1.472 (6)	C27—H27A	0.9700
N9—C29	1.482 (7)	C27—H27B	0.9700
N9—H9C	0.9100	C28—H28A	0.9700
C1—C2	1.375 (7)	C28—H28B	0.9700
C1—C6	1.448 (7)	C29—C30	1.533 (8)
C2—C3	1.376 (9)	C29—H29A	0.9700
C2—H2	0.9300	C29—H29B	0.9700
C3—C4	1.350 (8)	C30—H30A	0.9600
C3—H3	0.9300	C30—H30B	0.9600
C4—C5	1.368 (7)	C30—H30C	0.9600
N2—Ni1—N5	176.21 (14)	N2—C7—C8	108.2 (4)
N2—Ni1—N1	78.29 (14)	N2—C7—H7A	110.1
N5—Ni1—N1	101.70 (13)	C8—C7—H7A	110.1
N2—Ni1—N6	102.37 (14)	N2—C7—H7B	110.1
N5—Ni1—N6	81.42 (14)	C8—C7—H7B	110.1
N1—Ni1—N6	92.98 (13)	H7A—C7—H7B	108.4
N2—Ni1—N4	98.36 (13)	N3—C8—C7	110.1 (4)
N5—Ni1—N4	77.86 (13)	N3—C8—H8A	109.6
N1—Ni1—N4	86.88 (13)	C7—C8—H8A	109.6
N6—Ni1—N4	158.80 (13)	N3—C8—H8B	109.6
N2—Ni1—N3	80.81 (14)	C7—C8—H8B	109.6
N5—Ni1—N3	99.02 (13)	H8A—C8—H8B	108.1
N1—Ni1—N3	158.99 (13)	N3—C9—C10	114.9 (4)
N6—Ni1—N3	93.51 (13)	N3—C9—H9A	108.5
N4—Ni1—N3	94.12 (13)	C10—C9—H9A	108.5
N8^{i}—Ni2—N8	174.7 (2)	N3—C9—H9B	108.5

N8^{i}—Ni2—N9^{i}	81.35 (14)	C10—C9—H9B	108.5
N8—Ni2—N9^{i}	102.27 (14)	H9A—C9—H9B	107.5
N8^{i}—Ni2—N9	102.27 (14)	C9—C10—H10A	109.5
N8—Ni2—N9	81.35 (14)	C9—C10—H10B	109.5
N9^{i}—Ni2—N9	95.2 (2)	H10A—C10—H10B	109.5
N8^{i}—Ni2—N7	98.11 (13)	C9—C10—H10C	109.5
N8—Ni2—N7	77.91 (13)	H10A—C10—H10C	109.5
N9^{i}—Ni2—N7	94.05 (14)	H10B—C10—H10C	109.5
N9—Ni2—N7	158.65 (13)	N4—C11—C12	121.6 (4)
N8^{i}—Ni2—N7^{i}	77.91 (13)	N4—C11—C16	114.4 (4)
N8—Ni2—N7^{i}	98.11 (13)	C12—C11—C16	124.0 (4)
N9^{i}—Ni2—N7^{i}	158.65 (13)	C13—C12—C11	119.5 (4)
N9—Ni2—N7^{i}	94.05 (14)	C13—C12—H12	120.2
N7—Ni2—N7^{i}	83.98 (18)	C11—C12—H12	120.2
O2—Cl1—O1	110.6 (3)	C12—C13—C14	119.2 (4)
O2—Cl1—O4	110.8 (3)	C12—C13—H13	120.4
O1—Cl1—O4	106.4 (3)	C14—C13—H13	120.4
O2—Cl1—O3	111.1 (3)	C13—C14—C15	119.0 (5)
O1—Cl1—O3	109.1 (3)	C13—C14—H14	120.5
O4—Cl1—O3	108.6 (3)	C15—C14—H14	120.5
O7—Cl2—O6	114.4 (5)	N4—C15—C14	122.4 (4)
O7—Cl2—O8	101.2 (5)	N4—C15—H15	118.8
O6—Cl2—O8	109.5 (5)	C14—C15—H15	118.8
O7—Cl2—O5	112.4 (4)	N5—C16—C11	118.0 (3)
O6—Cl2—O5	109.4 (4)	N5—C16—H16	121.0
O8—Cl2—O5	109.6 (3)	C11—C16—H16	121.0
O10^{ii}—Cl3—O10	110.0 (4)	N5—C17—C18	107.7 (3)
O10^{ii}—Cl3—O9^{ii}	107.5 (2)	N5—C17—H17A	110.2
O10—Cl3—O9^{ii}	111.4 (3)	C18—C17—H17A	110.2
O10^{ii}—Cl3—O9	111.4 (3)	N5—C17—H17B	110.2
O10—Cl3—O9	107.5 (2)	C18—C17—H17B	110.2
O9^{ii}—Cl3—O9	109.1 (4)	H17A—C17—H17B	108.5
O11^{iii}—Cl4—O11	107.4 (12)	N6—C18—C17	109.7 (4)
O11^{iii}—Cl4—O12^{iii}	111.3 (7)	N6—C18—H18A	109.7
O11—Cl4—O12^{iii}	106.9 (6)	C17—C18—H18A	109.7
O11^{iii}—Cl4—O12	106.9 (6)	N6—C18—H18B	109.7
O11—Cl4—O12	111.3 (7)	C17—C18—H18B	109.7
O12^{iii}—Cl4—O12	112.9 (8)	H18A—C18—H18B	108.2
C5—N1—C1	117.8 (4)	N6—C19—C20	115.8 (5)
C5—N1—Ni1	130.5 (3)	N6—C19—H19A	108.3
C1—N1—Ni1	111.2 (3)	C20—C19—H19A	108.3
C6—N2—C7	127.0 (4)	N6—C19—H19B	108.3
C6—N2—Ni1	117.7 (3)	C20—C19—H19B	108.3
C7—N2—Ni1	115.3 (3)	H19A—C19—H19B	107.4
C8—N3—C9	114.5 (4)	C19—C20—H20A	109.5

C8—N3—Ni1	105.3 (3)	C19—C20—H20B	109.5
C9—N3—Ni1	118.2 (3)	H20A—C20—H20B	109.5
C8—N3—H3A	106.0	C19—C20—H20C	109.5
C9—N3—H3A	106.0	H20A—C20—H20C	109.5
Ni1—N3—H3A	106.0	H20B—C20—H20C	109.5
C15—N4—C11	118.2 (4)	C22—C21—N7	122.1 (4)
C15—N4—Ni1	129.7 (3)	C22—C21—C26	123.9 (4)
C11—N4—Ni1	111.7 (3)	N7—C21—C26	114.0 (4)
C16—N5—C17	126.8 (3)	C21—C22—C23	119.6 (5)
C16—N5—Ni1	118.0 (3)	C21—C22—H22	120.2
C17—N5—Ni1	115.2 (3)	C23—C22—H22	120.2
C18—N6—C19	113.3 (4)	C24—C23—C22	118.6 (5)
C18—N6—Ni1	106.2 (3)	C24—C23—H23	120.7
C19—N6—Ni1	116.6 (3)	C22—C23—H23	120.7
C18—N6—H6A	106.7	C23—C24—C25	119.4 (5)
C19—N6—H6A	106.7	C23—C24—H24	120.3
Ni1—N6—H6A	106.7	C25—C24—H24	120.3
C25—N7—C21	117.8 (4)	N7—C25—C24	122.5 (5)
C25—N7—Ni2	130.7 (3)	N7—C25—H25	118.7
C21—N7—Ni2	110.9 (3)	C24—C25—H25	118.7
C26—N8—C27	126.3 (4)	N8—C26—C21	118.1 (4)
C26—N8—Ni2	118.5 (3)	N8—C26—H26	121.0
C27—N8—Ni2	115.2 (3)	C21—C26—H26	121.0
C28—N9—C29	112.3 (4)	N8—C27—C28	107.9 (4)
C28—N9—Ni2	105.7 (3)	N8—C27—H27A	110.1
C29—N9—Ni2	115.3 (3)	C28—C27—H27A	110.1
C28—N9—H9C	107.8	N8—C27—H27B	110.1
C29—N9—H9C	107.8	C28—C27—H27B	110.1
Ni2—N9—H9C	107.8	H27A—C27—H27B	108.4
N1—C1—C2	121.0 (5)	N9—C28—C27	110.8 (4)
N1—C1—C6	114.7 (4)	N9—C28—H28A	109.5
C2—C1—C6	124.3 (4)	C27—C28—H28A	109.5
C1—C2—C3	120.6 (5)	N9—C28—H28B	109.5
C1—C2—H2	119.7	C27—C28—H28B	109.5
C3—C2—H2	119.7	H28A—C28—H28B	108.1
C4—C3—C2	117.0 (5)	N9—C29—C30	113.9 (5)
C4—C3—H3	121.5	N9—C29—H29A	108.8
C2—C3—H3	121.5	C30—C29—H29A	108.8
C3—C4—C5	120.9 (5)	N9—C29—H29B	108.8
C3—C4—H4	119.6	C30—C29—H29B	108.8
C5—C4—H4	119.6	H29A—C29—H29B	107.7
N1—C5—C4	122.6 (5)	C29—C30—H30A	109.5
N1—C5—H5	118.7	C29—C30—H30B	109.5
C4—C5—H5	118.7	H30A—C30—H30B	109.5
N2—C6—C1	117.7 (4)	C29—C30—H30C	109.5
N2—C6—H6	121.1	H30A—C30—H30C	109.5
C1—C6—H6	121.1	H30B—C30—H30C	109.5

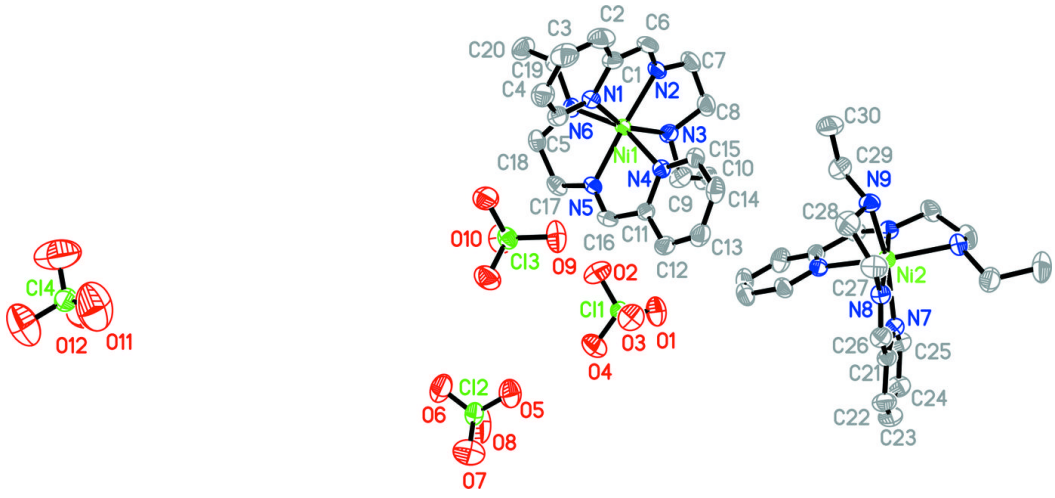
Symmetry codes: (i) $-x$, y, $-z+3/2$; (ii) $-x+1$, y, $-z+3/2$; (iii) $-x+2$, y, $-z+3/2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O4^{iv}	0.91	2.39	3.300 (6)	173
N6—H6A···O3^{iv}	0.91	2.51	3.359 (6)	156
N6—H6A···O4^{iv}	0.91	2.62	3.443 (6)	150
N9—H9C···O12^{v}	0.91	2.27	3.141 (9)	160

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

Fig. 1


C2
C6
C3
C20
C19
C4
C1
C7
N1
N2
C8
N6
N3
C5
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C15
C18
N4
C10
C17
N5
C9
C14
C16
C11
C13
C12
O10
Cl3
O9
O2
Cl1
O3
O1
O4
Cl4
O12
O11
Cl2
O6
O5
O8
O7
C30
C29
N9
C28
Ni2
C27
N8
N7
C26
C25
C21
C24
C22
C23