Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[*N*,*N*,*N*′,*N*′-Tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine]nickel(II) dichloride trimethanol solvate

Ya-Mei Pei, Xiang-Gao Meng, Chun-Shan Zhou and Wang Li*

Key Laboratory of Pestcide and Chemical Biology, Department of Chemistry, Central China Normal University, Wuhan, Hubei 430079, People's Republic of China
Correspondence e-mail: wl_928@mail.ccnu.edu.cn

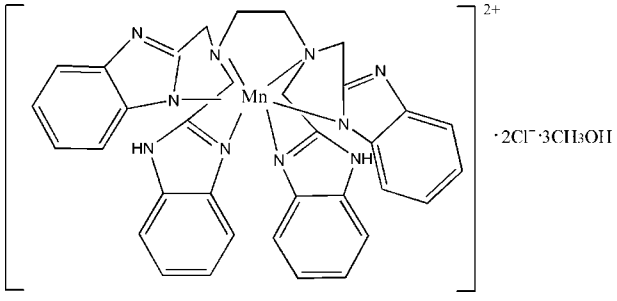
Received 16 April 2007; accepted 26 April 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.052; wR factor = 0.145; data-to-parameter ratio = 15.2.

In the title compound, $[Ni(C_{34}H_{32}N_{10})]Cl_2\cdot 3CH_4O$, the Ni^{II} atom is in a distorted octahedral coordination environment. In the crystal structure, extensive hydrogen bonding links the ions and molecules into a three-dimensional network.

Related literature

For related literature, see: Chen *et al.* (2004); Hendriks *et al.* (1982); Liao *et al.* (2001).



Experimental

Crystal data

$[Ni(C_{34}H_{32}N_{10})]Cl_2\cdot 3CH_4O$
M_r = 806.43
Triclinic, $P\overline{1}$
a = 10.8183 (5) Å
b = 11.7267 (6) Å
c = 16.8837 (8) Å
α = 74.3120 (10)°
β = 87.4910 (10)°
γ = 73.0650 (10)°
V = 1971.28 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
17041 measured reflections
7670 independent reflections
6229 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.145
S = 1.05
7670 reflections
505 parameters
26 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N5	2.076 (2)	Ni1—N7	2.097 (2)
Ni1—N3	2.078 (2)	Ni1—N1	2.167 (2)
Ni1—N13	2.082 (2)	Ni1—N2	2.175 (2)
N5—Ni1—N3	91.55 (10)	N13—Ni1—N1	93.27 (9)
N5—Ni1—N13	171.99 (10)	N7—Ni1—N1	159.13 (10)
N3—Ni1—N13	92.50 (10)	N5—Ni1—N2	93.07 (9)
N5—Ni1—N7	92.35 (10)	N3—Ni1—N2	159.90 (9)
N3—Ni1—N7	120.95 (10)	N13—Ni1—N2	80.83 (9)
N13—Ni1—N7	91.49 (10)	N7—Ni1—N2	78.41 (9)
N5—Ni1—N1	80.72 (9)	N1—Ni1—N2	82.31 (9)
N3—Ni1—N1	79.15 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···Cl1^{i}	0.82	2.30	3.117 (7)	171
N4—H4···Cl1^{ii}	0.86	2.29	3.140 (3)	172
N6—H6A···O3^{iii}	0.86	1.90	2.761 (5)	175
N12—H12···Cl1^{iv}	0.86	2.29	3.116 (3)	162
C2—H2B···O2^{iv}	0.97	2.25	3.145 (5)	154
C11—H11B···Cl2^{iii}	0.97	2.53	3.445 (3)	157
O1—H1···Cl2	0.82	2.27	3.065 (4)	163
O2—H2···Cl2	0.82	2.53	3.027 (5)	120
N8—H8A···O1	0.86	1.88	2.705 (4)	161
C27—H27B···Cl2	0.97	2.64	3.582 (3)	165

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

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

The authors thank Xiang-Gao Meng for help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2277).

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  doi:10.1107/S1600536807020879

supplementary materials

Acta Cryst. (2007). E**63**, m1568 [**doi:10.1107/S1600536807020879**]

[*N*,*N*,*N*',*N*'-Tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine]nickel(II) dichloride trimethanol solvate

Y.-M. Pei, X.-G. Meng, C.-S. Zhou and W. Li

Comment

Recently, study in the ligands containing-polybenzimidazoles and their metal coordination compounds has been widely carried on (Chen *et al.*, 2004; Liao *et al.*, 2001). As the continuing work of our workgroup, we report the crystallography structure of the title compound, [Ni(EDTB)]2 C l¯.3CH_3OH, (I); {EDTB = *N*,*N*,*N*',*N*'-tetrakis(2'-benzimidazolyl methyl)-1,2-ethanediamine}.

In the title molecular structure (I), Ni^{II} is coordinated by four four benzimidazole nitrogen atoms, two amino N atoms of EDTB, forming a distorted octahedron coordination geometry (Table 1 and Fig. 1).

In the supramolecular structure, there are a number of N(or O)–H···Cl, N–H···O and O–H···N hydrogen bonding interactions which link the molecules into a three-dimensional framwork (Table 2 and Fig.2.).

Experimental

The ligand *N,N,N ',N'*-tetrakis (2 '-benzimidazolyl methyl) -,2-ethanediamine (EDTB) was synthesized from reported literature earlier (Hendriks *et al.*, 1982). After, the ligand EDTB (0.58 g, 1.0 mmol) in 20 ml hot absolute methanol was added slowly to the $NiCl_2$.$6H_2O$ (0.24 g, 1.0 mmol) solution of 10 ml me thanol. The mixture was stirred for 1 h. After filtration, the purple solution was allowed to stand at room temperature. Purple block-shaped crystals suitable of (I) for X-ray analysis were obtained in several days in 45% yield.

Refinement

The atoms of one of the methanol molecules are disordered over two sites; the atoms involved are O3, C37 with their attached H atoms. Site occupancy factors refined to 0.75 (2):0.25 (2). The H atoms bonded C atoms were placed at their idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, with U_{iso}(H) = 1.2-1.5U_{eq}(C). H atoms bonded to N atoms were placed at their indicative positions with the U_{iso} value being set 1.2 times of their carrier atoms, N—H = 0.86 Å. The H atoms of the hydroxyl group were refined with the constraints of O–H = 0.82 Å, and U_{iso}(H) =1.5U_{eq}(O).

Figures

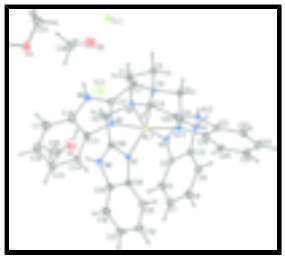

Fig. 1. View of the molecular structure of (I), showing 30% probability displacement ellipsoids. Only the major disorder component is shown.

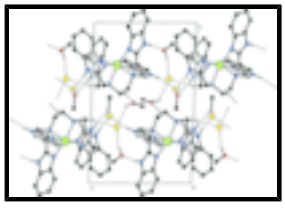

Fig. 2. Part of the crystal structure of (I), showing hydrogen bonds as dashed lines.

[*N*,*N*,*N*',*N*'-Tetrakis(benzimidazol-2-ylmethyl)ethane-1,2-diamine]nickel(II) dichloride trimethanol solvate

Crystal data

$[Ni(C_{34}H_{32}N_{10})]Cl_2·3CH_4O$	$Z = 2$
$M_r = 806.43$	$F_{000} = 844$
Triclinic, $P\overline{1}$	$D_x = 1.359$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.8183$ (5) Å	Cell parameters from 5644 reflections
$b = 11.7267$ (6) Å	$\theta = 0.00$–0.00°
$c = 16.8837$ (8) Å	$\mu = 0.68$ mm^{-1}
$\alpha = 74.3120$ (10)°	$T = 298$ (2) K
$\beta = 87.4910$ (10)°	Block, purple
$\gamma = 73.0650$ (10)°	0.30 × 0.20 × 0.20 mm
$V = 1971.28$ (16) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	6229 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.031$
Monochromator: graphite	$\theta_{max} = 26.0^\circ$
$T = 298(2)$ K	$\theta_{min} = 1.9^\circ$
φ and ω scans	$h = -13\rightarrow12$
Absorption correction: none	$k = -14\rightarrow14$
17041 measured reflections	$l = -20\rightarrow20$
7670 independent reflections	

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.145$

$S = 1.05$

7670 reflections

505 parameters

26 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.9889P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.52$ e Å^{-3}

$\Delta\rho_{min} = -0.50$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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)
Ni1	0.76117 (3)	0.88541 (3)	0.73720 (2)	0.03295 (13)	
C1	0.6510 (3)	0.8609 (3)	0.58813 (18)	0.0418 (7)	
H1A	0.5788	0.8775	0.5505	0.050*	
H1B	0.7081	0.7789	0.5909	0.050*	
C2	0.7239 (3)	0.9574 (3)	0.55753 (18)	0.0443 (7)	
H2A	0.7536	0.9567	0.5026	0.053*	
H2B	0.6670	1.0393	0.5553	0.053*	
C3	0.8848 (3)	1.0338 (3)	0.61055 (18)	0.0438 (7)	
H3A	0.8138	1.1096	0.6006	0.053*	
H3B	0.9443	1.0423	0.5662	0.053*	
C4	0.9526 (3)	1.0095 (3)	0.69153 (18)	0.0381 (6)	
C5	1.0036 (3)	0.9358 (3)	0.82128 (19)	0.0393 (7)	
C6	1.0163 (3)	0.8747 (3)	0.9047 (2)	0.0497 (8)	
H6	0.9621	0.8275	0.9291	0.060*	
C7	1.1123 (4)	0.8869 (3)	0.9498 (2)	0.0589 (9)	

H7	1.1221	0.8480	1.0059	0.071*
C8	1.1956 (4)	0.9562 (3)	0.9138 (3)	0.0608 (10)
H8	1.2601	0.9612	0.9462	0.073*
C9	1.1842 (3)	1.0169 (3)	0.8315 (2)	0.0520 (8)
H9	1.2397	1.0628	0.8074	0.062*
C10	1.0864 (3)	1.0070 (3)	0.7856 (2)	0.0423 (7)
C11	0.9413 (3)	0.8190 (3)	0.60412 (19)	0.0434 (7)
H11A	0.9297	0.8057	0.5510	0.052*
H11B	1.0239	0.8355	0.6054	0.052*
C12	0.9414 (3)	0.7065 (3)	0.67009 (19)	0.0404 (7)
C13	0.9106 (3)	0.5870 (3)	0.7870 (2)	0.0439 (7)
C14	0.8774 (4)	0.5367 (3)	0.8664 (2)	0.0524 (8)
H14	0.8228	0.5856	0.8962	0.063*
C15	0.9291 (4)	0.4106 (4)	0.8990 (3)	0.0700 (11)
H15	0.9104	0.3742	0.9525	0.084*
C16	1.0083 (4)	0.3365 (4)	0.8539 (3)	0.0775 (13)
H16	1.0393	0.2517	0.8776	0.093*
C17	1.0417 (4)	0.3846 (4)	0.7761 (3)	0.0730 (12)
H17	1.0950	0.3346	0.7465	0.088*
C18	0.9927 (3)	0.5121 (3)	0.7428 (2)	0.0527 (8)
C19	0.4865 (3)	0.9738 (3)	0.6662 (2)	0.0440 (7)
H19A	0.4238	0.9478	0.7042	0.053*
H19B	0.4474	1.0029	0.6110	0.053*
C20	0.5218 (3)	1.0769 (3)	0.68755 (18)	0.0386 (7)
C21	0.5050 (3)	1.2598 (3)	0.70313 (19)	0.0451 (7)
C22	0.4686 (4)	1.3832 (3)	0.7052 (2)	0.0587 (9)
H22	0.3867	1.4360	0.6869	0.070*
C23	0.5591 (4)	1.4227 (3)	0.7353 (3)	0.0648 (11)
H23	0.5379	1.5045	0.7375	0.078*
C24	0.6816 (4)	1.3445 (4)	0.7628 (2)	0.0622 (10)
H24	0.7403	1.3752	0.7828	0.075*
C25	0.7183 (4)	1.2220 (3)	0.7612 (2)	0.0498 (8)
H25	0.8004	1.1699	0.7799	0.060*
C26	0.6285 (3)	1.1797 (3)	0.73060 (18)	0.0403 (7)
C27	0.5784 (3)	0.7514 (3)	0.72125 (18)	0.0406 (7)
H27A	0.6449	0.6793	0.7140	0.049*
H27B	0.4950	0.7469	0.7058	0.049*
C28	0.5802 (3)	0.7576 (3)	0.80841 (18)	0.0380 (6)
C29	0.5324 (3)	0.7414 (3)	0.9378 (2)	0.0477 (8)
C30	0.4836 (4)	0.7203 (4)	1.0160 (2)	0.0644 (10)
H30	0.4234	0.6762	1.0302	0.077*
C31	0.5272 (5)	0.7664 (5)	1.0710 (2)	0.0750 (12)
H31	0.4957	0.7543	1.1238	0.090*
C32	0.6186 (5)	0.8317 (4)	1.0501 (2)	0.0728 (12)
H32	0.6461	0.8619	1.0895	0.087*
C33	0.6691 (4)	0.8527 (4)	0.9729 (2)	0.0560 (9)
H33	0.7302	0.8960	0.9594	0.067*
C34	0.6239 (3)	0.8058 (3)	0.91627 (18)	0.0395 (7)
C35	0.2331 (6)	0.5681 (6)	0.8657 (5)	0.122 (2)

H35A	0.2554	0.5382	0.9235	0.182*	
H35B	0.2409	0.4992	0.8434	0.182*	
H35C	0.1456	0.6209	0.8574	0.182*	
C36	0.4998 (6)	0.6466 (4)	0.5199 (3)	0.1029 (18)	
H36A	0.5832	0.6546	0.5022	0.154*	
H36B	0.4745	0.5954	0.4919	0.154*	
H36C	0.5041	0.6096	0.5782	0.154*	
Cl1	0.81962 (8)	0.76367 (8)	0.41547 (5)	0.0523 (2)	
Cl2	0.25611 (11)	0.79632 (15)	0.65016 (9)	0.0972 (4)	
N1	0.8357 (2)	0.9273 (2)	0.61481 (14)	0.0388 (6)	
N2	0.6035 (2)	0.8669 (2)	0.67068 (15)	0.0370 (5)	
N3	0.9191 (2)	0.9405 (2)	0.75989 (15)	0.0378 (5)	
N4	1.0494 (3)	1.0531 (2)	0.70377 (16)	0.0446 (6)	
H4	1.0824	1.1013	0.6671	0.053*	
N5	0.8790 (2)	0.7102 (2)	0.73796 (15)	0.0389 (6)	
N6	1.0092 (3)	0.5910 (3)	0.66900 (18)	0.0526 (7)	
H6A	1.0546	0.5701	0.6293	0.063*	
N7	0.6534 (2)	0.8140 (2)	0.83407 (15)	0.0386 (6)	
N8	0.5074 (3)	0.7112 (3)	0.86743 (16)	0.0488 (7)	
H8A	0.4552	0.6703	0.8626	0.059*	
N12	0.4403 (3)	1.1903 (2)	0.67747 (16)	0.0459 (6)	
H12	0.3618	1.2153	0.6584	0.055*	
N13	0.6354 (2)	1.0632 (2)	0.71968 (15)	0.0398 (6)	
O1	0.3132 (4)	0.6324 (5)	0.8274 (3)	0.1190 (14)	
H1	0.2816	0.6754	0.7820	0.178*	
O2	0.4147 (6)	0.7566 (4)	0.5025 (3)	0.154 (2)	
H2	0.3433	0.7497	0.5171	0.231*	
O3	0.1666 (6)	0.5150 (6)	0.5485 (3)	0.100 (3)	0.752 (18)
H3	0.1713	0.4426	0.5524	0.150*	0.752 (18)
C37	0.1726 (9)	0.5770 (9)	0.4660 (4)	0.101 (3)	0.752 (18)
H37A	0.1762	0.6592	0.4620	0.152*	0.752 (18)
H37B	0.0972	0.5814	0.4361	0.152*	0.752 (18)
H37C	0.2486	0.5331	0.4432	0.152*	0.752 (18)
C37'	0.143 (10)	0.581 (10)	0.460 (4)	0.37 (6)	0.248 (18)
H37D	0.0541	0.6280	0.4461	0.558*	0.248 (18)
H37E	0.1533	0.4957	0.4632	0.558*	0.248 (18)
H37F	0.1965	0.6126	0.4176	0.558*	0.248 (18)
O3'	0.178 (3)	0.591 (4)	0.5330 (19)	0.155 (11)	0.248 (18)
H3'	0.2517	0.5977	0.5310	0.232*	0.248 (18)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0340 (2)	0.0360 (2)	0.0319 (2)	−0.01547 (16)	0.00156 (14)	−0.00855 (15)
C1	0.0439 (18)	0.0517 (18)	0.0352 (15)	−0.0184 (15)	−0.0050 (13)	−0.0149 (13)
C2	0.0507 (19)	0.0497 (18)	0.0316 (15)	−0.0177 (15)	−0.0015 (13)	−0.0055 (13)
C3	0.0516 (19)	0.0449 (17)	0.0365 (16)	−0.0236 (15)	0.0040 (13)	−0.0033 (13)
C4	0.0415 (17)	0.0378 (15)	0.0390 (15)	−0.0174 (13)	0.0052 (13)	−0.0111 (12)

C5	0.0374 (16)	0.0394 (16)	0.0434 (16)	−0.0110 (13)	0.0013 (13)	−0.0150 (13)
C6	0.053 (2)	0.0480 (18)	0.0473 (18)	−0.0194 (16)	−0.0051 (15)	−0.0050 (15)
C7	0.067 (2)	0.060 (2)	0.051 (2)	−0.0205 (19)	−0.0133 (17)	−0.0106 (17)
C8	0.055 (2)	0.056 (2)	0.075 (3)	−0.0177 (18)	−0.0210 (19)	−0.0204 (19)
C9	0.048 (2)	0.052 (2)	0.066 (2)	−0.0231 (16)	0.0001 (16)	−0.0220 (17)
C10	0.0417 (18)	0.0412 (17)	0.0496 (18)	−0.0157 (14)	0.0017 (14)	−0.0174 (14)
C11	0.0413 (18)	0.0512 (18)	0.0395 (16)	−0.0166 (15)	0.0069 (13)	−0.0126 (14)
C12	0.0366 (16)	0.0449 (17)	0.0421 (16)	−0.0121 (13)	−0.0003 (13)	−0.0150 (13)
C13	0.0414 (18)	0.0388 (16)	0.0492 (18)	−0.0098 (14)	−0.0053 (14)	−0.0090 (14)
C14	0.058 (2)	0.0445 (18)	0.0509 (19)	−0.0137 (16)	0.0015 (16)	−0.0069 (15)
C15	0.085 (3)	0.050 (2)	0.063 (2)	−0.016 (2)	0.002 (2)	−0.0002 (18)
C16	0.078 (3)	0.039 (2)	0.094 (3)	−0.001 (2)	−0.001 (2)	0.001 (2)
C17	0.074 (3)	0.045 (2)	0.090 (3)	−0.0027 (19)	0.007 (2)	−0.019 (2)
C18	0.048 (2)	0.0436 (18)	0.063 (2)	−0.0085 (15)	0.0007 (16)	−0.0139 (16)
C19	0.0342 (16)	0.0456 (17)	0.0534 (18)	−0.0120 (14)	−0.0042 (14)	−0.0139 (14)
C20	0.0401 (17)	0.0357 (15)	0.0386 (15)	−0.0098 (13)	−0.0001 (13)	−0.0090 (12)
C21	0.056 (2)	0.0414 (17)	0.0386 (16)	−0.0147 (15)	0.0066 (14)	−0.0127 (13)
C22	0.069 (2)	0.0436 (19)	0.059 (2)	−0.0122 (18)	0.0079 (18)	−0.0116 (16)
C23	0.087 (3)	0.0391 (19)	0.077 (3)	−0.027 (2)	0.019 (2)	−0.0237 (18)
C24	0.077 (3)	0.060 (2)	0.069 (2)	−0.040 (2)	0.016 (2)	−0.0294 (19)
C25	0.053 (2)	0.0531 (19)	0.054 (2)	−0.0251 (16)	0.0080 (16)	−0.0231 (16)
C26	0.0471 (18)	0.0413 (16)	0.0365 (15)	−0.0190 (14)	0.0071 (13)	−0.0110 (13)
C27	0.0408 (17)	0.0426 (17)	0.0451 (17)	−0.0209 (14)	0.0008 (13)	−0.0132 (13)
C28	0.0386 (16)	0.0396 (16)	0.0390 (15)	−0.0176 (13)	0.0011 (12)	−0.0087 (12)
C29	0.0470 (19)	0.055 (2)	0.0418 (17)	−0.0215 (16)	0.0020 (14)	−0.0073 (14)
C30	0.069 (3)	0.085 (3)	0.048 (2)	−0.042 (2)	0.0133 (18)	−0.0127 (19)
C31	0.085 (3)	0.110 (4)	0.041 (2)	−0.048 (3)	0.0204 (19)	−0.020 (2)
C32	0.091 (3)	0.101 (3)	0.046 (2)	−0.046 (3)	0.014 (2)	−0.033 (2)
C33	0.067 (2)	0.068 (2)	0.0444 (18)	−0.033 (2)	0.0078 (16)	−0.0209 (17)
C34	0.0386 (16)	0.0450 (17)	0.0369 (15)	−0.0174 (14)	0.0042 (12)	−0.0089 (13)
C35	0.095 (4)	0.121 (5)	0.173 (7)	−0.059 (4)	0.020 (4)	−0.051 (4)
C36	0.152 (6)	0.059 (3)	0.088 (4)	−0.021 (3)	0.011 (3)	−0.015 (3)
Cl1	0.0505 (5)	0.0553 (5)	0.0541 (5)	−0.0238 (4)	0.0026 (4)	−0.0107 (4)
Cl2	0.0509 (6)	0.1369 (12)	0.1111 (10)	−0.0283 (7)	0.0003 (6)	−0.0437 (9)
N1	0.0427 (14)	0.0419 (14)	0.0340 (12)	−0.0185 (12)	0.0018 (10)	−0.0073 (10)
N2	0.0406 (14)	0.0362 (13)	0.0367 (13)	−0.0140 (11)	−0.0014 (10)	−0.0104 (10)
N3	0.0361 (13)	0.0414 (13)	0.0370 (13)	−0.0161 (11)	−0.0012 (10)	−0.0066 (10)
N4	0.0454 (15)	0.0476 (15)	0.0484 (15)	−0.0258 (13)	0.0095 (12)	−0.0135 (12)
N5	0.0383 (14)	0.0405 (14)	0.0377 (13)	−0.0118 (11)	0.0009 (10)	−0.0097 (11)
N6	0.0523 (17)	0.0521 (17)	0.0561 (17)	−0.0130 (14)	0.0134 (13)	−0.0233 (14)
N7	0.0419 (14)	0.0426 (14)	0.0370 (13)	−0.0196 (12)	0.0048 (11)	−0.0127 (11)
N8	0.0504 (16)	0.0591 (17)	0.0459 (15)	−0.0334 (14)	0.0044 (12)	−0.0106 (13)
N12	0.0435 (15)	0.0448 (15)	0.0465 (15)	−0.0085 (12)	−0.0026 (12)	−0.0116 (12)
N13	0.0432 (15)	0.0384 (13)	0.0419 (14)	−0.0158 (11)	0.0016 (11)	−0.0136 (11)
O1	0.098 (3)	0.168 (4)	0.120 (3)	−0.091 (3)	−0.016 (2)	−0.026 (3)
O2	0.187 (5)	0.101 (3)	0.107 (3)	0.023 (3)	0.025 (3)	0.009 (2)
O3	0.135 (4)	0.065 (3)	0.105 (4)	−0.028 (3)	0.051 (3)	−0.039 (3)
C37	0.082 (5)	0.094 (5)	0.094 (5)	−0.002 (4)	0.015 (4)	0.003 (4)
C37'	0.37 (6)	0.37 (6)	0.37 (6)	−0.11 (2)	0.009 (11)	−0.098 (19)

O3'	0.158 (13)	0.151 (15)	0.163 (14)	−0.052 (9)	0.017 (9)	−0.049 (10)

Geometric parameters (Å, °)

Ni1—N5	2.076 (2)	C21—N12	1.375 (4)
Ni1—N3	2.078 (2)	C21—C22	1.394 (5)
Ni1—N13	2.082 (2)	C21—C26	1.403 (5)
Ni1—N7	2.097 (2)	C22—C23	1.367 (6)
Ni1—N1	2.167 (2)	C22—H22	0.9300
Ni1—N2	2.175 (2)	C23—C24	1.389 (6)
C1—N2	1.476 (4)	C23—H23	0.9300
C1—C2	1.528 (4)	C24—C25	1.382 (5)
C1—H1A	0.9700	C24—H24	0.9300
C1—H1B	0.9700	C25—C26	1.385 (4)
C2—N1	1.481 (4)	C25—H25	0.9300
C2—H2A	0.9700	C26—N13	1.408 (4)
C2—H2B	0.9700	C27—N2	1.485 (4)
C3—N1	1.476 (4)	C27—C28	1.494 (4)
C3—C4	1.498 (4)	C27—H27A	0.9700
C3—H3A	0.9700	C27—H27B	0.9700
C3—H3B	0.9700	C28—N7	1.320 (4)
C4—N3	1.321 (4)	C28—N8	1.340 (4)
C4—N4	1.339 (4)	C29—C30	1.386 (5)
C5—C6	1.389 (4)	C29—N8	1.386 (4)
C5—N3	1.391 (4)	C29—C34	1.392 (4)
C5—C10	1.406 (4)	C30—C31	1.354 (6)
C6—C7	1.377 (5)	C30—H30	0.9300
C6—H6	0.9300	C31—C32	1.397 (6)
C7—C8	1.397 (5)	C31—H31	0.9300
C7—H7	0.9300	C32—C33	1.378 (5)
C8—C9	1.372 (5)	C32—H32	0.9300
C8—H8	0.9300	C33—C34	1.393 (5)
C9—C10	1.387 (5)	C33—H33	0.9300
C9—H9	0.9300	C34—N7	1.394 (4)
C10—N4	1.371 (4)	C35—O1	1.344 (6)
C11—C12	1.478 (4)	C35—H35A	0.9600
C11—N1	1.488 (4)	C35—H35B	0.9600
C11—H11A	0.9700	C35—H35C	0.9600
C11—H11B	0.9700	C36—O2	1.313 (6)
C12—N5	1.309 (4)	C36—H36A	0.9600
C12—N6	1.345 (4)	C36—H36B	0.9600
C13—C14	1.388 (5)	C36—H36C	0.9600
C13—C18	1.400 (5)	N4—H4	0.8600
C13—N5	1.407 (4)	N6—H6A	0.8600
C14—C15	1.381 (5)	N8—H8A	0.8600
C14—H14	0.9300	N12—H12	0.8600
C15—C16	1.390 (6)	O1—H1	0.8200
C15—H15	0.9300	O2—H2	0.8200
C16—C17	1.360 (6)	O3—C37	1.395 (7)

C16—H16	0.9300	O3—H3	0.8200
C17—C18	1.393 (5)	C37—H37A	0.9600
C17—H17	0.9300	C37—H37B	0.9600
C18—N6	1.376 (4)	C37—H37C	0.9600
C19—N2	1.488 (4)	C37'—O3'	1.358 (9)
C19—C20	1.502 (4)	C37'—H37D	0.9600
C19—H19A	0.9700	C37'—H37E	0.9600
C19—H19B	0.9700	C37'—H37F	0.9600
C20—N13	1.314 (4)	O3'—H3'	0.8200
C20—N12	1.335 (4)		
N5—Ni1—N3	91.55 (10)	C22—C23—C24	122.0 (3)
N5—Ni1—N13	171.99 (10)	C22—C23—H23	119.0
N3—Ni1—N13	92.50 (10)	C24—C23—H23	119.0
N5—Ni1—N7	92.35 (10)	C25—C24—C23	121.6 (4)
N3—Ni1—N7	120.95 (10)	C25—C24—H24	119.2
N13—Ni1—N7	91.49 (10)	C23—C24—H24	119.2
N5—Ni1—N1	80.72 (9)	C24—C25—C26	117.5 (4)
N3—Ni1—N1	79.15 (9)	C24—C25—H25	121.2
N13—Ni1—N1	93.27 (9)	C26—C25—H25	121.2
N7—Ni1—N1	159.13 (10)	C25—C26—C21	120.3 (3)
N5—Ni1—N2	93.07 (9)	C25—C26—N13	131.7 (3)
N3—Ni1—N2	159.90 (9)	C21—C26—N13	108.0 (3)
N13—Ni1—N2	80.83 (9)	N2—C27—C28	105.7 (2)
N7—Ni1—N2	78.41 (9)	N2—C27—H27A	110.6
N1—Ni1—N2	82.31 (9)	C28—C27—H27A	110.6
N2—C1—C2	108.7 (2)	N2—C27—H27B	110.6
N2—C1—H1A	110.0	C28—C27—H27B	110.6
C2—C1—H1A	110.0	H27A—C27—H27B	108.7
N2—C1—H1B	110.0	N7—C28—N8	113.1 (3)
C2—C1—H1B	110.0	N7—C28—C27	122.0 (3)
H1A—C1—H1B	108.3	N8—C28—C27	124.9 (3)
N1—C2—C1	108.6 (2)	C30—C29—N8	132.6 (3)
N1—C2—H2A	110.0	C30—C29—C34	121.8 (3)
C1—C2—H2A	110.0	N8—C29—C34	105.6 (3)
N1—C2—H2B	110.0	C31—C30—C29	117.4 (4)
C1—C2—H2B	110.0	C31—C30—H30	121.3
H2A—C2—H2B	108.3	C29—C30—H30	121.3
N1—C3—C4	107.2 (2)	C30—C31—C32	121.4 (3)
N1—C3—H3A	110.3	C30—C31—H31	119.3
C4—C3—H3A	110.3	C32—C31—H31	119.3
N1—C3—H3B	110.3	C33—C32—C31	122.2 (4)
C4—C3—H3B	110.3	C33—C32—H32	118.9
H3A—C3—H3B	108.5	C31—C32—H32	118.9
N3—C4—N4	113.0 (3)	C32—C33—C34	116.4 (3)
N3—C4—C3	121.3 (3)	C32—C33—H33	121.8
N4—C4—C3	125.7 (3)	C34—C33—H33	121.8
C6—C5—N3	131.2 (3)	C29—C34—C33	120.8 (3)
C6—C5—C10	120.4 (3)	C29—C34—N7	109.1 (3)
N3—C5—C10	108.3 (3)	C33—C34—N7	130.1 (3)

C7—C6—C5	117.3 (3)	O1—C35—H35A	109.5
C7—C6—H6	121.3	O1—C35—H35B	109.5
C5—C6—H6	121.3	H35A—C35—H35B	109.5
C6—C7—C8	122.0 (3)	O1—C35—H35C	109.5
C6—C7—H7	119.0	H35A—C35—H35C	109.5
C8—C7—H7	119.0	H35B—C35—H35C	109.5
C9—C8—C7	121.3 (3)	O2—C36—H36A	109.5
C9—C8—H8	119.4	O2—C36—H36B	109.5
C7—C8—H8	119.4	H36A—C36—H36B	109.5
C8—C9—C10	117.3 (3)	O2—C36—H36C	109.5
C8—C9—H9	121.4	H36A—C36—H36C	109.5
C10—C9—H9	121.4	H36B—C36—H36C	109.5
N4—C10—C9	132.5 (3)	C3—N1—C2	113.5 (2)
N4—C10—C5	105.8 (3)	C3—N1—C11	111.1 (2)
C9—C10—C5	121.7 (3)	C2—N1—C11	111.7 (2)
C12—C11—N1	110.6 (2)	C3—N1—Ni1	104.52 (17)
C12—C11—H11A	109.5	C2—N1—Ni1	105.47 (18)
N1—C11—H11A	109.5	C11—N1—Ni1	110.16 (17)
C12—C11—H11B	109.5	C1—N2—C27	114.3 (2)
N1—C11—H11B	109.5	C1—N2—C19	111.8 (2)
H11A—C11—H11B	108.1	C27—N2—C19	109.8 (2)
N5—C12—N6	112.8 (3)	C1—N2—Ni1	106.06 (18)
N5—C12—C11	122.9 (3)	C27—N2—Ni1	104.33 (17)
N6—C12—C11	124.3 (3)	C19—N2—Ni1	110.27 (17)
C14—C13—C18	120.8 (3)	C4—N3—C5	105.3 (2)
C14—C13—N5	131.1 (3)	C4—N3—Ni1	110.72 (19)
C18—C13—N5	108.0 (3)	C5—N3—Ni1	143.9 (2)
C15—C14—C13	116.9 (3)	C4—N4—C10	107.4 (2)
C15—C14—H14	121.5	C4—N4—H4	126.3
C13—C14—H14	121.5	C10—N4—H4	126.3
C14—C15—C16	121.8 (4)	C12—N5—C13	105.7 (3)
C14—C15—H15	119.1	C12—N5—Ni1	113.6 (2)
C16—C15—H15	119.1	C13—N5—Ni1	140.5 (2)
C17—C16—C15	121.9 (4)	C12—N6—C18	107.6 (3)
C17—C16—H16	119.1	C12—N6—H6A	126.2
C15—C16—H16	119.1	C18—N6—H6A	126.2
C16—C17—C18	117.2 (4)	C28—N7—C34	105.1 (2)
C16—C17—H17	121.4	C28—N7—Ni1	110.24 (19)
C18—C17—H17	121.4	C34—N7—Ni1	144.6 (2)
N6—C18—C17	132.8 (4)	C28—N8—C29	107.1 (3)
N6—C18—C13	105.8 (3)	C28—N8—H8A	126.4
C17—C18—C13	121.3 (4)	C29—N8—H8A	126.4
N2—C19—C20	110.3 (2)	C20—N12—C21	107.5 (3)
N2—C19—H19A	109.6	C20—N12—H12	126.3
C20—C19—H19A	109.6	C21—N12—H12	126.3
N2—C19—H19B	109.6	C20—N13—C26	105.1 (3)
C20—C19—H19B	109.6	C20—N13—Ni1	113.40 (19)
H19A—C19—H19B	108.1	C26—N13—Ni1	141.5 (2)
N13—C20—N12	113.5 (3)	C35—O1—H1	109.5

N13—C20—C19	123.1 (3)	C36—O2—H2	109.5
N12—C20—C19	123.4 (3)	O3'—C37'—H37D	109.5
N12—C21—C22	132.3 (3)	O3'—C37'—H37E	109.5
N12—C21—C26	105.9 (3)	H37D—C37'—H37E	109.5
C22—C21—C26	121.8 (3)	O3'—C37'—H37F	109.5
C23—C22—C21	116.8 (4)	H37D—C37'—H37F	109.5
C23—C22—H22	121.6	H37E—C37'—H37F	109.5
C21—C22—H22	121.6	C37'—O3'—H3'	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···Cl1^{i}	0.82	2.30	3.117 (7)	171
N4—H4···Cl1^{ii}	0.86	2.29	3.140 (3)	172
N6—H6A···O3^{iii}	0.86	1.90	2.761 (5)	175
N12—H12···Cl1^{iv}	0.86	2.29	3.116 (3)	162
C2—H2B···O2^{iv}	0.97	2.25	3.145 (5)	154
C11—H11B···Cl2^{iii}	0.97	2.53	3.445 (3)	157
O1—H1···Cl2	0.82	2.27	3.065 (4)	163
O2—H2···Cl2	0.82	2.53	3.027 (5)	120
N8—H8A···O1	0.86	1.88	2.705 (4)	161
C27—H27B···Cl2	0.97	2.64	3.582 (3)	165

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

Fig. 1

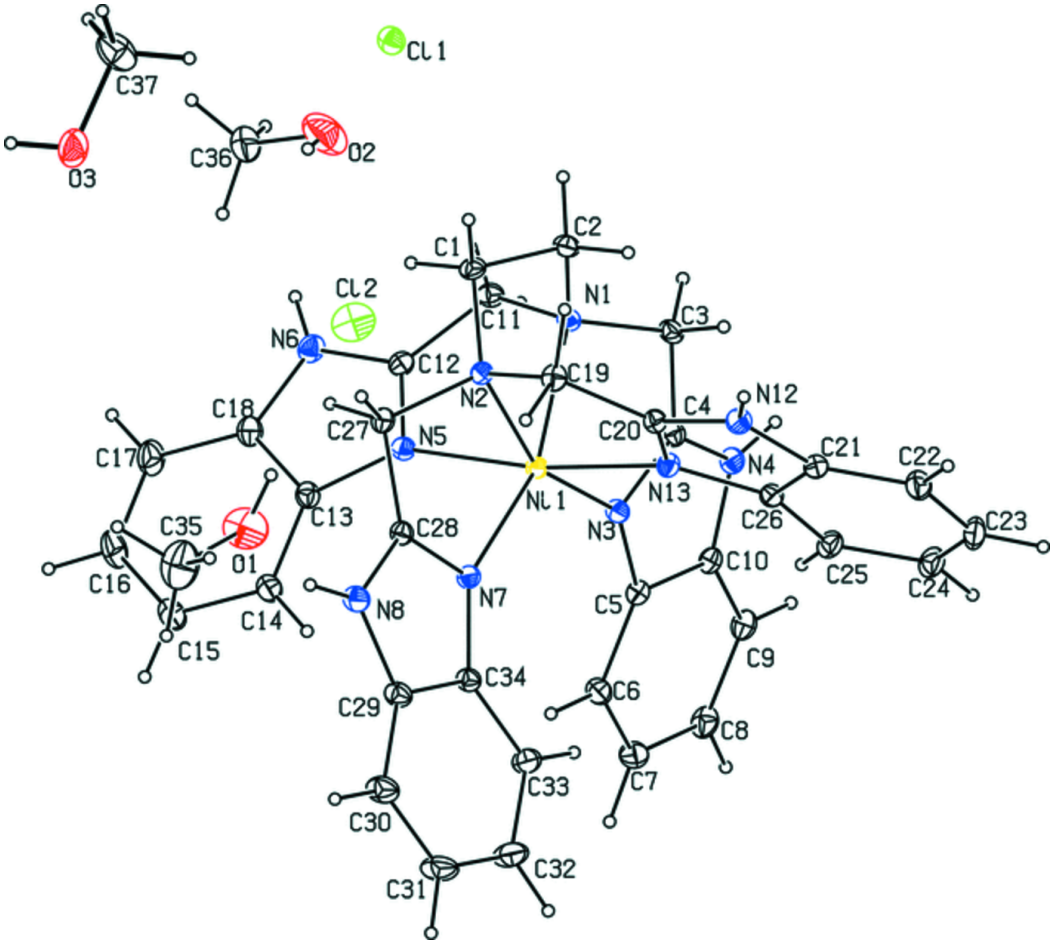
Cl1
C37
O3
C36
O2
C1
C2
Cl2
C11
N1
C3
N6
C12
N2
C19
C18
C27
N5
C4
N12
C20
C17
N4
C21
C22
Ni1
N13
C13
C28
N3
C26
C23
C35
O1
C10
C25
C24
C16
N8
N7
C5
C14
C9
C15
C34
C6
C29
C8
C33
C7
C30
C32
C31

Fig. 2