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Aquachloridobis[2-(1,3-thiazol-4-yl-κN)-1*H*-benzimidazole-κN^3]nickel(II) nitrate

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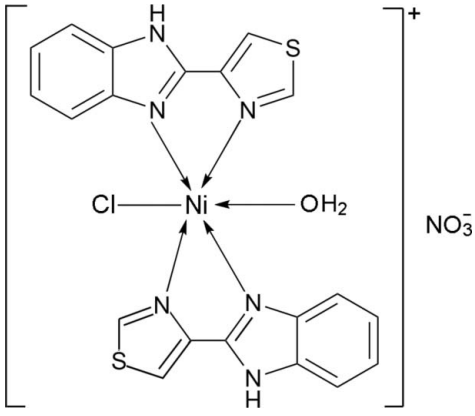
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.054; wR factor = 0.174; data-to-parameter ratio = 12.8.

In the title compound, $[NiCl(C_{10}H_7N_3S)_2(H_2O)]NO_3$, the Ni^{II} ion is coordinated by four N atoms from two chelating 2-(1,3-thiazol-4-yl)-1*H*-benzimidazole ligands, one Cl atom and one water molecule in a distorted octahedral geometry. In the crystal, O—H···O, N—H···O and N—H···Cl hydrogen bonds link the complex cations and nitrate anions into a three-dimensional network. π–π interactions between the thiazole and imidazole rings and between the thiazole and benzene rings are observed [centroid–centroid distances = 3.592 (3) and 3.735 (3) Å].

Related literature

For background to the synthesis and properties of benzimidazole derivatives, see: Agh-Atabay *et al.* (2003); Devereux *et al.* (2004); Inoue *et al.* (2002). For a related structure, see: Mothilal *et al.* (2004).



Experimental

Crystal data

$[NiCl(C_{10}H_7N_3S)_2(H_2O)]NO_3$ M_r = 576.68
Monoclinic, $P2_1/c$
a = 16.091 (5) Å
b = 11.189 (3) Å
c = 13.931 (3) Å
β = 113.275 (3)°
V = 2304.1 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 296 K
0.26 × 0.25 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.748, T_{max} = 0.764
11654 measured reflections
4050 independent reflections
3129 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.174
S = 1.07
4050 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O3^{i}	0.84	2.00	2.751 (5)	149
O1—H1B···O2^{ii}	0.79	2.53	3.293 (6)	160
O1—H1B···O4^{ii}	0.79	2.38	3.025 (5)	139
N4—H4···O3^{iii}	0.86	2.35	2.962 (5)	129
N4—H4···O4^{iii}	0.86	2.14	2.996 (5)	173
N7—H7···Cl1^{iv}	0.86	2.35	3.159 (4)	157

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

Data collection: *SMART* (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: HY2553).

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supplementary materials

Acta Cryst. (2012). E**68**, m1029 [doi:10.1107/S1600536812029728]

Aquachloridobis[2-(1,3-thiazol-4-yl-κN)-1*H*-benzimidazole-κN^3]nickel(II) nitrate

Peng Liang, Wei Wu, Wei-Man Tian and Xian-Hong Yin

Comment

Thiabendazole (TBZ) aroused considerable interest in biology and medicine due to its antiproliferative activities. It is an antimicrobial drug belonging to the benzimidazole derivatives and exhibits wide applications in human and veterinary medicine (Agh-Atabay *et al.*, 2003; Devereux *et al.*, 2004; Inoue *et al.*, 2002). As part of our studies of the synthesis and characterization of these compounds, we report here the synthesis and crystal structure of the title compound (Fig. 1).

In the crystal, intermolecular O—H···O, N—H···O and N—H···Cl hydrogen bonds link the complex cations and nitrate anions into a three-dimensional network (Table 1, Fig. 2) (Mothilal *et al.*, 2004). π–π interactions between the thiazole and imidazole rings and between the thiazole and benzene rings are observed [centroid–centroid distances = 3.592 (3) and 3.735 (3) Å]. In the complex cation, the two ligand planes are nearly perpendicular to each other, with a dihedral angle of 89.14 (7)°.

Experimental

A solution of TBZ (0.201 g, 1 mmol) in 3 ml DMF was added dropwise with stirring at room temperature to a solution of $Ni(NO_3)_2.6H_2O$ (0.290 g, 1 mmol) and $NiCl_2.6H_2O$ (0.237 g, 1 mmol) in a mixture of 10 ml water and 5 ml ethanol. Then an aqueous solution of sodium hydroxide was added dropwise with stirring to adjust the pH value of the solution being 6. The resulting mixture was sealed in a 23 ml Teflon-lined stainless reactor, kept under autogenous pressure at 403 K for 72 h, and then slowly cooled to room temperature at a rate of 5 K per hour. Dark-green block crystals suitable for X-ray diffraction were isolated, washed with ethanol and dried in air (yield: 65% based on Ni).

Refinement

H atoms on C and N atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and N—H = 0.86 Å and with U_{iso}(H) = 1.2U_{eq}(C, N). The water H atoms were located from a difference Fourier map and refined as riding with U_{iso}(H) = 0.079 Å^2.

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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).

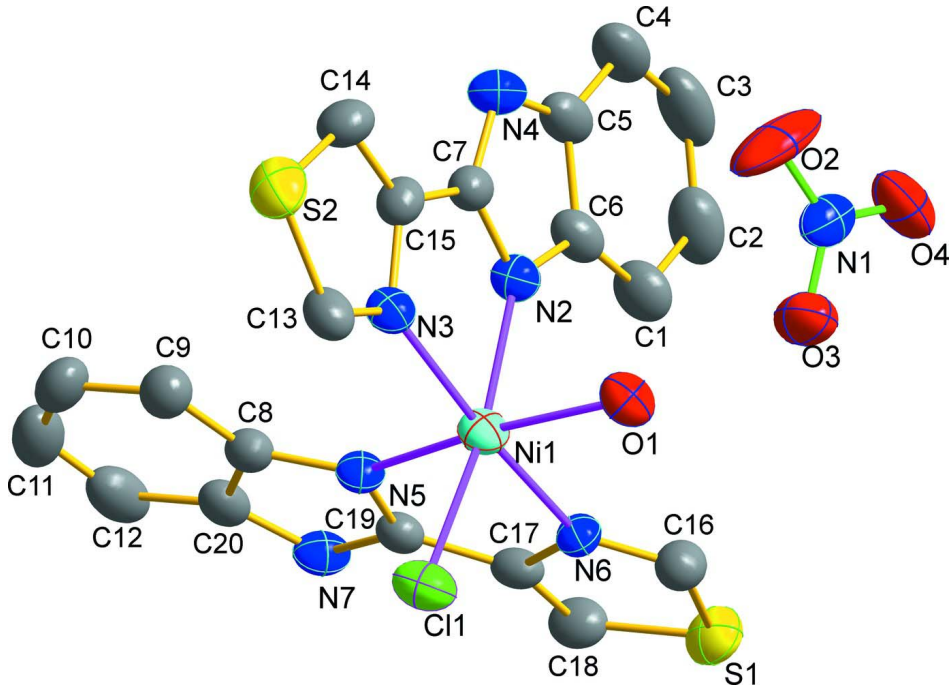

Figure 1

The Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

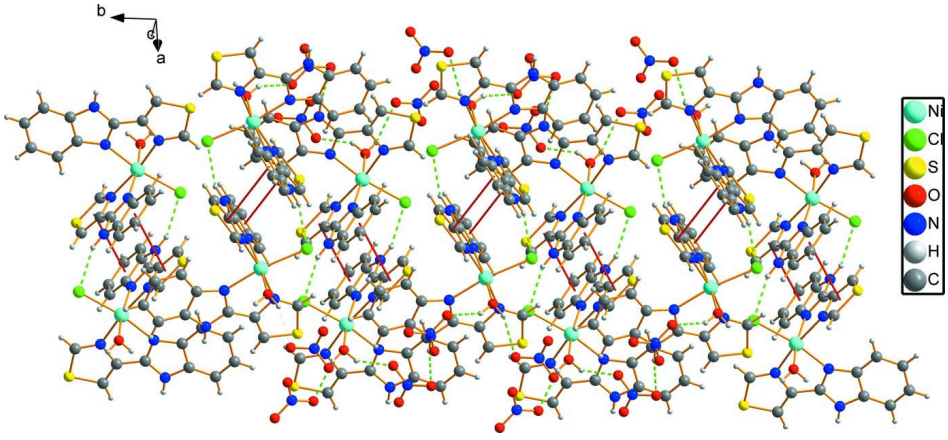

Figure 2

Crystal packing of the title compound. Dashed lines denote hydrogen bonds.

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Crystal data

$[NiCl(C_{10}H_7N_3S)_2(H_2O)]NO_3$
$M_r = 576.68$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.091$ (5) Å
$b = 11.189$ (3) Å
$c = 13.931$ (3) Å
$\beta = 113.275$ (3)°
$V = 2304.1$ (11) Å^3
$Z = 4$
$F(000) = 1176$
$D_x = 1.662$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2584 reflections

θ = 2.3–26.6°
μ = 1.18 mm^{-1}
T = 296 K

Block, green
0.26 × 0.25 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.748, T_{max} = 0.764

11654 measured reflections
4050 independent reflections
3129 reflections with $I > 2\sigma(I)$
R_{int} = 0.072
θ_{max} = 25.0°, θ_{min} = 1.4°
h = −18→19
k = −13→13
l = −14→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.174
S = 1.07
4050 reflections
316 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.083P)^2 + 1.4424P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.045
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 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	0.26114 (3)	0.47368 (5)	0.32612 (4)	0.0352 (2)
Cl1	0.31740 (8)	0.27662 (10)	0.40665 (10)	0.0490 (4)
S1	0.36620 (9)	0.71229 (11)	0.62788 (10)	0.0507 (4)
S2	0.13043 (9)	0.27528 (12)	0.00588 (11)	0.0552 (4)
O1	0.13949 (19)	0.4517 (3)	0.3478 (3)	0.0412 (7)
O3	1.0666 (2)	0.6635 (3)	0.3784 (3)	0.0606 (10)
O4	1.0018 (2)	0.8339 (3)	0.3421 (3)	0.0693 (11)
O2	0.9808 (3)	0.7045 (5)	0.2204 (3)	0.0964 (18)
N3	0.2001 (2)	0.3971 (3)	0.1739 (3)	0.0344 (8)
N5	0.3884 (2)	0.5240 (3)	0.3241 (3)	0.0313 (8)
N6	0.3205 (2)	0.5777 (3)	0.4687 (3)	0.0324 (8)
N2	0.2024 (2)	0.6272 (3)	0.2292 (3)	0.0343 (8)
N7	0.5158 (2)	0.6289 (3)	0.3975 (3)	0.0370 (9)
H7	0.5562	0.6742	0.4414	0.044*

N4	0.1133 (2)	0.6929 (3)	0.0713 (3)	0.0430 (9)
H4	0.0801	0.6916	0.0054	0.052*
N1	1.0157 (2)	0.7334 (4)	0.3117 (3)	0.0447 (10)
C8	0.4375 (3)	0.5129 (4)	0.2623 (3)	0.0343 (10)
C15	0.1532 (3)	0.4763 (4)	0.0953 (4)	0.0368 (10)
C20	0.5192 (3)	0.5792 (4)	0.3096 (4)	0.0371 (10)
C7	0.1553 (3)	0.5995 (4)	0.1300 (3)	0.0339 (9)
C19	0.4372 (2)	0.5941 (3)	0.4029 (3)	0.0321 (9)
C17	0.4038 (2)	0.6273 (3)	0.4827 (3)	0.0327 (9)
C6	0.1899 (3)	0.7514 (4)	0.2356 (4)	0.0388 (10)
C13	0.1927 (3)	0.2884 (4)	0.1364 (4)	0.0419 (11)
H13	0.2196	0.2229	0.1783	0.050*
C5	0.1327 (3)	0.7920 (4)	0.1353 (4)	0.0441 (11)
C18	0.4377 (3)	0.7027 (4)	0.5649 (4)	0.0421 (11)
H18	0.4923	0.7435	0.5842	0.051*
C11	0.5629 (4)	0.5228 (5)	0.1731 (5)	0.0571 (14)
H11	0.6040	0.5248	0.1412	0.069*
C1	0.2222 (3)	0.8290 (4)	0.3202 (4)	0.0495 (12)
H1	0.2602	0.8024	0.3862	0.059*
C12	0.5820 (3)	0.5849 (5)	0.2636 (5)	0.0540 (14)
H12	0.6349	0.6294	0.2935	0.065*
C14	0.1106 (3)	0.4261 (5)	−0.0009 (4)	0.0467 (12)
H14	0.0759	0.4676	−0.0613	0.056*
C10	0.4830 (4)	0.4559 (5)	0.1265 (4)	0.0507 (12)
H10	0.4723	0.4144	0.0649	0.061*
C9	0.4209 (3)	0.4511 (4)	0.1705 (4)	0.0443 (11)
H9	0.3681	0.4069	0.1392	0.053*
C16	0.2942 (3)	0.6140 (4)	0.5385 (4)	0.0412 (11)
H16	0.2400	0.5892	0.5412	0.049*
C4	0.1057 (4)	0.9106 (5)	0.1180 (5)	0.0562 (14)
H4A	0.0679	0.9375	0.0520	0.067*
C2	0.1958 (4)	0.9471 (4)	0.3023 (5)	0.0612 (15)
H2	0.2169	1.0019	0.3569	0.073*
C3	0.1367 (4)	0.9856 (4)	0.2012 (6)	0.0661 (18)
H3	0.1186	1.0652	0.1916	0.079*
H1A	0.1016	0.5069	0.3358	0.079*
H1B	0.1000	0.4040	0.3241	0.079*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0293 (3)	0.0361 (3)	0.0344 (4)	−0.0022 (2)	0.0065 (3)	−0.0048 (2)
Cl1	0.0429 (6)	0.0411 (6)	0.0506 (8)	0.0038 (5)	0.0053 (5)	0.0024 (5)
S1	0.0636 (8)	0.0451 (6)	0.0402 (8)	−0.0015 (5)	0.0170 (6)	−0.0142 (5)
S2	0.0516 (7)	0.0592 (8)	0.0476 (8)	−0.0047 (6)	0.0119 (6)	−0.0238 (6)
O1	0.0344 (15)	0.0363 (15)	0.051 (2)	−0.0037 (12)	0.0148 (14)	−0.0003 (14)
O3	0.072 (2)	0.054 (2)	0.046 (2)	0.0172 (18)	0.0134 (19)	0.0004 (17)
O4	0.059 (2)	0.057 (2)	0.093 (3)	0.0218 (18)	0.032 (2)	0.011 (2)
O2	0.090 (3)	0.159 (5)	0.025 (2)	−0.052 (3)	0.006 (2)	−0.010 (2)
N3	0.0294 (16)	0.0339 (17)	0.034 (2)	−0.0017 (14)	0.0065 (15)	−0.0072 (15)

N5	0.0255 (16)	0.0344 (17)	0.029 (2)	−0.0029 (13)	0.0058 (15)	−0.0020 (15)
N6	0.0306 (17)	0.0380 (18)	0.025 (2)	0.0000 (14)	0.0077 (15)	−0.0059 (15)
N2	0.0346 (17)	0.0303 (17)	0.035 (2)	−0.0006 (14)	0.0104 (16)	−0.0017 (15)
N7	0.0291 (16)	0.0394 (18)	0.036 (2)	−0.0067 (14)	0.0055 (16)	0.0033 (16)
N4	0.042 (2)	0.045 (2)	0.036 (2)	0.0034 (17)	0.0087 (17)	0.0068 (18)
N1	0.0357 (19)	0.061 (3)	0.038 (2)	−0.0123 (18)	0.0146 (18)	0.001 (2)
C8	0.032 (2)	0.035 (2)	0.033 (2)	0.0016 (17)	0.0102 (19)	0.0018 (18)
C15	0.032 (2)	0.045 (2)	0.032 (3)	−0.0053 (17)	0.0113 (19)	−0.0058 (19)
C20	0.034 (2)	0.034 (2)	0.044 (3)	0.0039 (17)	0.0153 (19)	0.010 (2)
C7	0.0296 (19)	0.040 (2)	0.033 (2)	0.0007 (17)	0.0126 (18)	0.0016 (18)
C19	0.0265 (18)	0.033 (2)	0.033 (2)	0.0024 (16)	0.0076 (18)	0.0031 (18)
C17	0.0296 (19)	0.0275 (18)	0.032 (2)	−0.0016 (16)	0.0032 (17)	0.0002 (17)
C6	0.033 (2)	0.030 (2)	0.054 (3)	−0.0005 (17)	0.017 (2)	0.004 (2)
C13	0.031 (2)	0.044 (2)	0.046 (3)	−0.0004 (18)	0.010 (2)	−0.009 (2)
C5	0.039 (2)	0.045 (3)	0.054 (3)	0.0063 (19)	0.024 (2)	0.018 (2)
C18	0.042 (2)	0.037 (2)	0.040 (3)	−0.0067 (18)	0.007 (2)	−0.0074 (19)
C11	0.069 (3)	0.057 (3)	0.062 (4)	0.013 (3)	0.043 (3)	0.017 (3)
C1	0.048 (3)	0.035 (2)	0.065 (3)	0.001 (2)	0.021 (2)	−0.003 (2)
C12	0.040 (2)	0.053 (3)	0.071 (4)	0.003 (2)	0.024 (3)	0.023 (3)
C14	0.045 (2)	0.057 (3)	0.033 (3)	−0.002 (2)	0.010 (2)	0.001 (2)
C10	0.064 (3)	0.055 (3)	0.040 (3)	0.004 (2)	0.028 (3)	0.006 (2)
C9	0.046 (3)	0.043 (2)	0.043 (3)	0.001 (2)	0.018 (2)	−0.001 (2)
C16	0.036 (2)	0.046 (2)	0.038 (3)	−0.0030 (19)	0.012 (2)	−0.004 (2)
C4	0.060 (3)	0.045 (3)	0.071 (4)	0.016 (2)	0.035 (3)	0.022 (3)
C2	0.069 (3)	0.038 (2)	0.092 (5)	−0.002 (2)	0.048 (3)	−0.005 (3)
C3	0.067 (3)	0.034 (2)	0.116 (6)	0.011 (2)	0.057 (4)	0.013 (3)

Geometric parameters (Å, º)

Ni1—O1	2.109 (3)	C8—C9	1.383 (6)
Ni1—N3	2.133 (3)	C8—C20	1.424 (6)
Ni1—N5	2.134 (3)	C15—C14	1.361 (6)
Ni1—N2	2.159 (3)	C15—C7	1.456 (6)
Ni1—N6	2.171 (3)	C20—C12	1.396 (7)
Ni1—Cl1	2.4772 (13)	C19—C17	1.461 (6)
S1—C18	1.704 (5)	C17—C18	1.351 (6)
S1—C16	1.721 (4)	C6—C1	1.389 (7)
S2—C13	1.700 (5)	C6—C5	1.410 (6)
S2—C14	1.713 (5)	C13—H13	0.9300
O1—H1A	0.8372	C5—C4	1.387 (7)
O1—H1B	0.7947	C18—H18	0.9300
O3—N1	1.244 (5)	C11—C12	1.364 (8)
O4—N1	1.252 (5)	C11—C10	1.406 (8)
O2—N1	1.214 (5)	C11—H11	0.9300
N3—C13	1.310 (5)	C1—C2	1.381 (7)
N3—C15	1.380 (5)	C1—H1	0.9300
N5—C19	1.326 (5)	C12—H12	0.9300
N5—C8	1.386 (6)	C14—H14	0.9300
N6—C16	1.271 (6)	C10—C9	1.364 (7)
N6—C17	1.391 (5)	C10—H10	0.9300

N2—C7	1.324 (5)	C9—H9	0.9300
N2—C6	1.412 (5)	C16—H16	0.9300
N7—C19	1.354 (5)	C4—C3	1.356 (8)
N7—C20	1.367 (6)	C4—H4A	0.9300
N7—H7	0.8600	C2—C3	1.420 (8)
N4—C7	1.335 (5)	C2—H2	0.9300
N4—C5	1.379 (6)	C3—H3	0.9300
N4—H4	0.8600		

O1—Ni1—N3	90.37 (13)	N2—C7—C15	119.8 (4)
O1—Ni1—N5	169.10 (12)	N4—C7—C15	126.7 (4)
N3—Ni1—N5	99.19 (13)	N5—C19—N7	112.6 (4)
O1—Ni1—N2	88.88 (12)	N5—C19—C17	120.3 (3)
N3—Ni1—N2	77.42 (13)	N7—C19—C17	127.0 (4)
N5—Ni1—N2	88.12 (13)	C18—C17—N6	114.4 (4)
O1—Ni1—N6	91.69 (12)	C18—C17—C19	131.0 (4)
N3—Ni1—N6	171.22 (14)	N6—C17—C19	114.5 (3)
N5—Ni1—N6	78.08 (13)	C1—C6—C5	121.2 (4)
N2—Ni1—N6	94.09 (13)	C1—C6—N2	130.8 (4)
O1—Ni1—Cl1	91.44 (9)	C5—C6—N2	107.9 (4)
N3—Ni1—Cl1	91.99 (10)	N3—C13—S2	115.4 (4)
N5—Ni1—Cl1	93.43 (9)	N3—C13—H13	122.3
N2—Ni1—Cl1	169.41 (10)	S2—C13—H13	122.3
N6—Ni1—Cl1	96.48 (10)	N4—C5—C4	132.9 (5)
C18—S1—C16	89.2 (2)	N4—C5—C6	105.9 (4)
C13—S2—C14	89.5 (2)	C4—C5—C6	121.1 (5)
Ni1—O1—H1A	122.0	C17—C18—S1	110.3 (3)
Ni1—O1—H1B	130.8	C17—C18—H18	124.9
H1A—O1—H1B	90.7	S1—C18—H18	124.9
C13—N3—C15	110.2 (4)	C12—C11—C10	121.9 (5)
C13—N3—Ni1	134.7 (3)	C12—C11—H11	119.0
C15—N3—Ni1	115.1 (3)	C10—C11—H11	119.0
C19—N5—C8	105.7 (3)	C2—C1—C6	117.4 (5)
C19—N5—Ni1	113.7 (3)	C2—C1—H1	121.3
C8—N5—Ni1	140.4 (3)	C6—C1—H1	121.3
C16—N6—C17	111.0 (4)	C11—C12—C20	117.5 (5)
C16—N6—Ni1	135.5 (3)	C11—C12—H12	121.3
C17—N6—Ni1	113.2 (3)	C20—C12—H12	121.3
C7—N2—C6	105.0 (3)	C15—C14—S2	110.0 (4)
C7—N2—Ni1	113.3 (3)	C15—C14—H14	125.0
C6—N2—Ni1	141.4 (3)	S2—C14—H14	125.0
C19—N7—C20	107.6 (3)	C9—C10—C11	120.8 (5)
C19—N7—H7	126.2	C9—C10—H10	119.6
C20—N7—H7	126.2	C11—C10—H10	119.6
C7—N4—C5	107.6 (4)	C10—C9—C8	119.2 (5)
C7—N4—H4	126.2	C10—C9—H9	120.4
C5—N4—H4	126.2	C8—C9—H9	120.4
O2—N1—O3	120.7 (5)	N6—C16—S1	115.2 (3)
O2—N1—O4	121.6 (5)	N6—C16—H16	122.4

O3—N1—O4	117.7 (4)	S1—C16—H16	122.4
C9—C8—N5	132.1 (4)	C3—C4—C5	117.4 (5)
C9—C8—C20	119.5 (4)	C3—C4—H4A	121.3
N5—C8—C20	108.4 (4)	C5—C4—H4A	121.3
C14—C15—N3	114.9 (4)	C1—C2—C3	120.5 (5)
C14—C15—C7	130.8 (4)	C1—C2—H2	119.8
N3—C15—C7	114.3 (4)	C3—C2—H2	119.8
N7—C20—C12	133.3 (4)	C4—C3—C2	122.4 (5)
N7—C20—C8	105.7 (4)	C4—C3—H3	118.8
C12—C20—C8	121.0 (5)	C2—C3—H3	118.8
N2—C7—N4	113.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O3^{i}	0.84	2.00	2.751 (5)	149
O1—H1*B*···O2^{ii}	0.79	2.53	3.293 (6)	160
O1—H1*B*···O4^{ii}	0.79	2.38	3.025 (5)	139
N4—H4···O3^{iii}	0.86	2.35	2.962 (5)	129
N4—H4···O4^{iii}	0.86	2.14	2.996 (5)	173
N7—H7···Cl1^{iv}	0.86	2.35	3.159 (4)	157

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