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Aquachloridobis[5-(2-pyridyl)-1*H*-tetrazolato-κN^1]iron(III)

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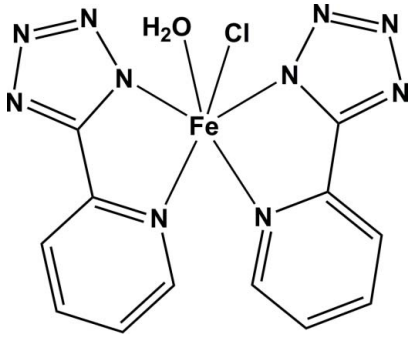
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.080; data-to-parameter ratio = 16.3.

The title compound, $[Fe(C_6H_4N_5)_2Cl(H_2O)]$, was synthesized by hydrothermal reaction of $FeCl_3$ with 2-(1*H*-tetrazol-5-yl)-pyridine. The iron(III) metal centre exhibits a distorted octahedral coordination geometry provided by four N atoms from two bidentate organic ligands, one water O atom and one chloride anion. The pyridine and tetrazole rings are nearly coplanar [dihedral angles = 4.32 (15) and 5.04 (14)°]. In the crystal structure, intermolecular O—H···N hydrogen bonds link the complex molecules into a two-dimensional network parallel to (100).

Related literature

For physical properties such as permittivity, fluorescence, magnetism and optical properties of metal-organic coordination compounds, see: Fu *et al.* (2007); Huang *et al.* (1999); Liu *et al.* (1999); Xie *et al.* (2003); Zhang *et al.* (2000, 2001). For the structure of a related tetrazole compound, see: Fu *et al.* (2008).



Experimental

Crystal data

$[Fe(C_6H_4N_5)_2Cl(H_2O)]$ M_r = 401.60
Monoclinic, $P2_1/c$
a = 17.072 (3) Å
b = 7.1905 (14) Å
c = 14.292 (3) Å
β = 113.85 (3)°
V = 1604.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 298 K
0.15 × 0.10 × 0.10 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.867, T_{max} = 0.894
15693 measured reflections
3678 independent reflections
3226 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.080
S = 1.13
3678 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···N4^{i}	0.98	1.67	2.652 (2)	178
O1W—H1WB···N9^{ii}	0.82	1.80	2.626 (2)	176

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC*.

This work was supported by a start-up grant from Southeast University to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2339).

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supplementary materials

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Aquachloridobis[5-(2-pyridyl)-1*H*-tetrazolato-κN^1]iron(III)

B. Wang

Comment

The construction of metal-organic coordination compounds has attracted much attention owing to their potential propertiess, such as permittivity, fluorescence, magnetism and optical properties. (Fu *et al.*, 2007; Huang *et al.*, 1999; Liu *et al.*, 1999; Xie *et al.*, 2003; Zhang *et al.*,2001; Zhang *et al.*,2000). Tetrazole compounds are a class of excellent ligands for the construction of novel metal-organic frameworks, because of their various coordination modes. (Fu *et al.*, 2008). Herein the crystal structure of the title compound is reported.

In the title compound (Fig. 1), the distorted octahedral coordination geometry around the iron(III) metal centre is provided by four N atoms from two bidentate 2-(1H-tetrazol-5-yl)pyridine ligands, one water O atom and one chloride ion. The pyridine and tetrazole rings are nearly coplanar and only twisted by a dihedral angle of 4.32 (15) and 5.04 (14)°. The geometric parameters of the tetrazole rings are comparable to those observed in a related molecule (Fu *et al.*, 2008). The water molecules are involved in intermolecular O—H···N hydrogen bonds (Table 1) generating a two-dimensional network (Fig. 2).

Experimental

A mixture of 2-(1H-tetrazol-5-yl)pyridine (0.2 mmol), $FeCl_3$ (0.1 mmol), distilled water (1 ml) and a few drops of ethanol sealed in a glass tube was heated at 85 °C. Colourless block crystals suitable for X-ray analysis were obtained after 10 days.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C-H = 0.93 Å with $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference Fourier map refined as riding, with $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

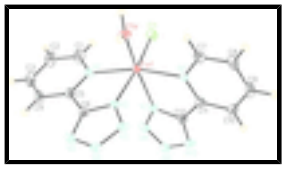

Fig. 1. The molecular view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

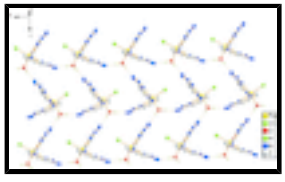

Fig. 2. The crystal packing of the title compound viewed along the *a* axis, showing the two dimensionnal hydrogen bondings network (dashed line). Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

Aquachloridobis[5-(2-pyridyl)-1*H*-tetrazolato-κN^1]iron(III)

Crystal data

$[Fe(C_6H_4N_5)_2Cl(H_2O)]$	F_{000} = 812
M_r = 401.60	D_x = 1.662 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3226 reflections
a = 17.072 (3) Å	θ = 3.1–27.5º
b = 7.1905 (14) Å	μ = 1.13 mm^{-1}
c = 14.292 (3) Å	T = 298 K
β = 113.85 (3)º	Block, colourless
V = 1604.6 (7) Å^3	0.15 × 0.10 × 0.10 mm
Z = 4	

Data collection

Rigaku Mercury2 diffractometer	3678 independent reflections
Radiation source: fine-focus sealed tube	3226 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 27.5º
T = 298 K	θ_{min} = 3.1º
CCD profile fitting scans	h = −22→22
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −9→9
T_{min} = 0.867, T_{max} = 0.894	l = −18→18
15693 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.034	H-atom parameters constrained
$wR(F^2)$ = 0.080	$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 0.8976P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.13	$(\Delta/\sigma)_{max} < 0.001$
3678 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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}
Fe1	0.244652 (16)	0.52062 (4)	0.23914 (2)	0.02111 (9)
Cl1	0.23959 (4)	0.25457 (8)	0.15658 (4)	0.04015 (15)
O1W	0.24124 (9)	0.4003 (2)	0.36157 (10)	0.0298 (3)
H1WA	0.2559	0.2685	0.3733	0.045*
H1WB	0.2346	0.4617	0.4065	0.045*
N6	0.10878 (10)	0.5759 (2)	0.17945 (13)	0.0252 (4)
N2	0.26988 (10)	0.7731 (2)	0.32361 (13)	0.0233 (3)
N1	0.38334 (10)	0.5417 (2)	0.30588 (13)	0.0277 (4)
N4	0.28121 (13)	1.0424 (2)	0.39005 (15)	0.0369 (5)
C11	0.07709 (12)	0.6877 (3)	0.09684 (15)	0.0250 (4)
N10	0.13543 (12)	0.8769 (3)	−0.00850 (13)	0.0332 (4)
N3	0.22568 (11)	0.9153 (2)	0.33720 (14)	0.0310 (4)
N7	0.22328 (10)	0.6973 (2)	0.11379 (13)	0.0260 (4)
N9	0.21594 (12)	0.8912 (3)	−0.00236 (14)	0.0338 (4)
N8	0.26901 (11)	0.7850 (3)	0.07022 (14)	0.0324 (4)
N5	0.36207 (12)	0.9877 (3)	0.41089 (16)	0.0391 (5)
C5	0.41688 (12)	0.6927 (3)	0.36392 (16)	0.0277 (4)
C6	0.35228 (13)	0.8211 (3)	0.36874 (15)	0.0266 (4)
C12	0.14278 (13)	0.7567 (3)	0.06464 (15)	0.0251 (4)
C10	−0.00933 (13)	0.7286 (3)	0.04887 (17)	0.0345 (5)
H10A	−0.0299	0.8074	−0.0075	0.041*
C4	0.50448 (14)	0.7199 (4)	0.41376 (19)	0.0412 (6)
H4A	0.5264	0.8261	0.4527	0.049*
C8	−0.03227 (14)	0.5360 (4)	0.1706 (2)	0.0419 (6)
H8A	−0.0686	0.4823	0.1970	0.050*
C9	−0.06443 (14)	0.6492 (4)	0.08684 (19)	0.0403 (6)
H9A	−0.1229	0.6729	0.0555	0.048*
C7	0.05448 (14)	0.5021 (3)	0.21553 (18)	0.0370 (5)
H7A	0.0761	0.4255	0.2728	0.044*
C3	0.55837 (15)	0.5858 (4)	0.4041 (2)	0.0501 (7)
H3A	0.6174	0.6006	0.4367	0.060*
C2	0.52448 (15)	0.4307 (4)	0.3465 (2)	0.0524 (7)
H2A	0.5602	0.3387	0.3398	0.063*

C1	0.43723 (15)	0.4126 (4)	0.2986 (2)	0.0436 (6)
H1A	0.4146	0.3068	0.2595	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01986 (15)	0.01999 (15)	0.02244 (15)	0.00008 (11)	0.00748 (11)	−0.00171 (11)
Cl1	0.0484 (3)	0.0314 (3)	0.0355 (3)	0.0008 (2)	0.0116 (3)	−0.0137 (2)
O1W	0.0454 (9)	0.0204 (7)	0.0275 (7)	0.0062 (6)	0.0188 (7)	0.0003 (6)
N6	0.0206 (8)	0.0261 (9)	0.0284 (9)	−0.0020 (7)	0.0095 (7)	0.0006 (7)
N2	0.0231 (8)	0.0186 (8)	0.0289 (9)	0.0013 (6)	0.0114 (7)	−0.0012 (7)
N1	0.0222 (8)	0.0314 (9)	0.0288 (9)	0.0024 (7)	0.0095 (7)	−0.0064 (7)
N4	0.0465 (11)	0.0195 (9)	0.0431 (11)	0.0034 (8)	0.0165 (9)	−0.0044 (8)
C11	0.0244 (10)	0.0242 (10)	0.0260 (10)	0.0006 (8)	0.0098 (8)	−0.0027 (8)
N10	0.0421 (11)	0.0280 (10)	0.0302 (9)	0.0018 (8)	0.0155 (8)	0.0042 (8)
N3	0.0358 (10)	0.0210 (9)	0.0396 (10)	0.0064 (7)	0.0186 (8)	0.0011 (8)
N7	0.0255 (8)	0.0282 (9)	0.0279 (9)	−0.0033 (7)	0.0145 (7)	0.0021 (7)
N9	0.0472 (11)	0.0292 (10)	0.0319 (10)	−0.0045 (8)	0.0229 (9)	0.0008 (8)
N8	0.0349 (10)	0.0340 (10)	0.0348 (10)	−0.0060 (8)	0.0210 (8)	−0.0001 (8)
N5	0.0390 (11)	0.0251 (10)	0.0456 (12)	−0.0034 (8)	0.0094 (9)	−0.0092 (8)
C5	0.0237 (10)	0.0301 (11)	0.0272 (10)	−0.0002 (8)	0.0080 (8)	−0.0018 (9)
C6	0.0264 (10)	0.0234 (10)	0.0266 (10)	−0.0021 (8)	0.0071 (8)	−0.0030 (8)
C12	0.0292 (10)	0.0224 (10)	0.0238 (10)	−0.0002 (8)	0.0108 (8)	−0.0005 (8)
C10	0.0280 (11)	0.0368 (12)	0.0335 (12)	0.0073 (9)	0.0071 (9)	0.0005 (10)
C4	0.0252 (11)	0.0490 (15)	0.0417 (13)	−0.0075 (10)	0.0056 (10)	−0.0078 (11)
C8	0.0263 (11)	0.0538 (16)	0.0512 (15)	−0.0093 (10)	0.0214 (11)	−0.0024 (12)
C9	0.0198 (10)	0.0519 (16)	0.0456 (14)	0.0028 (10)	0.0094 (10)	−0.0113 (12)
C7	0.0292 (11)	0.0443 (14)	0.0401 (13)	−0.0043 (10)	0.0167 (10)	0.0092 (11)
C3	0.0188 (11)	0.078 (2)	0.0485 (15)	0.0031 (12)	0.0083 (10)	−0.0018 (14)
C2	0.0288 (12)	0.0694 (19)	0.0582 (17)	0.0176 (12)	0.0168 (12)	−0.0098 (15)
C1	0.0325 (12)	0.0460 (15)	0.0503 (15)	0.0093 (11)	0.0146 (11)	−0.0157 (12)

Geometric parameters (Å, °)

Fe1—O1W	1.9737 (14)	N7—C12	1.336 (3)
Fe1—N7	2.1041 (17)	N7—N8	1.337 (2)
Fe1—N2	2.1256 (16)	N9—N8	1.312 (3)
Fe1—N6	2.1602 (17)	N5—C6	1.321 (3)
Fe1—N1	2.1708 (18)	C5—C4	1.386 (3)
Fe1—Cl1	2.2308 (7)	C5—C6	1.461 (3)
O1W—H1WA	0.9774	C10—C9	1.385 (3)
O1W—H1WB	0.8241	C10—H10A	0.9300
N6—C7	1.339 (3)	C4—C3	1.377 (4)
N6—C11	1.347 (3)	C4—H4A	0.9300
N2—N3	1.331 (2)	C8—C9	1.366 (4)
N2—C6	1.334 (2)	C8—C7	1.377 (3)
N1—C1	1.340 (3)	C8—H8A	0.9300
N1—C5	1.345 (3)	C9—H9A	0.9300
N4—N3	1.313 (3)	C7—H7A	0.9300

N4—N5	1.348 (3)	C3—C2	1.368 (4)
C11—C10	1.384 (3)	C3—H3A	0.9300
C11—C12	1.461 (3)	C2—C1	1.371 (3)
N10—C12	1.322 (3)	C2—H2A	0.9300
N10—N9	1.345 (3)	C1—H1A	0.9300
O1W—Fe1—N7	164.20 (6)	N8—N9—N10	111.58 (17)
O1W—Fe1—N2	86.71 (6)	N9—N8—N7	107.23 (16)
N7—Fe1—N2	83.89 (7)	C6—N5—N4	103.55 (17)
O1W—Fe1—N6	91.08 (7)	N1—C5—C4	122.2 (2)
N7—Fe1—N6	76.34 (7)	N1—C5—C6	113.45 (17)
N2—Fe1—N6	90.32 (6)	C4—C5—C6	124.4 (2)
O1W—Fe1—N1	93.38 (7)	N5—C6—N2	111.68 (19)
N7—Fe1—N1	96.59 (7)	N5—C6—C5	129.50 (19)
N2—Fe1—N1	75.90 (6)	N2—C6—C5	118.81 (18)
N6—Fe1—N1	165.22 (7)	N10—C12—N7	111.92 (18)
O1W—Fe1—Cl1	94.84 (5)	N10—C12—C11	129.17 (19)
N7—Fe1—Cl1	96.38 (5)	N7—C12—C11	118.91 (18)
N2—Fe1—Cl1	171.26 (5)	C11—C10—C9	118.4 (2)
N6—Fe1—Cl1	98.24 (5)	C11—C10—H10A	120.8
N1—Fe1—Cl1	95.41 (5)	C9—C10—H10A	120.8
Fe1—O1W—H1WA	118.7	C3—C4—C5	118.4 (2)
Fe1—O1W—H1WB	121.3	C3—C4—H4A	120.8
H1WA—O1W—H1WB	119.5	C5—C4—H4A	120.8
C7—N6—C11	118.60 (17)	C9—C8—C7	119.3 (2)
C7—N6—Fe1	125.09 (15)	C9—C8—H8A	120.3
C11—N6—Fe1	116.26 (13)	C7—C8—H8A	120.3
N3—N2—C6	106.24 (16)	C8—C9—C10	119.5 (2)
N3—N2—Fe1	137.95 (13)	C8—C9—H9A	120.2
C6—N2—Fe1	115.30 (13)	C10—C9—H9A	120.2
C1—N1—C5	118.19 (19)	N6—C7—C8	122.1 (2)
C1—N1—Fe1	125.34 (15)	N6—C7—H7A	118.9
C5—N1—Fe1	116.35 (13)	C8—C7—H7A	118.9
N3—N4—N5	111.16 (17)	C2—C3—C4	119.6 (2)
N6—C11—C10	122.05 (19)	C2—C3—H3A	120.2
N6—C11—C12	113.04 (17)	C4—C3—H3A	120.2
C10—C11—C12	124.90 (19)	C3—C2—C1	119.2 (2)
C12—N10—N9	103.34 (17)	C3—C2—H2A	120.4
N4—N3—N2	107.37 (16)	C1—C2—H2A	120.4
C12—N7—N8	105.94 (17)	N1—C1—C2	122.5 (2)
C12—N7—Fe1	115.35 (13)	N1—C1—H1A	118.8
N8—N7—Fe1	138.44 (14)	C2—C1—H1A	118.8

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···N4^{i}	0.98	1.67	2.652 (2)	178
O1W—H1WB···N9^{ii}	0.82	1.80	2.626 (2)	176

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

Fig. 1

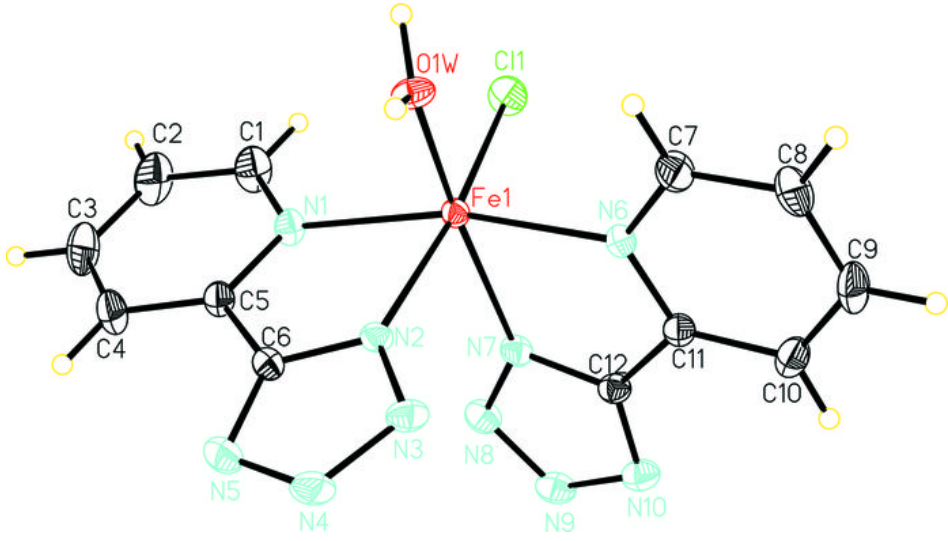
O1W
Cl1
C2
C1
C7
C8
C3
N1
Fe1
N6
C9
C5
C6
N2
N7
C12
C11
C4
C10
N3
N8
N5
N4
N9
N10

Fig. 2