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[*N,N*-Bis(2-pyridylmethyl)glycinato- κ^4 *N,N',N'',O*]dichloridoiron(III)–[*N,N*-bis(2-pyridylmethyl)glycine- κ^4 *N,N',N'',O*]dichloridozinc(II) (1/1)

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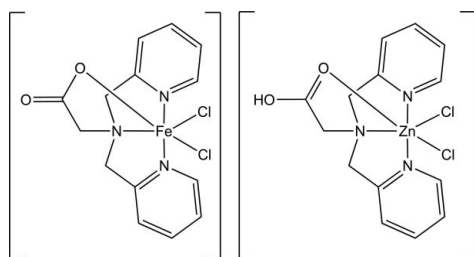
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Key indicators: single-crystal X-ray study; $T = 180$ K; mean $\sigma(\text{C}–\text{C}) = 0.006$ Å; disorder in main residue; R factor = 0.053; wR factor = 0.132; data-to-parameter ratio = 24.0.

The title compound, $[\text{Fe}(\text{C}_{14}\text{H}_{14}\text{N}_3\text{O}_2)\text{Cl}_2] \cdot [\text{ZnCl}_2(\text{C}_{14}\text{H}_{15}\text{N}_3\text{O}_2)]$, is formulated as $[\text{Fe}^{\text{III}}(\text{bpg})\text{Cl}_2][\text{Zn}^{\text{II}}\text{Cl}_2(\text{bpgH})]$, where bpg is the tetradentate ligand *N,N*-bis(2-pyridylmethyl)glycine. The structure contains one crystallographically distinct complex with Fe^{III} and Zn^{II} atoms present in a 50:50 ratio in a single-atom site. The non-coordinated O atoms of the carboxyl groups of bpg meet across crystallographic inversion centres, forming $\text{O}–\text{H} \cdots \text{O}$ hydrogen bonds that include only one H atom per two complexes, consistent with the 1:1 disorder of Fe^{III} and Zn^{II} .

Related literature

For related Fe^{III} structures of bpg, see: Mortensen *et al.* (2004).
For details of the synthesis, see: Suzuki *et al.* (1988).



Experimental

Crystal data

$[\text{Fe}(\text{C}_{14}\text{H}_{14}\text{N}_3\text{O}_2)\text{Cl}_2] \cdot [\text{ZnCl}_2(\text{C}_{14}\text{H}_{15}\text{N}_3\text{O}_2)]$
 $M_r = 776.59$
Monoclinic, $P2_1/c$
 $a = 8.8710$ (3) Å
 $b = 13.1898$ (5) Å
 $c = 13.3983$ (4) Å
 $\beta = 91.737$ (2) $^\circ$
 $V = 1566.97$ (9) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.62$ mm⁻¹
 $T = 180$ K
 $0.20 \times 0.20 \times 0.15$ mm

Data collection

Bruker–Nonius X8APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
 $T_{\text{min}} = 0.701$, $T_{\text{max}} = 0.794$
32580 measured reflections
4775 independent reflections
4248 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.132$
 $S = 1.36$
4775 reflections
199 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.71$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D–H \cdots A$	$D–H$	$H \cdots A$	$D \cdots A$	$D–H \cdots A$
$\text{O2}–\text{H2} \cdots \text{O2}^i$	0.93	1.64	2.559 (6)	169

Symmetry code: (i) $-x + 1, -y + 1, -z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the Danish Natural Sciences Research Council and the Carlsberg Foundation for provision of the X-ray equipment.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2118).

References

- Bruker (2003). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Mortensen, M. N., Jensen, B., Hazell, A., Bond, A. D. & McKenzie, C. J. (2004). *Dalton Trans.* pp. 3396–3402.
Sheldrick, G. M. (2003). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Suzuki, M., Senda, H., Kobayashi, Y., Oshio, H. & Uehara, A. (1988). *Chem. Lett.* pp. 1763–1766.

supporting information

Acta Cryst. (2009). E65, m1706 [doi:10.1107/S1600536809051022]

[*N,N*-Bis(2-pyridylmethyl)glycinato- κ^4 *N,N',N'',O*]dichloridoiron(III)–[*N,N*-bis(2-pyridylmethyl)glycine- κ^4 *N,N',N'',O*]dichloridozinc(II) (1/1)

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S1. Comment

Crystallization of the title compound, [FeCl₂(bpg)][ZnCl₂(bpgH)] (where bpg denotes the tetradentate ligand *N,N*-bis(2-pyridylmethyl)glycine), was surprising given the presence of water in its preparation. In our hands, simple binary mixtures of bpgH and FeCl₃ in water-containing solutions do not yield the complex [FeCl₂(bpg)]. If only chloride ions but not Zn^{II} are present in equivalent reaction mixtures (*i.e.* aerobic conditions and containing water), oligomeric (hydr)oxo-bridged Fe^{III} complexes are formed, such as [Fe₂(O)(bpg)₂(H₂O)₂](ClO₄)₂ and [Fe₃(O)₂(OH)(bpg)₃](ClO₄) (Mortensen *et al.*, 2004). Addition of Zn^{II} has in this case enabled isolation of [FeCl₂(bpg)] from water as one component of the co-crystal.

S2. Experimental

N,N-Bis(2-pyridylmethyl)glycine (bpgH) was prepared according to a literature method (Suzuki *et al.*, 1988). BpgH (125 mg, 49 mmol) was then dissolved in hot acetonitrile (5 ml) and water (0.5 ml), before Fe(NO₃)₃·9H₂O (99 mg, 24 mmol), ZnCl₂ (67 mg, 49 mmol) and NH₄Cl (78 mg, 15 mmol) were added. A few yellow crystals of the title compound were deposited overnight.

S3. Refinement

H atoms bound to C atoms were placed in idealized positions with C—H = 0.95 or 0.99 Å and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom of the OH group was included in a position identified from a difference Fourier map, then allowed to ride on atom O2 with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The 50:50 disorder of atoms Fe1 and Zn1 is required for charge balance in the structure, but it is also supported by the diffraction data: refinement of the atom solely as Fe gives a comparatively small displacement ellipsoid while refinement solely as Zn gives a comparatively large ellipsoid. In both cases, the *R*-factors increase compared to the disordered refinement.

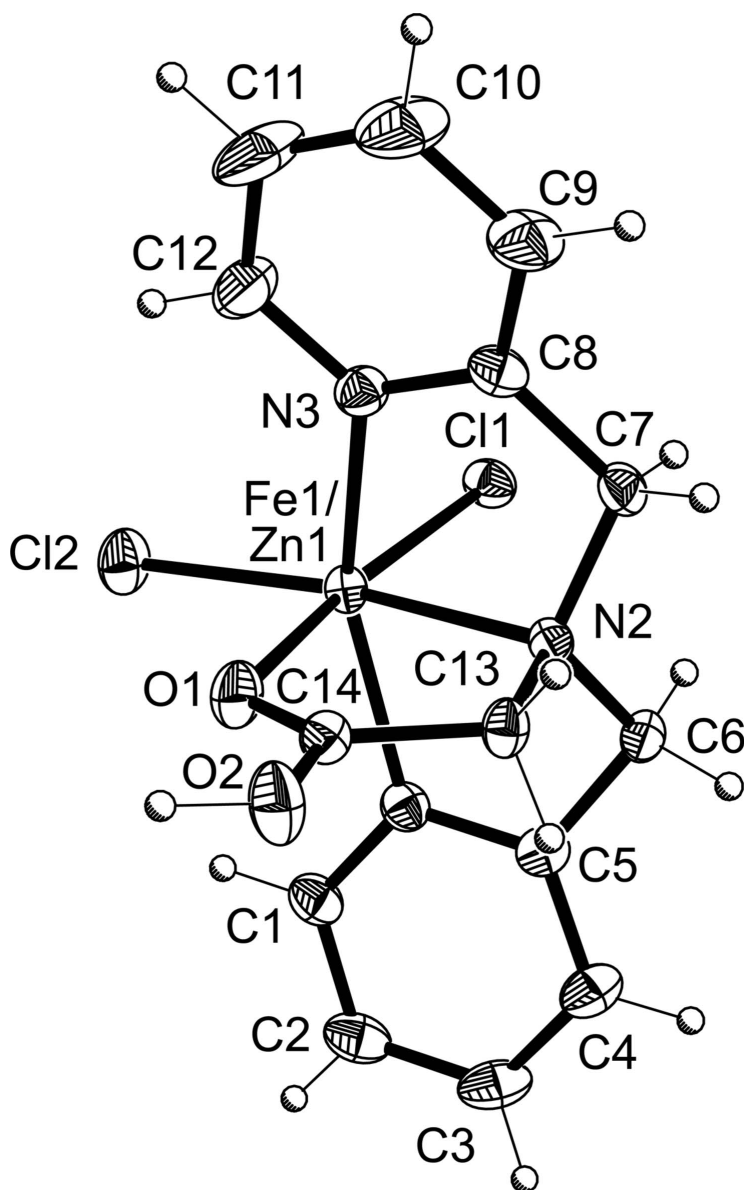


Figure 1

Molecular structure with displacement ellipsoids shown at 50% probability for non-H atoms.

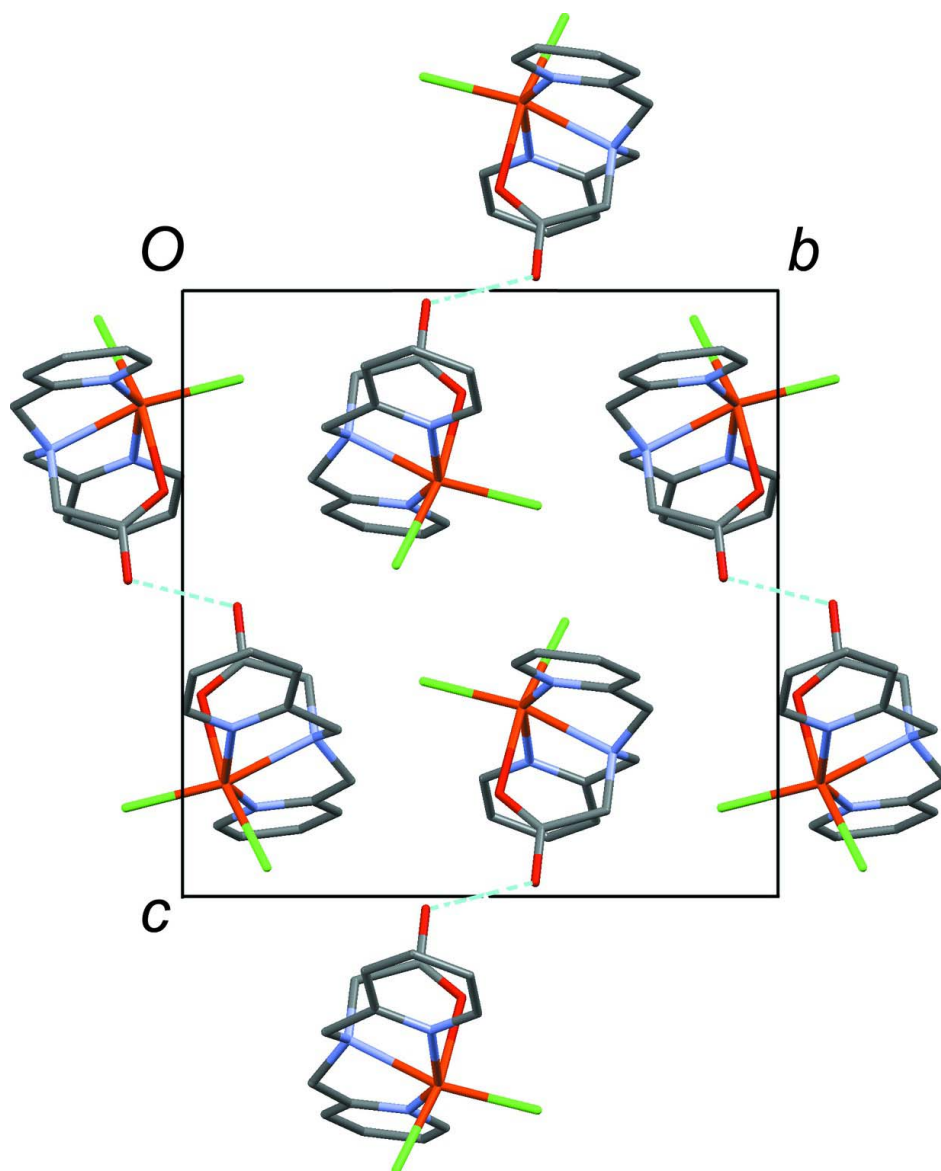


Figure 2

Projection along the a axis showing hydrogen bonds (dashed lines) formed between bpg(H) ligands across crystallographic inversion centres.

[N,N -Bis(2-pyridylmethyl)glycinato- κ^4N,N',N'',O]dichloridoiron(III)– [N,N -bis(2-pyridylmethyl)glycine- κ^4N,N',N'',O]dichloridozinc(II) (1/1)

Crystal data

[Fe(C₁₄H₁₄N₃O₂)Cl₂] \cdot [ZnCl₂(C₁₄H₁₃N₃O₂)]

$M_r = 776.59$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 8.8710$ (3) Å

$b = 13.1898$ (5) Å

$c = 13.3983$ (4) Å

$\beta = 91.737$ (2)°

$V = 1566.97$ (9) Å³

$Z = 2$

$F(000) = 790$

$D_x = 1.646$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5945 reflections

$\theta = 2.3$ – 29.9 °

$\mu = 1.62$ mm⁻¹

$T = 180$ K $0.20 \times 0.20 \times 0.15$ mm
 Block, yellow

Data collection

Bruker–Nonius X8APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator Thin-slice ω and φ scans Absorption correction: multi-scan (SADABS; Sheldrick, 2003) $T_{\min} = 0.701$, $T_{\max} = 0.794$	32580 measured reflections 4775 independent reflections 4248 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.031$ $\theta_{\text{max}} = 30.5^\circ$, $\theta_{\text{min}} = 3.8^\circ$ $h = -12 \rightarrow 12$ $k = -18 \rightarrow 18$ $l = -19 \rightarrow 18$
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Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.053$ $wR(F^2) = 0.132$ $S = 1.36$ 4775 reflections 199 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 $w = 1/[\sigma^2(F_o^2) + 7.0062P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.55 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.71 \text{ e } \text{\AA}^{-3}$
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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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Fe1	0.30263 (5)	0.42993 (3)	0.31348 (3)	0.01709 (11)	0.50
Zn1	0.30263 (5)	0.42993 (3)	0.31348 (3)	0.01709 (11)	0.50
Cl1	0.19027 (10)	0.35846 (7)	0.45311 (7)	0.02319 (19)	
Cl2	0.30370 (13)	0.59544 (7)	0.35454 (8)	0.0290 (2)	
O1	0.3982 (4)	0.4689 (2)	0.1686 (2)	0.0295 (6)	
O2	0.4679 (4)	0.4082 (2)	0.0219 (2)	0.0326 (7)	
H2	0.4790	0.4759	0.0050	0.049*	0.50
N1	0.5237 (4)	0.3803 (2)	0.3539 (2)	0.0204 (6)	
N2	0.3235 (3)	0.2778 (2)	0.2375 (2)	0.0171 (6)	
N3	0.0989 (4)	0.4170 (3)	0.2225 (2)	0.0215 (6)	
C1	0.6376 (4)	0.4414 (3)	0.3838 (3)	0.0245 (8)	
H1A	0.6184	0.5117	0.3927	0.029*	
C2	0.7825 (5)	0.4048 (4)	0.4022 (3)	0.0291 (9)	
H2A	0.8617	0.4493	0.4228	0.035*	

C3	0.8095 (5)	0.3026 (4)	0.3899 (3)	0.0320 (10)
H3A	0.9081	0.2759	0.4010	0.038*
C4	0.6917 (5)	0.2392 (3)	0.3615 (3)	0.0280 (8)
H4A	0.7076	0.1684	0.3548	0.034*
C5	0.5506 (4)	0.2805 (3)	0.3429 (3)	0.0208 (7)
C6	0.4167 (4)	0.2175 (3)	0.3096 (3)	0.0202 (7)
H6A	0.4512	0.1543	0.2775	0.024*
H6B	0.3564	0.1989	0.3678	0.024*
C7	0.1677 (4)	0.2401 (3)	0.2253 (3)	0.0215 (7)
H7A	0.1323	0.2150	0.2901	0.026*
H7B	0.1647	0.1829	0.1774	0.026*
C8	0.0656 (4)	0.3237 (3)	0.1875 (3)	0.0230 (7)
C9	-0.0583 (5)	0.3063 (4)	0.1241 (3)	0.0340 (10)
H9A	-0.0797	0.2399	0.1001	0.041*
C10	-0.1499 (6)	0.3865 (5)	0.0964 (4)	0.0445 (13)
H10A	-0.2355	0.3759	0.0534	0.053*
C11	-0.1162 (6)	0.4821 (4)	0.1318 (4)	0.0465 (14)
H11A	-0.1784	0.5382	0.1137	0.056*
C12	0.0097 (5)	0.4952 (4)	0.1942 (4)	0.0336 (10)
H12A	0.0338	0.5613	0.2178	0.040*
C13	0.3965 (4)	0.2893 (3)	0.1407 (3)	0.0198 (7)
H13A	0.3337	0.2553	0.0883	0.024*
H13B	0.4956	0.2548	0.1442	0.024*
C14	0.4195 (4)	0.3982 (3)	0.1113 (3)	0.0190 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0191 (2)	0.0150 (2)	0.0172 (2)	-0.00111 (17)	0.00049 (15)	0.00011 (17)
Zn1	0.0191 (2)	0.0150 (2)	0.0172 (2)	-0.00111 (17)	0.00049 (15)	0.00011 (17)
Cl1	0.0217 (4)	0.0273 (5)	0.0207 (4)	-0.0020 (3)	0.0013 (3)	0.0032 (3)
Cl2	0.0400 (6)	0.0201 (4)	0.0272 (5)	0.0007 (4)	0.0063 (4)	-0.0067 (4)
O1	0.0351 (16)	0.0169 (13)	0.0363 (17)	0.0000 (12)	0.0006 (13)	-0.0069 (12)
O2	0.0476 (19)	0.0233 (15)	0.0271 (15)	-0.0051 (13)	0.0057 (13)	0.0043 (12)
N1	0.0204 (15)	0.0210 (15)	0.0196 (14)	-0.0020 (12)	-0.0012 (11)	-0.0008 (12)
N2	0.0173 (14)	0.0162 (14)	0.0178 (13)	-0.0016 (11)	-0.0002 (11)	0.0006 (11)
N3	0.0205 (15)	0.0223 (16)	0.0216 (15)	0.0013 (12)	-0.0015 (12)	-0.0004 (12)
C1	0.0231 (18)	0.0261 (19)	0.0243 (18)	-0.0055 (15)	0.0003 (14)	-0.0037 (15)
C2	0.0209 (18)	0.041 (2)	0.0253 (19)	-0.0060 (17)	-0.0018 (15)	-0.0064 (17)
C3	0.0211 (19)	0.047 (3)	0.028 (2)	0.0080 (18)	-0.0049 (15)	-0.0064 (19)
C4	0.026 (2)	0.031 (2)	0.0268 (19)	0.0081 (16)	-0.0041 (15)	-0.0039 (16)
C5	0.0213 (17)	0.0243 (18)	0.0166 (15)	0.0013 (14)	-0.0013 (13)	-0.0016 (13)
C6	0.0226 (17)	0.0161 (16)	0.0218 (17)	0.0015 (13)	-0.0010 (13)	0.0005 (13)
C7	0.0208 (17)	0.0186 (17)	0.0249 (17)	-0.0041 (14)	-0.0034 (13)	-0.0010 (14)
C8	0.0193 (17)	0.0273 (19)	0.0223 (17)	-0.0033 (15)	-0.0014 (13)	-0.0025 (15)
C9	0.027 (2)	0.040 (3)	0.034 (2)	-0.0024 (18)	-0.0101 (17)	-0.0074 (19)
C10	0.030 (2)	0.057 (3)	0.045 (3)	0.010 (2)	-0.018 (2)	-0.011 (2)
C11	0.036 (3)	0.051 (3)	0.052 (3)	0.022 (2)	-0.020 (2)	-0.011 (2)

C12	0.031 (2)	0.029 (2)	0.041 (3)	0.0087 (18)	-0.0066 (18)	-0.0021 (19)
C13	0.0267 (18)	0.0161 (16)	0.0168 (15)	0.0002 (13)	0.0028 (13)	0.0007 (12)
C14	0.0204 (16)	0.0185 (16)	0.0179 (16)	0.0000 (13)	-0.0005 (13)	-0.0019 (13)

Geometric parameters (Å, °)

Fe1—N1	2.122 (3)	C3—H3A	0.950
Fe1—N3	2.156 (3)	C4—C5	1.381 (5)
Fe1—O1	2.202 (3)	C4—H4A	0.950
Fe1—Cl2	2.2512 (11)	C5—C6	1.506 (5)
Fe1—N2	2.260 (3)	C6—H6A	0.990
Fe1—Cl1	2.3441 (10)	C6—H6B	0.990
O1—C14	1.226 (5)	C7—C8	1.505 (5)
O2—C14	1.291 (5)	C7—H7A	0.990
O2—H2	0.927	C7—H7B	0.990
N1—C1	1.345 (5)	C8—C9	1.387 (5)
N1—C5	1.346 (5)	C9—C10	1.378 (7)
N2—C7	1.473 (5)	C9—H9A	0.950
N2—C13	1.475 (5)	C10—C11	1.377 (8)
N2—C6	1.483 (5)	C10—H10A	0.950
N3—C8	1.347 (5)	C11—C12	1.386 (6)
N3—C12	1.348 (5)	C11—H11A	0.950
C1—C2	1.388 (6)	C12—H12A	0.950
C1—H1A	0.950	C13—C14	1.504 (5)
C2—C3	1.381 (7)	C13—H13A	0.990
C2—H2A	0.950	C13—H13B	0.990
C3—C4	1.382 (6)		
N1—Fe1—N3	150.70 (12)	C3—C4—H4A	120.5
N1—Fe1—O1	85.37 (12)	N1—C5—C4	121.9 (4)
N3—Fe1—O1	81.87 (12)	N1—C5—C6	115.5 (3)
N1—Fe1—Cl2	103.88 (9)	C4—C5—C6	122.6 (4)
N3—Fe1—Cl2	102.26 (9)	N2—C6—C5	108.4 (3)
O1—Fe1—Cl2	89.45 (8)	N2—C6—H6A	110.0
N1—Fe1—N2	75.71 (11)	C5—C6—H6A	110.0
N3—Fe1—N2	75.74 (12)	N2—C6—H6B	110.0
O1—Fe1—N2	76.77 (11)	C5—C6—H6B	110.0
Cl2—Fe1—N2	166.22 (8)	H6A—C6—H6B	108.4
N1—Fe1—Cl1	94.84 (9)	N2—C7—C8	110.1 (3)
N3—Fe1—Cl1	92.86 (9)	N2—C7—H7A	109.6
O1—Fe1—Cl1	168.98 (8)	C8—C7—H7A	109.6
Cl2—Fe1—Cl1	101.17 (4)	N2—C7—H7B	109.6
N2—Fe1—Cl1	92.57 (8)	C8—C7—H7B	109.6
C14—O1—Fe1	116.5 (3)	H7A—C7—H7B	108.2
C14—O2—H2	111.5	N3—C8—C9	121.7 (4)
C1—N1—C5	119.0 (3)	N3—C8—C7	115.4 (3)
C1—N1—Fe1	124.9 (3)	C9—C8—C7	122.8 (4)
C5—N1—Fe1	116.1 (2)	C10—C9—C8	119.2 (4)

C7—N2—C13	111.8 (3)	C10—C9—H9A	120.4
C7—N2—C6	113.2 (3)	C8—C9—H9A	120.4
C13—N2—C6	112.1 (3)	C11—C10—C9	119.4 (4)
C7—N2—Fe1	105.1 (2)	C11—C10—H10A	120.3
C13—N2—Fe1	110.4 (2)	C9—C10—H10A	120.3
C6—N2—Fe1	103.6 (2)	C10—C11—C12	119.0 (5)
C8—N3—C12	118.7 (4)	C10—C11—H11A	120.5
C8—N3—Fe1	116.2 (3)	C12—C11—H11A	120.5
C12—N3—Fe1	125.0 (3)	N3—C12—C11	122.0 (5)
N1—C1—C2	121.9 (4)	N3—C12—H12A	119.0
N1—C1—H1A	119.1	C11—C12—H12A	119.0
C2—C1—H1A	119.1	N2—C13—C14	113.3 (3)
C3—C2—C1	118.8 (4)	N2—C13—H13A	108.9
C3—C2—H2A	120.6	C14—C13—H13A	108.9
C1—C2—H2A	120.6	N2—C13—H13B	108.9
C2—C3—C4	119.4 (4)	C14—C13—H13B	108.9
C2—C3—H3A	120.3	H13A—C13—H13B	107.7
C4—C3—H3A	120.3	O1—C14—O2	124.4 (4)
C5—C4—C3	119.0 (4)	O1—C14—C13	122.5 (3)
C5—C4—H4A	120.5	O2—C14—C13	113.1 (3)
N1—Fe1—O1—C14	77.2 (3)	C5—N1—C1—C2	1.1 (6)
N3—Fe1—O1—C14	-76.3 (3)	Fe1—N1—C1—C2	-175.2 (3)
C12—Fe1—O1—C14	-178.8 (3)	N1—C1—C2—C3	-0.5 (6)
N2—Fe1—O1—C14	0.8 (3)	C1—C2—C3—C4	-1.0 (7)
C11—Fe1—O1—C14	-14.3 (7)	C2—C3—C4—C5	2.0 (6)
N3—Fe1—N1—C1	144.7 (3)	C1—N1—C5—C4	-0.1 (6)
O1—Fe1—N1—C1	80.4 (3)	Fe1—N1—C5—C4	176.5 (3)
C12—Fe1—N1—C1	-7.9 (3)	C1—N1—C5—C6	179.8 (3)
N2—Fe1—N1—C1	157.9 (3)	Fe1—N1—C5—C6	-3.7 (4)
C11—Fe1—N1—C1	-110.7 (3)	C3—C4—C5—N1	-1.5 (6)
N3—Fe1—N1—C5	-31.7 (4)	C3—C4—C5—C6	178.7 (4)
O1—Fe1—N1—C5	-96.0 (3)	C7—N2—C6—C5	-160.8 (3)
C12—Fe1—N1—C5	175.7 (3)	C13—N2—C6—C5	71.5 (4)
N2—Fe1—N1—C5	-18.5 (3)	Fe1—N2—C6—C5	-47.5 (3)
C11—Fe1—N1—C5	73.0 (3)	N1—C5—C6—N2	36.7 (4)
N1—Fe1—N2—C7	154.6 (2)	C4—C5—C6—N2	-143.5 (4)
N3—Fe1—N2—C7	-32.0 (2)	C13—N2—C7—C8	-75.2 (4)
O1—Fe1—N2—C7	-116.9 (2)	C6—N2—C7—C8	157.0 (3)
C12—Fe1—N2—C7	-115.3 (4)	Fe1—N2—C7—C8	44.6 (3)
C11—Fe1—N2—C7	60.3 (2)	C12—N3—C8—C9	-0.5 (6)
N1—Fe1—N2—C13	-84.6 (2)	Fe1—N3—C8—C9	-176.8 (3)
N3—Fe1—N2—C13	88.7 (2)	C12—N3—C8—C7	-178.1 (4)
O1—Fe1—N2—C13	3.9 (2)	Fe1—N3—C8—C7	5.6 (4)
C12—Fe1—N2—C13	5.4 (5)	N2—C7—C8—N3	-35.6 (5)
C11—Fe1—N2—C13	-179.0 (2)	N2—C7—C8—C9	146.9 (4)
N1—Fe1—N2—C6	35.6 (2)	N3—C8—C9—C10	-0.2 (7)
N3—Fe1—N2—C6	-151.1 (2)	C7—C8—C9—C10	177.2 (4)

O1—Fe1—N2—C6	124.1 (2)	C8—C9—C10—C11	0.3 (8)
Cl2—Fe1—N2—C6	125.6 (3)	C9—C10—C11—C12	0.2 (9)
Cl1—Fe1—N2—C6	-58.8 (2)	C8—N3—C12—C11	1.1 (7)
N1—Fe1—N3—C8	28.4 (4)	Fe1—N3—C12—C11	177.0 (4)
O1—Fe1—N3—C8	93.5 (3)	C10—C11—C12—N3	-1.0 (9)
Cl2—Fe1—N3—C8	-178.8 (3)	C7—N2—C13—C14	109.1 (3)
N2—Fe1—N3—C8	15.2 (3)	C6—N2—C13—C14	-122.4 (3)
Cl1—Fe1—N3—C8	-76.7 (3)	Fe1—N2—C13—C14	-7.5 (4)
N1—Fe1—N3—C12	-147.6 (3)	Fe1—O1—C14—O2	176.6 (3)
O1—Fe1—N3—C12	-82.5 (4)	Fe1—O1—C14—C13	-5.8 (5)
Cl2—Fe1—N3—C12	5.2 (4)	N2—C13—C14—O1	9.3 (5)
N2—Fe1—N3—C12	-160.8 (4)	N2—C13—C14—O2	-172.8 (3)
Cl1—Fe1—N3—C12	107.3 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2...O2 ⁱ	0.93	1.64	2.559 (6)	169

Symmetry code: (i) $-x+1, -y+1, -z$.