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Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Poly[diaquadi-μ_3-malonato-μ-pyrazine-dinickel(II)]	Liu *et al.* (2005)	10.1107/S1600536805026358	GATWAA
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)samarium(II)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]	Liu *et al.* (2006)	10.1107/S1600536806038141	FONCUH03
Poly[[[μ_4-4,4′-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)-dipalladium(II)] dihydrate]	Li, Wang, Zhang & Yu (2007*e*)	10.1107/S1600536807039050	AFELAZ
Poly[diaqua-μ_3-malonato-μ-pyrazine-diiron(II)]	Li, Liu *et al.* (2007)	10.1107/S1600536807038743	AFELON
Poly[diaqua-di-μ_3-malonato-μ-pyrazine-dimanganese(II)]	Li, Wang, Zhang & Yu (2007*f*)	10.1107/S1600536807039773	VIJZAQ
Poly[[aqua(2,2-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]	Li, Wang, Zhang & Yu (2007*g*)	10.1107/S1600536807040275	VIKCIC
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)holmium(III)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]	Li, Wang, Zhang & Yu (2007*a*)	10.1107/S1600536807041657	DILGEL
catena-Poly[[(2,2′-bipyridine-κ^2N,N')iron(II)]-μ-5-carboxy-4-carboxylatoimidazol-1-ido-$\kappa^4N^3,O^4{:}N^1,O^5$]	Li, Wang, Zhang & Yu (2007*h*)	10.1107/S1600536807042122	XIKWAQ
Poly[[aqua(2,2′-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]	Li, Wang, Zhang & Yu (2007*b*)	10.1107/S1600536807046466	LEVZAO01
2-(Benzyliminomethyl)-6-methoxyphenol	Li, Wang, Zhang & Yu (2007*i*)	10.1107/S1600536807042134	SILDEX
Poly[aqua(2,2′-bipyridine)(μ_3-pyridine-2,4-dicarboxylato)palladium(II)]	Li, Wang, Zhang & Yu (2007*c*)	10.1107/S1600536807047575	SILXAN
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]iron(III)} bis(hexafluoridophosphate)	Liu, Dou, Li & Zhang (2007)	10.1107/S1600536807049665	TINRIS
μ-Oxido-bis({4,4′-dibromo-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-manganese(III))	Liu, Dou, Niu & Zhang (2007*a*)	10.1107/S1600536807051008	GIMZAE
Bis[N-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate	Li, Wang, Zhang & Yu (2007*d*)	10.1107/S1600536807048556	WIMZIC
μ-Oxido-bis({4,4′-dibromo-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-chromium(III))	Liu, Dou, Niu & Zhang (2007*b*)	10.1107/S1600536807057996	HIQFIX
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis(hexafluorido-phosphate)	Li, Wang *et al.* (2008)	10.1107/S1600536807061296	MIRNAD
μ-Oxido-bis({4,4′-dibromo-2,2′-ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-iron(III))	Meng *et al.* (2008*a*)	10.1107/S1600536807063143	MIRWUG
catena-Poly[[bis(1H-benzimidazole-κN^3)palladium(II)]-μ-benzene-1,4-dicarboxylato-$\kappa^2O^1{:}O^4$]	Meng *et al.* (2008*b*)	10.1107/S1600536807065051	XISCAE
Oxalatobis(propane-1,3-diamine)manganese(II) chloride monohydrate	Meng *et al.* (2008*e*)	10.1107/S1600536807065361	SISWIB
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]manganese(III)} bis(hexafluorido-phosphate)	Meng *et al.* (2008*c*)	10.1107/S1600536807066512	RISRIV
Bis[N-(8-quinolyl)pyridine-2-carboxamidato-κ^3N,N',N'']manganese(III) perchlorate monohydrate	Meng *et al.* (2008*d*)	10.1107/S1600536808000287	GISLEA
Diaquabis(pyridine-2-carboxylato-κ^2N,O)cobalt(II)	Huang (2008)	10.1107/S1600536808010507	WIZPOL
Tetra-μ-2,5-difluorobenzoato-bis[(2,2′-bipyridine)(2,5-difluorobenzoato)gadolinium(III)]	Li, Zhang *et al.* (2008)	10.1107/S1600536808023507	BOFQIX
catena-Poly[[(2,2′-bipyridine-κ^2N,N')nickel(II)]-μ-oxalato-$\kappa^4O^1,O^2{:}O^{1'},O^{2'}$]	Li, Yan *et al.* (2008)	10.1107/S1600536808028389	NOHYUF
catena-Poly[[aqua(2,2′-bipyridyl)cobalt(II)]-μ-5-nitroisophthlalato]	Liu *et al.* (2008)	10.1107/S1600536808038178	AFIREN
Diaquabis(pyridine-2-carboxylato-κ^2N,O)iron(II)	Xia & Sun (2009)	10.1107/S1600536809005765	RONFEG
catena-Poly[[[diaquathulium(III)]-μ-6-carboxynicotinato-μ-pyridine-2,5-dicarboxylato] dihydrate]	Li *et al.* (2009)	10.1107/S1600536809008836	NOQNIR
1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one	Liu *et al.* (2009)	10.1107/S1600536809040227	PUGLOT

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Bis[*N*-(8-quinolyl)pyridine-2-carboxamidato-κ^3N,N',N'']manganese(III) perchlorate monohydrate

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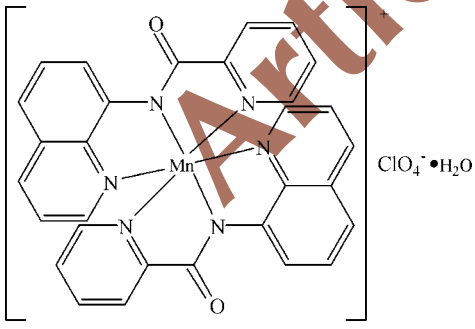
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; H-atom completeness 91%; R factor = 0.066; wR factor = 0.190; data-to-parameter ratio = 12.1.

The Mn^{III} ion in the title complex, $[Mn(C_{15}H_{10}N_3O)_2]ClO_4\cdot H_2O$, is coordinated meridionally by six N atoms from two tridentate *N*-(8-quinolyl)pyridine-2-carboxamidate ligands, yielding a distorted octahedral coordination geometry. The two ligands are nearly planar and their mean planes are almost perpendicular, with a dihedral angle of 86.7 (2)°.

Related literature

For related literature, see: Dutta *et al.* (2000); Ni *et al.* (2006); Ni (2007); Zhang *et al.* (2001).



Experimental

Crystal data

$[Mn(C_{15}H_{10}N_3O)_2]ClO_4\cdot H_2O$
M_r = 668.93
Triclinic, $P\overline{1}$
a = 9.2314 (5) Å
b = 12.9987 (10) Å
c = 12.0126 (5) Å
α = 95.786 (1)°
β = 91.592 (2)°
γ = 90.486 (1)°
V = 1433.48 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 293 (2) K
0.28 × 0.22 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.847, T_{max} = 0.898
5004 measured reflections
4920 independent reflections
3731 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.189
S = 1.00
4920 reflections
406 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Bruker, 2001); 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: CF2173).

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supporting information

Acta Cryst. (2008). E**64**, m332 [doi:10.1107/S1600536808000287]

Bis[*N*-(8-quinolyl)pyridine-2-carboxamidato-κ^3N,N',N'']manganese(III) perchlorate monohydrate

Qingguo Meng, Lintong Wang, Yanzhen Liu and Yan Pang

S1. Comment

To date, many symmetrical pyridinecarboxamide ligands and their coordination complexes have been synthesized (Ni *et al.*, 2006). However, unsymetrical pyridinecarboxamide ligands are limited (Zhang *et al.*, 2001). Here we report a new Mn^{III} complex, $[Mn(C_{15}H_{10}N_3O)_2]ClO_4.H_2O$, (I), containing two unsymmetrical pyridinecarboxamide tridentate ligands, 8-(pyridine-2-carboxamido)quinoline.

The structure and labeling scheme for the title complex are shown in Figure 1. The title compound comprises a $[Mn^{III}(pcq)_2]^+$ (Hpcq = 8-(pyridine-2-carboxamido)quinoline) cation and a ClO_4^- anion as well as an uncoordinated water molecule. The Mn^{III} ion in the cation is coordinated by six nitrogen atoms from two *mer* pcq^- ligands, giving a distorted octahedral coordination environment. The C—O, $C_{pyridine}$—N, and $C_{carboxy}$—N bond distances in the title complex agree well with those reported for other complexes containing pyridinecarboxamide ligands (Dutta *et al.*, 2000; Ni, 2007) and with the ligand precursor Hpcq (Zhang *et al.*, 2001). The average Mn—$N_{pyridine}$ bond distance is 1.914 Å and the average Mn—N_{amide} bond length is 2.028 Å. The two pcq^- ligands in (I) are both nearly planar, and the two mean planes are almost perpendicular, with a dihedral angle of 86.7 (2)°. There is probably a hydrogen bond between water and perchlorate, but the H atoms of the water molecule could not be located.

S2. Experimental

The material Hpcq was synthesized according to the literature (Zhang *et al.*, 2001). Solid Hpcq (500 mg, 2 mmol) was added to a methanol/water solution (20 ml, $MeOH/H_2O$ = 4:1 *v*/*v*) of Mn^{III} acetate (326 mg, 1 mmol) containing 0.5 ml pyridine The mixture was stirred for about 0.5 h. The mixture was then filtered and the resulting solution was kept at room temperature for about one week, giving rise to pink block crystals. Yield: 50%. Elemental analysis [found (calculated)] for $C_{30}H_{22}ClMnN_6O_7$: C 53.65 (53.79), H 3.35 (3.31), N 12.39% (12.55%).

S3. Refinement

The H atoms of the water molecule were not located. H atoms bound to C atoms were positioned geometrically, with C—H = 0.93 Å and refined as riding atoms with $U_{iso}(H) = 1.2U_{eq}(C)$.

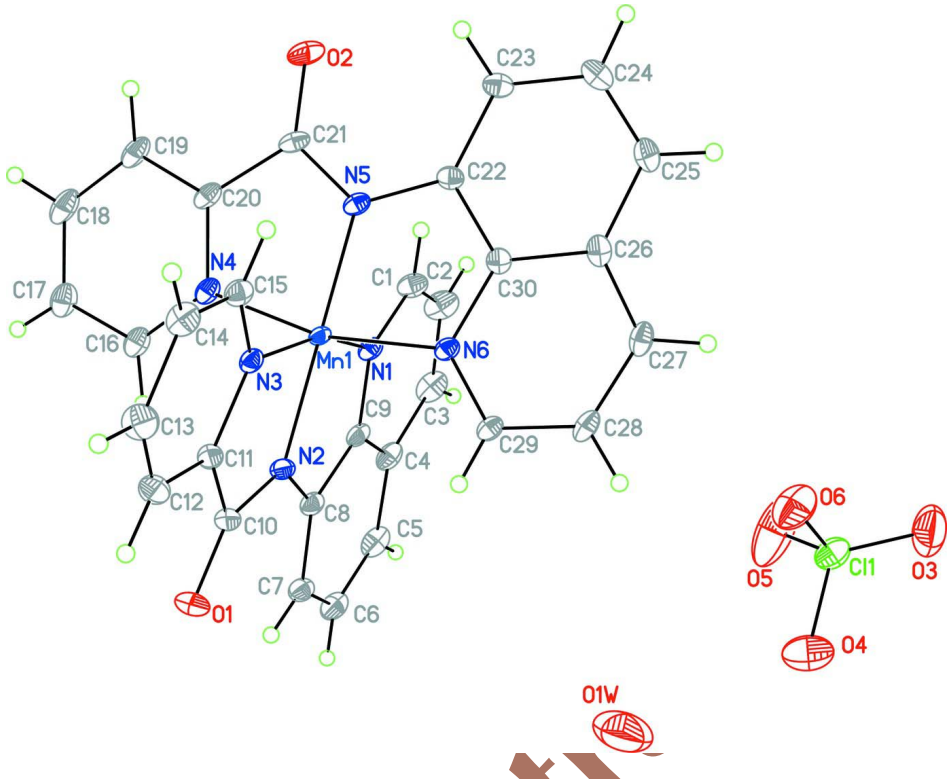

Figure 1

A view of (I) with the unique atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Bis[*N*-(8-quinolyl)pyridine-2-carboxamidato-κ^3N,N',N'']manganate(III) perchlorate monohydrate

Crystal data

$[Mn(C_{15}H_{10}N_3O)_2]ClO_4 \cdot H_2O$
$M_r = 668.93$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.2314\ (5)$ Å
$b = 12.9987\ (10)$ Å
$c = 12.0126\ (5)$ Å
$\alpha = 95.786\ (1)°$
$\beta = 91.592\ (2)°$
$\gamma = 90.486\ (1)°$
$V = 1433.48\ (15)$ Å^3
$Z = 2$
$F(000) = 684$
$D_x = 1.550$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4924 reflections
$\theta = 3.1–25.0°$
$\mu = 0.61$ mm^{-1}
$T = 293$ K
Block, pink
0.28 × 0.22 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.847$, $T_{max} = 0.898$
5004 measured reflections
4920 independent reflections
3731 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.1°$
$h = -10 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.189$
$S = 1.00$
4920 reflections
406 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
$w = 1/[\sigma^2(F_o^2) + (0.1288P)^2 + 0.5125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	1.01973 (6)	0.24180 (4)	0.24794 (4)	0.0384 (2)
Cl1	0.51979 (17)	0.11333 (15)	0.74568 (15)	0.0909 (5)
N2	0.9935 (4)	0.3931 (3)	0.3109 (3)	0.0518 (9)
N6	0.9288 (4)	0.1667 (3)	0.3589 (3)	0.0475 (8)
N5	1.0500 (4)	0.0939 (3)	0.1904 (3)	0.0495 (8)
N4	1.1108 (4)	0.2804 (3)	0.1203 (3)	0.0527 (9)
N1	0.8270 (4)	0.2620 (3)	0.1907 (3)	0.0531 (9)
C21	1.1198 (5)	0.0783 (4)	0.0992 (4)	0.0574 (12)
C8	0.8606 (5)	0.4385 (4)	0.2926 (4)	0.0551 (11)
C30	0.9270 (5)	0.0526 (3)	0.3384 (3)	0.0490 (10)
C22	0.9966 (5)	0.0084 (3)	0.2476 (3)	0.0493 (10)
O1	1.1111 (5)	0.5442 (3)	0.4079 (4)	0.0856 (12)
O2	1.1503 (5)	−0.0117 (3)	0.0524 (3)	0.0824 (11)
N3	1.2070 (4)	0.2650 (3)	0.3217 (3)	0.0475 (8)
C20	1.1555 (5)	0.1885 (4)	0.0605 (3)	0.0564 (12)
C29	0.8639 (5)	0.2116 (4)	0.4435 (3)	0.0538 (11)
H29A	0.8655	0.2831	0.4598	0.065*
C10	1.1042 (5)	0.4462 (4)	0.3671 (4)	0.0581 (11)
C26	0.8586 (5)	−0.0202 (4)	0.4046 (4)	0.0599 (12)
C9	0.7712 (5)	0.3641 (4)	0.2238 (4)	0.0542 (11)
C19	1.2233 (6)	0.1982 (6)	−0.0317 (4)	0.0755 (16)
H19A	1.2555	0.1408	−0.0763	0.091*
C16	1.1330 (6)	0.3830 (5)	0.0897 (4)	0.0669 (14)
H16A	1.0992	0.4398	0.1346	0.080*
C3	0.5529 (7)	0.3131 (6)	0.1275 (5)	0.0885 (19)

H3A	0.4579	0.3260	0.1054	0.106*
C4	0.6317 (6)	0.3950 (5)	0.1946 (4)	0.0683 (14)
C27	0.7876 (5)	0.0330 (5)	0.4904 (4)	0.0675 (14)
H27A	0.7353	−0.0039	0.5385	0.081*
C25	0.8682 (6)	−0.1357 (4)	0.3793 (5)	0.0711 (15)
H25A	0.8232	−0.1787	0.4255	0.085*
C1	0.7488 (6)	0.1890 (5)	0.1282 (4)	0.0686 (14)
H1A	0.7861	0.1235	0.1091	0.082*
C7	0.8077 (6)	0.5402 (4)	0.3300 (4)	0.0646 (13)
H7A	0.8676	0.5861	0.3748	0.078*
C15	1.3127 (5)	0.1909 (4)	0.3235 (4)	0.0577 (11)
H15A	1.2969	0.1248	0.2878	0.069*
C28	0.7912 (6)	0.1470 (5)	0.5094 (4)	0.0690 (14)
H28A	0.7411	0.1780	0.5698	0.083*
C24	0.9389 (7)	−0.1761 (4)	0.2934 (6)	0.0758 (16)
H24A	0.9466	−0.2473	0.2773	0.091*
C11	1.2259 (5)	0.3692 (4)	0.3732 (4)	0.0572 (11)
C12	1.3534 (6)	0.3970 (5)	0.4287 (5)	0.0775 (16)
H12A	1.3695	0.4635	0.4636	0.093*
C17	1.2026 (7)	0.3964 (6)	−0.0036 (5)	0.0810 (17)
H17A	1.2204	0.4610	−0.0277	0.097*
C23	1.0035 (6)	−0.1057 (4)	0.2258 (4)	0.0623 (12)
H23A	1.0534	−0.1331	0.1636	0.075*
C2	0.6104 (7)	0.2143 (6)	0.0929 (5)	0.094 (2)
H2A	0.5552	0.1666	0.0465	0.112*
C18	1.2466 (7)	0.3029 (7)	−0.0623 (5)	0.091 (2)
H18A	1.2960	0.3086	−0.1278	0.109*
C14	1.4402 (6)	0.2164 (5)	0.3784 (5)	0.0732 (15)
H14A	1.5138	0.1684	0.3824	0.088*
C13	1.4573 (7)	0.3211 (6)	0.4304 (6)	0.0904 (19)
H13A	1.5449	0.3388	0.4679	0.108*
C5	0.5839 (7)	0.5006 (6)	0.2351 (5)	0.0828 (18)
H5A	0.4908	0.5198	0.2149	0.099*
C6	0.6675 (7)	0.5712 (5)	0.3000 (5)	0.0816 (17)
H6A	0.6336	0.6368	0.3233	0.098*
O3	0.4151 (9)	0.0401 (7)	0.7756 (7)	0.182 (3)
O6	0.6578 (6)	0.0767 (6)	0.7331 (6)	0.142 (2)
O5	0.4784 (9)	0.1497 (12)	0.6457 (8)	0.258 (7)
O4	0.5174 (12)	0.2145 (7)	0.8072 (9)	0.220 (4)
O1W	0.7670 (12)	0.3638 (8)	0.8063 (11)	0.254 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0473 (4)	0.0421 (4)	0.0250 (3)	0.0047 (2)	0.0057 (2)	−0.0016 (2)
Cl1	0.0727 (9)	0.1085 (13)	0.0909 (11)	0.0234 (9)	0.0159 (8)	0.0013 (9)
N2	0.067 (2)	0.0450 (19)	0.0427 (19)	0.0049 (17)	0.0095 (17)	−0.0011 (16)
N6	0.052 (2)	0.056 (2)	0.0325 (17)	0.0015 (16)	0.0008 (14)	−0.0011 (15)

N5	0.052 (2)	0.062 (2)	0.0333 (17)	0.0084 (17)	0.0005 (14)	−0.0034 (16)
N4	0.053 (2)	0.076 (3)	0.0299 (17)	0.0037 (18)	0.0016 (14)	0.0087 (17)
N1	0.058 (2)	0.069 (2)	0.0309 (17)	0.0032 (18)	0.0042 (15)	0.0008 (16)
C21	0.062 (3)	0.068 (3)	0.038 (2)	0.019 (2)	−0.0008 (19)	−0.013 (2)
C8	0.068 (3)	0.058 (3)	0.041 (2)	0.008 (2)	0.011 (2)	0.011 (2)
C30	0.049 (2)	0.058 (3)	0.040 (2)	−0.0046 (19)	−0.0094 (17)	0.0057 (19)
C22	0.050 (2)	0.051 (2)	0.044 (2)	0.0004 (19)	−0.0096 (18)	−0.0038 (19)
O1	0.106 (3)	0.055 (2)	0.090 (3)	0.000 (2)	−0.003 (2)	−0.0202 (19)
O2	0.107 (3)	0.089 (3)	0.0469 (19)	0.027 (2)	0.0061 (19)	−0.0160 (18)
N3	0.050 (2)	0.059 (2)	0.0334 (17)	−0.0011 (16)	0.0063 (14)	0.0023 (15)
C20	0.048 (2)	0.091 (4)	0.029 (2)	0.007 (2)	−0.0020 (16)	−0.004 (2)
C29	0.058 (3)	0.068 (3)	0.035 (2)	0.006 (2)	0.0039 (18)	0.003 (2)
C10	0.068 (3)	0.054 (3)	0.051 (3)	−0.003 (2)	0.007 (2)	−0.006 (2)
C26	0.057 (3)	0.074 (3)	0.050 (3)	−0.015 (2)	−0.012 (2)	0.018 (2)
C9	0.064 (3)	0.063 (3)	0.037 (2)	0.013 (2)	0.0147 (19)	0.0106 (19)
C19	0.067 (3)	0.127 (5)	0.031 (2)	0.003 (3)	0.010 (2)	0.000 (3)
C16	0.068 (3)	0.093 (4)	0.042 (3)	0.005 (3)	0.003 (2)	0.020 (3)
C3	0.065 (4)	0.130 (6)	0.071 (4)	0.024 (4)	−0.006 (3)	0.015 (4)
C4	0.066 (3)	0.093 (4)	0.051 (3)	0.023 (3)	0.009 (2)	0.023 (3)
C27	0.056 (3)	0.101 (4)	0.049 (3)	−0.011 (3)	0.001 (2)	0.026 (3)
C25	0.075 (4)	0.068 (3)	0.073 (4)	−0.014 (3)	−0.007 (3)	0.026 (3)
C1	0.065 (3)	0.083 (4)	0.054 (3)	0.014 (3)	−0.008 (2)	−0.009 (3)
C7	0.087 (4)	0.053 (3)	0.056 (3)	0.014 (2)	0.017 (2)	0.010 (2)
C15	0.068 (3)	0.063 (3)	0.043 (2)	0.008 (2)	0.003 (2)	0.008 (2)
C28	0.063 (3)	0.106 (4)	0.041 (2)	0.004 (3)	0.012 (2)	0.014 (3)
C24	0.087 (4)	0.051 (3)	0.089 (4)	−0.005 (3)	−0.013 (3)	0.009 (3)
C11	0.067 (3)	0.058 (3)	0.045 (2)	−0.009 (2)	0.006 (2)	−0.002 (2)
C12	0.073 (4)	0.083 (4)	0.071 (3)	−0.018 (3)	−0.006 (3)	−0.015 (3)
C17	0.082 (4)	0.114 (5)	0.051 (3)	−0.006 (3)	0.003 (3)	0.027 (3)
C23	0.073 (3)	0.055 (3)	0.056 (3)	0.005 (2)	−0.006 (2)	−0.005 (2)
C2	0.078 (4)	0.133 (6)	0.064 (4)	0.009 (4)	−0.021 (3)	−0.013 (4)
C18	0.077 (4)	0.154 (7)	0.042 (3)	0.002 (4)	0.014 (3)	0.014 (4)
C14	0.052 (3)	0.099 (4)	0.067 (3)	0.008 (3)	−0.011 (2)	0.005 (3)
C13	0.069 (4)	0.108 (5)	0.091 (4)	0.000 (3)	−0.015 (3)	−0.003 (4)
C5	0.077 (4)	0.109 (5)	0.068 (4)	0.032 (4)	0.011 (3)	0.030 (3)
C6	0.096 (4)	0.082 (4)	0.072 (4)	0.026 (3)	0.026 (3)	0.021 (3)
O3	0.164 (7)	0.217 (8)	0.172 (7)	−0.050 (6)	0.047 (5)	0.050 (6)
O6	0.109 (4)	0.176 (6)	0.146 (5)	0.063 (4)	0.029 (4)	0.034 (5)
O5	0.138 (7)	0.51 (2)	0.150 (7)	0.019 (9)	0.001 (5)	0.155 (10)
O4	0.280 (11)	0.141 (6)	0.231 (10)	0.035 (7)	0.097 (8)	−0.047 (6)
O1W	0.240 (11)	0.150 (7)	0.350 (16)	−0.003 (7)	0.052 (10)	−0.088 (9)

Geometric parameters (Å, º)

Mn1—N4	1.878 (3)	C9—C4	1.398 (7)
Mn1—N1	1.919 (4)	C19—C18	1.461 (10)
Mn1—N3	1.928 (4)	C19—H19A	0.930
Mn1—N6	1.935 (4)	C16—C17	1.334 (7)

Mn1—N5	2.000 (4)	C16—H16A	0.930
Mn1—N2	2.054 (4)	C3—C2	1.421 (10)
Cl1—O6	1.371 (5)	C3—C4	1.447 (9)
Cl1—O5	1.380 (8)	C3—H3A	0.930
Cl1—O3	1.429 (7)	C4—C5	1.485 (9)
Cl1—O4	1.442 (8)	C27—C28	1.477 (8)
N2—C10	1.353 (6)	C27—H27A	0.930
N2—C8	1.388 (6)	C25—C24	1.303 (9)
N6—C29	1.286 (6)	C25—H25A	0.930
N6—C30	1.478 (6)	C1—C2	1.388 (8)
N5—C21	1.286 (6)	C1—H1A	0.930
N5—C22	1.454 (6)	C7—C6	1.406 (9)
N4—C20	1.402 (6)	C7—H7A	0.930
N4—C16	1.433 (7)	C15—C14	1.355 (7)
N1—C1	1.342 (6)	C15—H15A	0.930
N1—C9	1.450 (6)	C28—H28A	0.930
C21—O2	1.283 (6)	C24—C23	1.422 (8)
C21—C20	1.585 (8)	C24—H24A	0.930
C8—C9	1.445 (7)	C11—C12	1.364 (7)
C8—C7	1.446 (7)	C12—C13	1.384 (9)
C30—C22	1.360 (6)	C12—H12A	0.930
C30—C26	1.449 (6)	C17—C18	1.411 (10)
C22—C23	1.481 (6)	C17—H17A	0.930
O1—C10	1.318 (6)	C23—H23A	0.930
N3—C15	1.378 (6)	C2—H2A	0.930
N3—C11	1.438 (6)	C18—H18A	0.930
C20—C19	1.304 (6)	C14—C13	1.444 (9)
C29—C28	1.391 (7)	C14—H14A	0.930
C29—H29A	0.930	C13—H13A	0.930
C10—C11	1.516 (7)	C5—C6	1.362 (9)
C26—C27	1.369 (8)	C5—H5A	0.930
C26—C25	1.505 (8)	C6—H6A	0.930

N4—Mn1—N1	94.61 (15)	C8—C9—N1	119.6 (4)
N4—Mn1—N3	85.35 (14)	C20—C19—C18	117.4 (6)
N1—Mn1—N3	162.60 (16)	C20—C19—H19A	121.3
N4—Mn1—N6	165.15 (17)	C18—C19—H19A	121.3
N1—Mn1—N6	86.06 (15)	C17—C16—N4	119.4 (6)
N3—Mn1—N6	98.42 (14)	C17—C16—H16A	120.3
N4—Mn1—N5	88.36 (16)	N4—C16—H16A	120.3
N1—Mn1—N5	100.50 (16)	C2—C3—C4	124.5 (5)
N3—Mn1—N5	96.89 (15)	C2—C3—H3A	117.7
N6—Mn1—N5	76.95 (15)	C4—C3—H3A	117.7
N4—Mn1—N2	92.24 (16)	C9—C4—C3	111.5 (5)
N1—Mn1—N2	81.17 (16)	C9—C4—C5	119.0 (6)
N3—Mn1—N2	81.45 (16)	C3—C4—C5	129.4 (5)
N6—Mn1—N2	102.51 (15)	C26—C27—C28	122.3 (5)
N5—Mn1—N2	178.18 (15)	C26—C27—H27A	118.8

O6—Cl1—O5	106.8 (5)	C28—C27—H27A	118.9
O6—Cl1—O3	115.4 (5)	C24—C25—C26	120.8 (5)
O5—Cl1—O3	110.0 (6)	C24—C25—H25A	119.6
O6—Cl1—O4	112.3 (6)	C26—C25—H25A	119.6
O5—Cl1—O4	93.5 (8)	N1—C1—C2	117.8 (6)
O3—Cl1—O4	116.3 (5)	N1—C1—H1A	121.1
C10—N2—C8	121.8 (4)	C2—C1—H1A	121.1
C10—N2—Mn1	120.3 (3)	C6—C7—C8	121.4 (5)
C8—N2—Mn1	117.9 (3)	C6—C7—H7A	119.3
C29—N6—C30	120.0 (4)	C8—C7—H7A	119.3
C29—N6—Mn1	123.0 (3)	C14—C15—N3	118.6 (5)
C30—N6—Mn1	116.8 (3)	C14—C15—H15A	120.7
C21—N5—C22	121.4 (4)	N3—C15—H15A	120.7
C21—N5—Mn1	116.1 (3)	C29—C28—C27	124.8 (5)
C22—N5—Mn1	122.5 (3)	C29—C28—H28A	117.6
C20—N4—C16	126.2 (4)	C27—C28—H28A	117.6
C20—N4—Mn1	106.4 (3)	C25—C24—C23	116.6 (5)
C16—N4—Mn1	127.4 (3)	C25—C24—H24A	121.7
C1—N1—C9	122.6 (4)	C23—C24—H24A	121.7
C1—N1—Mn1	124.1 (4)	C12—C11—N3	119.2 (5)
C9—N1—Mn1	113.4 (3)	C12—C11—C10	120.7 (5)
O2—C21—N5	123.9 (5)	N3—C11—C10	120.1 (4)
O2—C21—C20	129.2 (4)	C11—C12—C13	116.4 (5)
N5—C21—C20	106.9 (4)	C11—C12—H12A	121.8
N2—C8—C9	107.8 (4)	C13—C12—H12A	121.8
N2—C8—C7	130.8 (5)	C16—C17—C18	113.3 (6)
C9—C8—C7	121.4 (5)	C16—C17—H17A	123.3
C22—C30—C26	114.5 (4)	C18—C17—H17A	123.3
C22—C30—N6	118.1 (4)	C24—C23—C22	124.4 (5)
C26—C30—N6	127.4 (4)	C24—C23—H23A	117.8
C30—C22—N5	105.6 (4)	C22—C23—H23A	117.8
C30—C22—C23	120.3 (4)	C1—C2—C3	120.2 (6)
N5—C22—C23	134.1 (4)	C1—C2—H2A	119.9
C15—N3—C11	123.4 (4)	C3—C2—H2A	119.9
C15—N3—Mn1	124.0 (3)	C17—C18—C19	127.4 (5)
C11—N3—Mn1	112.6 (3)	C17—C18—H18A	116.3
C19—C20—N4	116.3 (5)	C19—C18—H18A	116.3
C19—C20—C21	121.5 (5)	C15—C14—C13	117.4 (5)
N4—C20—C21	122.1 (4)	C15—C14—H14A	121.3
N6—C29—C28	116.1 (5)	C13—C14—H14A	121.3
N6—C29—H29A	121.9	C12—C13—C14	125.0 (5)
C28—C29—H29A	121.9	C12—C13—H13A	117.5
O1—C10—N2	129.2 (5)	C14—C13—H13A	117.5
O1—C10—C11	125.3 (4)	C6—C5—C4	124.3 (6)
N2—C10—C11	105.5 (4)	C6—C5—H5A	117.9
C27—C26—C30	109.2 (5)	C4—C5—H5A	117.8
C27—C26—C25	127.4 (5)	C5—C6—C7	116.8 (6)
C30—C26—C25	123.4 (5)	C5—C6—H6A	121.6

C4—C9—C8	117.0 (5)	C7—C6—H6A	121.6
C4—C9—N1	123.3 (5)		