Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

  doi:10.1107/S1600536811037603

References

Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Huang, G. S. (2008). *Acta Cryst.* E**64**, m685–m686.
Li, S., Chen, Y., He, H.-M. & Ma, Y.-F. (2009). *Acta Cryst.* E**65**, m411.
Li, S., Wang, S.-B., Zhang, F.-L. & Tang, K. (2008). *Acta Cryst.* E**64**, m2.
Li, S., Yan, X.-L., Wang, S.-B. & Ma, Y.-F. (2008). *Acta Cryst.* E**64**, m1258.
Li, S., Zhang, F.-L., Tang, K. & Ma, Y.-F. (2008). *Acta Cryst.* E**64**, m1142.
Li, Z., Wang, S., Zhang, Q. & Yu, X. (2007*a*). *Acta Cryst.* E**63**, m2438–m2439.
Li, Z., Wang, S., Zhang, Q. & Yu, X. (2007*b*). *Acta Cryst.* E**63**, m2604.
Li, Z., Wang, S., Zhang, Q. & Yu, X. (2007*c*). *Acta Cryst.* E**63**, m2642.
Li, Z., Wang, S., Zhang, Q. & Yu, X. (2007*d*). *Acta Cryst.* E**63**, m2781.
Li, Z.-F., Liu, Y., Zhang, Q. & Yu, X.-J. (2007). *Acta Cryst.* E**63**, m2315.
Li, Z.-F., Wang, S.-W., Zhang, Q. & Yu, X.-J. (2007*e*). *Acta Cryst.* E**63**, m2312.
Li, Z.-F., Wang, S.-W., Zhang, Q. & Yu, X.-J. (2007*f*). *Acta Cryst.* E**63**, m2360.
Li, Z.-F., Wang, S.-W., Zhang, Q. & Yu, X.-J. (2007*g*). *Acta Cryst.* E**63**, m2373.
Li, Z.-F., Wang, S.-W., Zhang, Q. & Yu, X.-J. (2007*h*). *Acta Cryst.* E**63**, m2445.
Li, Z.-F., Wang, S.-W., Zhang, Q. & Yu, X.-J. (2007*i*). *Acta Cryst.* E**63**, o3930.
Liu, Y., Dou, J., Li, D. & Zhang, X. (2007). *Acta Cryst.* E**63**, m2722.
Liu, Y., Dou, J., Niu, M. & Zhang, X. (2007*a*). *Acta Cryst.* E**63**, m2771.
Liu, Y., Dou, J., Niu, M. & Zhang, X. (2007*b*). *Acta Cryst.* E**63**, m3032.
Liu, Y., Dou, J., Wang, D., Ma, G. & Li, D. (2005). *Acta Cryst.* E**61**, m1834–m1836.
Liu, Y., Dou, J.-M., Wang, D.-Q., Zhang, X.-X. & Zhou, L. (2006). *Acta Cryst.* E**62**, m2794–m2795.
Liu, Y., He, Q., Zhang, X., Xue, Z. & Lv, C. (2008). *Acta Cryst.* E**64**, m1605–m1606.
Liu, Y., Zhang, X., Xue, Z. & Lv, C. (2009). *Acta Cryst.* E**65**, o2724.
Meng, Q., Wang, L., Liu, Y. & Pang, Y. (2008*a*). *Acta Cryst.* E**64**, m63.
Meng, Q., Wang, L., Liu, Y. & Pang, Y. (2008*b*). *Acta Cryst.* E**64**, m133.
Meng, Q., Wang, L., Liu, Y. & Pang, Y. (2008*c*). *Acta Cryst.* E**64**, m204.
Meng, Q., Wang, L., Liu, Y. & Pang, Y. (2008*d*). *Acta Cryst.* E**64**, m332.
Meng, Q.-G., Wang, L.-T., Liu, Y.-Z. & Pang, Y. (2008*e*). *Acta Cryst.* E**64**, m170–m171.
Xia, G. & Sun, Z. (2009). *Acta Cryst.* E**65**, m315–m316.

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]manganese(III)} bis(hexafluoridophosphate)

Qingguo Meng,* Lintong Wang, Yanzhen Liu and Yan Pang

College of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: qgmeng_weifang@yahoo.cn

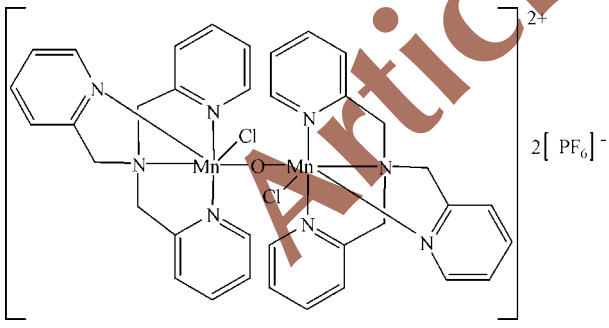
Received 11 November 2007; accepted 11 December 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.076; data-to-parameter ratio = 14.4.

In the title compound, $[Mn_2O(C_{18}H_{18}ClN_4)_2](PF_6)_2$, the Mn atom is chelated by a tetradentate ligand *via* four N atoms, and further bonded to one chloride ion and one bridging oxide, to give a centrosymmetric cation and distorted octahedral coordination geometry.

Related literature

For related literature, see: Scapin *et al.* (1997); Okabe *et al.* (2000); Serre *et al.* (2005).



Experimental

Crystal data

$[Mn_2O(C_{18}H_{18}ClN_4)_2](PF_6)_2$
M_r = 1067.45
Triclinic, $P\overline{1}$
a = 8.5517 (12) Å
b = 11.3128 (18) Å
c = 12.914 (2) Å
α = 115.51 (2)°
β = 107.44 (2)°
γ = 91.49 (2)°
V = 1058.1 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 293 (2) K
0.28 × 0.22 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.788, T_{max} = 0.856
9180 measured reflections
4125 independent reflections
3801 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
S = 1.00
4125 reflections
287 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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, 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 Liaocheng University for financial support and Professor Jianmin Dou for his help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2174).

References

Bruker (2001). *SADABS*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Okabe, N. & Oya, N. (2000). *Acta Cryst.* C**56**, 1416–1417.
Scapin, G., Reddy, S. G., Zheng, R. & Blanchard, J. S. (1997). *Biochemistry*, **36**, 15081–15088.
Serre, C., Marrot, J. & Ferey, G. (2005). *Inorg. Chem.* **44**, 654–658.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807066512

supporting information

Acta Cryst. (2008). E**64**, m204 [https://doi.org/10.1107/S1600536807066512]

μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]manganese(III)} bis(hexafluoridophosphate)

Qingguo Meng, Lintong Wang, Yanzhen Liu and Yan Pang

S1. Comment

In recent years, many symmetrical polypyridine ligands and their coordination complexes have been synthesized (Scapin *et al.*, 1997; Okabe *et al.*, 2000; Serre *et al.*, 2005). In this paper, we report the structure of the title compound, (I), containing an unsymmetrical polypyridine ligand.

As shown in Fig. 1, the Mn atom is chelated by the tetradentate ligand *via* four N atoms, and further bonded to one chloride ion and one bridging oxide, to give a centrosymmetric cation and distorted octahedral coordination geometry.

S2. Experimental

A mixture of manganese(III) acetate (1 mmol) and tris(2-pyridylmethyl)amine (1 mmol) in 20 ml me thanol was refluxed for two hours. The cooled solution was filtered and the filtrate allowed to evaporate at room temperature. Two days later, pink blocks of (I) were obtained with a yield of 30%. Anal. Calc. for $C_{36}H_{36}Cl_2F_{12}Mn_2N_8OP_2$: C 40.48, H 3.37, N 10.50%; Found: C 40.42, H 3.38, N 10.44%.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

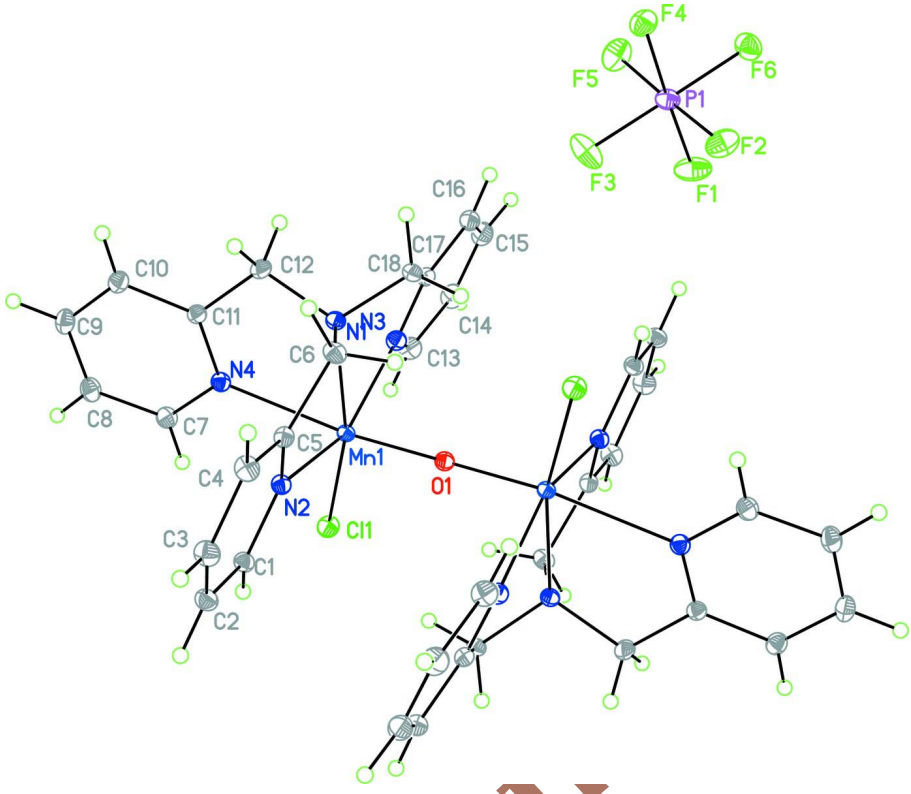


Figure 1

The molecular structure of (I), drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms.

μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]manganese(III)} bis(hexafluoridophosphate)

Crystal data

$[Mn_2O(C_{18}H_{18}ClN_4)_2](PF_6)_2$
$M_r = 1067.45$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.5517\ (12)$ Å
$b = 11.3128\ (18)$ Å
$c = 12.914\ (2)$ Å
$\alpha = 115.51\ (2)°$
$\beta = 107.44\ (2)°$
$\gamma = 91.49\ (2)°$
$V = 1058.1\ (3)$ Å^3
$Z = 1$
$F(000) = 538$
$D_x = 1.675$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4125 reflections
$\theta = 3.0–26.0°$
$\mu = 0.89$ mm^{-1}
$T = 293$ K
Block, pink
0.28 × 0.22 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.788$, $T_{max} = 0.856$
9180 measured reflections
4125 independent reflections
3801 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 26.0°$, $\theta_{min} = 3.0°$
$h = -8\rightarrow10$
$k = -13\rightarrow13$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.076$
$S = 1.00$
4125 reflections
287 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
$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.508P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0273 (16)

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}
Mn1	1.03744 (3)	0.34680 (2)	0.39271 (2)	0.0591 (3)
C16	0.9137 (3)	0.5294 (2)	0.15470 (19)	0.0579 (6)
H16	0.8144	0.5473	0.1147	0.070*
C15	1.0631 (4)	0.5736 (2)	0.1515 (2)	0.0698 (7)
H15	1.0656	0.6240	0.1109	0.084*
C12	0.7465 (3)	0.1753 (2)	0.14497 (19)	0.0547 (5)
H12A	0.7451	0.2011	0.0822	0.066*
H12B	0.6370	0.1255	0.1212	0.066*
C14	1.2072 (4)	0.5437 (3)	0.2077 (2)	0.0693 (7)
H14	1.3080	0.5723	0.2048	0.083*
C13	1.2008 (3)	0.4705 (2)	0.2687 (2)	0.0586 (5)
H13	1.2989	0.4497	0.3070	0.070*
C9	0.9549 (3)	−0.1237 (2)	0.0608 (2)	0.0591 (6)
H9	0.9333	−0.2116	0.0007	0.071*
C7	1.1344 (3)	0.0604 (2)	0.2403 (2)	0.0506 (5)
H7	1.2376	0.0959	0.3026	0.061*
C10	0.8352 (3)	−0.0448 (2)	0.05877 (19)	0.0503 (5)
H10	0.7312	−0.0789	−0.0027	0.060*
C8	1.1067 (3)	−0.0700 (2)	0.1531 (2)	0.0589 (6)
H8	1.1897	−0.1211	0.1567	0.071*
C6	0.6719 (2)	0.2876 (2)	0.33136 (19)	0.0473 (5)
H6A	0.5632	0.2359	0.2740	0.057*
H6B	0.6564	0.3760	0.3821	0.057*

C3	0.7291 (3)	0.1172 (2)	0.5339 (2)	0.0583 (5)
H3	0.6660	0.0777	0.5619	0.070*
C1	0.9874 (2)	0.18989 (19)	0.53077 (17)	0.0432 (4)
H1	1.1028	0.1989	0.5575	0.052*
C17	0.9146 (3)	0.45733 (19)	0.21901 (16)	0.0442 (4)
C2	0.8988 (3)	0.1304 (2)	0.57405 (19)	0.0509 (5)
H2	0.9530	0.0998	0.6292	0.061*
C4	0.6514 (3)	0.1631 (2)	0.4512 (2)	0.0528 (5)
H4	0.5359	0.1536	0.4227	0.063*
C18	0.7604 (3)	0.41495 (19)	0.23735 (18)	0.0450 (4)
H18A	0.7428	0.4883	0.3054	0.054*
H18B	0.6641	0.3918	0.1647	0.054*
C5	0.7463 (2)	0.22291 (18)	0.41146 (17)	0.0400 (4)
C11	0.8713 (2)	0.08589 (18)	0.14917 (16)	0.0398 (4)
Cl1	1.31393 (6)	0.35086 (5)	0.48444 (5)	0.05319 (15)
F3	0.5826 (2)	0.6606 (2)	0.1912 (2)	0.1062 (6)
F5	0.6040 (2)	0.71991 (18)	0.04862 (16)	0.0904 (5)
F2	0.4876 (2)	0.84879 (19)	0.27957 (14)	0.0865 (5)
F1	0.73275 (18)	0.8610 (2)	0.24889 (16)	0.0976 (6)
F6	0.5112 (2)	0.90781 (15)	0.13872 (16)	0.0796 (4)
F4	0.36039 (17)	0.71075 (14)	0.08069 (13)	0.0705 (4)
N3	1.0566 (2)	0.42831 (16)	0.27464 (15)	0.0455 (4)
N1	0.77789 (18)	0.29832 (15)	0.26229 (14)	0.0395 (3)
N4	1.01895 (19)	0.13923 (15)	0.23967 (14)	0.0415 (3)
N2	0.91299 (18)	0.23567 (15)	0.45101 (14)	0.0386 (3)
O1	1.0000	0.5000	0.5000	0.0399 (4)
P1	0.54877 (7)	0.78428 (6)	0.16552 (5)	0.05074 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0639 (6)	0.0610 (6)	0.0547 (6)	0.0008 (4)	0.0176 (5)	−0.0068 (4)
C16	0.0825 (17)	0.0485 (11)	0.0445 (11)	0.0145 (11)	0.0199 (11)	0.0241 (9)
C15	0.109 (2)	0.0528 (13)	0.0546 (13)	0.0012 (13)	0.0329 (14)	0.0282 (11)
C12	0.0490 (12)	0.0473 (11)	0.0438 (11)	0.0091 (9)	−0.0021 (9)	0.0119 (9)
C14	0.0823 (18)	0.0680 (15)	0.0664 (15)	−0.0023 (13)	0.0354 (14)	0.0328 (13)
C13	0.0575 (13)	0.0637 (13)	0.0599 (13)	0.0039 (10)	0.0251 (11)	0.0302 (11)
C9	0.0717 (15)	0.0427 (11)	0.0615 (13)	0.0130 (10)	0.0313 (12)	0.0171 (10)
C7	0.0432 (11)	0.0545 (11)	0.0568 (12)	0.0165 (9)	0.0196 (9)	0.0259 (10)
C10	0.0524 (12)	0.0457 (10)	0.0480 (11)	0.0023 (9)	0.0171 (9)	0.0179 (9)
C8	0.0620 (14)	0.0535 (12)	0.0700 (14)	0.0251 (10)	0.0329 (12)	0.0285 (11)
C6	0.0285 (9)	0.0554 (11)	0.0601 (12)	0.0089 (8)	0.0103 (8)	0.0316 (10)
C3	0.0582 (13)	0.0635 (13)	0.0647 (14)	0.0047 (10)	0.0273 (11)	0.0360 (11)
C1	0.0405 (10)	0.0443 (10)	0.0450 (10)	0.0095 (8)	0.0116 (8)	0.0226 (8)
C17	0.0552 (12)	0.0401 (9)	0.0348 (9)	0.0102 (8)	0.0153 (8)	0.0152 (8)
C2	0.0555 (12)	0.0529 (11)	0.0510 (11)	0.0101 (9)	0.0184 (9)	0.0297 (10)
C4	0.0355 (10)	0.0582 (12)	0.0680 (13)	0.0054 (9)	0.0189 (9)	0.0314 (11)
C18	0.0469 (11)	0.0461 (10)	0.0402 (10)	0.0158 (8)	0.0092 (8)	0.0218 (8)

C5	0.0315 (9)	0.0392 (9)	0.0446 (10)	0.0053 (7)	0.0113 (7)	0.0164 (8)
C11	0.0410 (10)	0.0412 (9)	0.0388 (9)	0.0051 (7)	0.0143 (7)	0.0197 (8)
Cl1	0.0309 (2)	0.0587 (3)	0.0585 (3)	0.0126 (2)	0.0094 (2)	0.0207 (2)
F3	0.0981 (14)	0.1209 (15)	0.1660 (19)	0.0536 (12)	0.0649 (13)	0.1092 (15)
F5	0.0931 (12)	0.0951 (12)	0.0853 (11)	0.0077 (9)	0.0564 (10)	0.0269 (9)
F2	0.0790 (11)	0.1126 (13)	0.0617 (9)	0.0061 (9)	0.0342 (8)	0.0286 (9)
F1	0.0443 (8)	0.1515 (17)	0.0847 (11)	−0.0079 (9)	0.0016 (7)	0.0586 (11)
F6	0.0760 (10)	0.0695 (9)	0.0981 (11)	0.0058 (7)	0.0193 (8)	0.0500 (9)
F4	0.0522 (8)	0.0690 (8)	0.0724 (9)	−0.0055 (6)	0.0123 (7)	0.0238 (7)
N3	0.0483 (9)	0.0479 (9)	0.0439 (9)	0.0075 (7)	0.0187 (7)	0.0225 (7)
N1	0.0332 (8)	0.0421 (8)	0.0402 (8)	0.0094 (6)	0.0078 (6)	0.0193 (7)
N4	0.0391 (8)	0.0433 (8)	0.0436 (8)	0.0111 (6)	0.0153 (7)	0.0205 (7)
N2	0.0325 (8)	0.0400 (8)	0.0429 (8)	0.0076 (6)	0.0113 (6)	0.0197 (7)
O1	0.0350 (9)	0.0409 (9)	0.0411 (9)	0.0076 (7)	0.0104 (7)	0.0185 (8)
P1	0.0402 (3)	0.0644 (3)	0.0516 (3)	0.0071 (2)	0.0144 (2)	0.0312 (3)

Geometric parameters (Å, º)

Mn1—O1	1.8034 (5)	C6—N1	1.485 (3)
Mn1—N2	2.1227 (16)	C6—C5	1.514 (3)
Mn1—N3	2.1341 (17)	C6—H6A	0.970
Mn1—N1	2.2280 (16)	C6—H6B	0.970
Mn1—N4	2.2893 (17)	C3—C2	1.367 (3)
Mn1—Cl1	2.2944 (7)	C3—C4	1.386 (3)
C16—C15	1.379 (4)	C3—H3	0.930
C16—C17	1.390 (3)	C1—N2	1.348 (2)
C16—H16	0.930	C1—C2	1.375 (3)
C15—C14	1.361 (4)	C1—H1	0.930
C15—H15	0.930	C17—N3	1.341 (3)
C12—N1	1.491 (2)	C17—C18	1.509 (3)
C12—C11	1.495 (3)	C2—H2	0.930
C12—H12A	0.970	C4—C5	1.378 (3)
C12—H12B	0.970	C4—H4	0.930
C14—C13	1.377 (3)	C18—N1	1.488 (2)
C14—H14	0.930	C18—H18A	0.970
C13—N3	1.346 (3)	C18—H18B	0.970
C13—H13	0.930	C5—N2	1.343 (2)
C9—C8	1.372 (3)	C11—N4	1.339 (2)
C9—C10	1.377 (3)	F3—P1	1.5854 (18)
C9—H9	0.930	F5—P1	1.5906 (16)
C7—N4	1.348 (3)	F2—P1	1.5908 (16)
C7—C8	1.375 (3)	F1—P1	1.5799 (16)
C7—H7	0.930	F6—P1	1.5966 (16)
C10—C11	1.385 (3)	F4—P1	1.6046 (15)
C10—H10	0.930	O1—Mn1^{i}	1.8034 (5)
C8—H8	0.930		
O1—Mn1—N2	90.82 (4)	N2—C1—H1	118.8

O1—Mn1—N3	92.87 (5)	C2—C1—H1	118.8
N2—Mn1—N3	154.78 (6)	N3—C17—C16	121.2 (2)
O1—Mn1—N1	91.90 (5)	N3—C17—C18	116.09 (17)
N2—Mn1—N1	78.71 (6)	C16—C17—C18	122.6 (2)
N3—Mn1—N1	76.24 (6)	C1—C2—C3	118.3 (2)
O1—Mn1—N4	166.67 (4)	C1—C2—H2	120.8
N2—Mn1—N4	82.20 (6)	C3—C2—H2	120.8
N3—Mn1—N4	88.79 (6)	C5—C4—C3	119.6 (2)
N1—Mn1—N4	75.64 (6)	C5—C4—H4	120.2
O1—Mn1—Cl1	102.88 (3)	C3—C4—H4	120.2
N2—Mn1—Cl1	103.45 (5)	N1—C18—C17	110.49 (15)
N3—Mn1—Cl1	100.01 (5)	N1—C18—H18A	109.6
N1—Mn1—Cl1	164.97 (4)	C17—C18—H18A	109.6
N4—Mn1—Cl1	89.83 (5)	N1—C18—H18B	109.6
C15—C16—C17	118.5 (2)	C17—C18—H18B	109.6
C15—C16—H16	120.7	H18A—C18—H18B	108.1
C17—C16—H16	120.7	N2—C5—C4	120.59 (18)
C16—C15—C14	120.3 (2)	N2—C5—C6	116.63 (17)
C16—C15—H15	119.9	C4—C5—C6	122.56 (17)
C14—C15—H15	119.9	N4—C11—C10	122.48 (18)
N1—C12—C11	114.72 (15)	N4—C11—C12	117.29 (16)
N1—C12—H12A	108.6	C10—C11—C12	120.17 (18)
C11—C12—H12A	108.6	C17—N3—C13	119.35 (19)
N1—C12—H12B	108.6	C17—N3—Mn1	114.96 (13)
C11—C12—H12B	108.6	C13—N3—Mn1	124.77 (15)
H12A—C12—H12B	107.6	C12—N1—C6	112.81 (17)
C13—C14—C15	118.8 (2)	C12—N1—C18	109.20 (15)
C13—C14—H14	120.6	C6—N1—C18	112.67 (15)
C15—C14—H14	120.6	C12—N1—Mn1	113.32 (12)
N3—C13—C14	121.8 (2)	C6—N1—Mn1	104.27 (11)
N3—C13—H13	119.1	C18—N1—Mn1	104.25 (11)
C14—C13—H13	119.1	C7—N4—C11	117.38 (17)
C8—C9—C10	118.7 (2)	C7—N4—Mn1	125.96 (14)
C8—C9—H9	120.7	C11—N4—Mn1	116.09 (12)
C10—C9—H9	120.7	C5—N2—C1	119.34 (17)
N4—C7—C8	123.0 (2)	C5—N2—Mn1	114.73 (12)
N4—C7—H7	118.5	C1—N2—Mn1	125.63 (13)
C8—C7—H7	118.5	Mn1^{i}—O1—Mn1	180
C11—C10—C9	119.3 (2)	F3—P1—F1	91.72 (12)
C11—C10—H10	120.3	F3—P1—F2	90.05 (11)
C9—C10—H10	120.3	F1—P1—F2	90.83 (10)
C9—C8—C7	119.1 (2)	F3—P1—F6	179.00 (10)
C9—C8—H8	120.4	F1—P1—F6	89.26 (10)
C7—C8—H8	120.4	F2—P1—F6	89.71 (10)
N1—C6—C5	112.64 (15)	F3—P1—F5	90.98 (11)
N1—C6—H6A	109.1	F1—P1—F5	90.78 (10)
C5—C6—H6A	109.1	F2—P1—F5	178.06 (10)
N1—C6—H6B	109.1	F6—P1—F5	89.23 (10)

C5—C6—H6B	109.1	F3—P1—F4	90.10 (11)
H6A—C6—H6B	107.8	F1—P1—F4	178.14 (11)
C2—C3—C4	119.6 (2)	F2—P1—F4	88.82 (9)
C2—C3—H3	120.2	F6—P1—F4	88.92 (9)
C4—C3—H3	120.2	F5—P1—F4	89.54 (9)
N2—C1—C2	122.44 (19)		

Symmetry code: (i) $-x+2, -y+1, -z+1$.