Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Tetraaquabis(4,4′-bipyridine)manganese(II) pyridine-2,6-dicarboxylate tetrahydrate

Yu-Xiang Gao,* Li-Bin Wang and Yan-Ling Niu

Department of Chemistry, Tonghua Teachers' College, Tonghua 134002, People's Republic of China
Correspondence e-mail: yxgao_tonghua@yahoo.com.cn

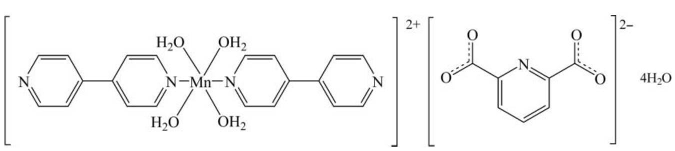
Received 14 July 2007; accepted 31 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.091; data-to-parameter ratio = 7.4.

The title compound, $[Mn(C_{10}H_8N_2)_2(H_2O)_4](C_7H_3NO_4)\cdot 4H_2O$, prepared by hydrothermal synthesis, is isostructural with its Fe^{II} analogue. The compound contains isolated tetraaquabis(4,4′-bipyridine)manganese(II) cations, with two 4,4′-bipyridine molecules bound to Mn^{II} in a *trans* manner. The cations lie in layers, with pyridine-2,6-dicarboxylate dianions and water molecules forming an extensive hydrogen-bond network between them. The cations exhibit noncrystallographic inversion symmetry. The crystal was a partial inversion twin.

Related literature

For the analogous Fe^{II} compound, see: Gao *et al.* (2007).



Experimental

Crystal data

$[Mn(C_{10}H_8N_2)_2(H_2O)_4]$-
$(C_7H_3NO_4)\cdot 4H_2O$
M_r = 676.54
Monoclinic, Cc
a = 18.407 (2) Å
b = 6.8231 (10) Å
c = 25.2925 (10) Å
β = 99.40 (2)°
V = 3133.9 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 293 (2) K
0.15 × 0.15 × 0.15 mm

Data collection

Bruker APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.930, T_{max} = 0.930
5104 measured reflections
3349 independent reflections
2946 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.05
3349 reflections
455 parameters
26 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 530 Friedel pairs
Flack parameter: 0.39 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11···O8^{i}	0.82 (1)	2.10 (3)	2.848 (6)	152 (6)
O1—H12···N3^{ii}	0.82 (1)	1.98 (2)	2.787 (5)	167 (6)
O2—H21···O5^{iii}	0.82 (1)	1.97 (1)	2.781 (5)	171 (5)
O2—H22···O7^{iii}	0.82 (1)	1.98 (1)	2.799 (5)	179 (7)
O3—H31···O5^{iv}	0.82 (1)	2.05 (1)	2.864 (6)	175 (6)
O3—H32···N5^{v}	0.81 (1)	1.96 (1)	2.772 (5)	177 (7)
O4—H41···O8	0.83 (1)	1.93 (1)	2.760 (4)	177 (5)
O4—H42···O11^{vi}	0.82 (1)	1.93 (1)	2.751 (4)	173 (5)
O5—H52···O6	0.82 (1)	1.96 (2)	2.773 (7)	169 (6)
O5—H51···O11^{vi}	0.82 (1)	1.97 (2)	2.770 (6)	165 (6)
O6—H62···O9	0.82 (1)	2.41 (7)	2.933 (6)	123 (7)
O6—H61···O10^{i}	0.82 (1)	2.01 (2)	2.821 (5)	169 (7)
O7—H72···O5^{vii}	0.82 (1)	2.56 (2)	3.330 (6)	158 (5)
O7—H71···O9	0.82 (1)	1.84 (2)	2.645 (5)	168 (6)
O8—H81···O7	0.82 (1)	2.04 (2)	2.844 (6)	166 (6)
O8—H82···O12^{viii}	0.82 (1)	1.98 (1)	2.787 (5)	172 (6)

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

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 the Natural Science Foundation of China (grant No. 20501017) and Tonghua Teachers' College.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2217).

References

Bruker (2001). *SADABS*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gao, Y.-X., Wang, L.-B. & Niu, Y.-L. (2007). *Acta Cryst.* E**63**, m1845–m1846.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

 doi:10.1107/S160053680703766X

supplementary materials

Acta Cryst. (2007). E**63**, m2283 [**doi:10.1107/S160053680703766X**]

Tetraaquabis(4,4'-bipyridine)manganese(II) pyridine-2,6-dicarboxylate tetrahydrate

Y.-X. Gao, L.-B. Wang and Y.-L. Niu

Comment

The title compound is isostructural with its Fe^{II} analogue (Gao *et al.*, 2007). In the $[Mn(C_{10}H_8N_2)_2(H_2O)_4]^{2+}$ cations, Mn^{II} is hexacoordinated in an octahedral manner by four water molecules in the equatorial plane and two N atoms in the axial positions from two 4,4'-bipyridine molecules (Figure 1). The Mn—N and Mn—O bond lengths are in the range 2.284 (4)–2.291 (4) and 2.144 (3)–2.222 (3) Å, respectively. The cations lie in layers in the *bc* planes. Pyridine-2,6-dicarboxylate anions and water molecules lie between these layers, forming an extensive hydrogen-bond network (Figure 2).

Experimental

A mixture of $MnSO_4$ (0.5 mmol), pyridine-2,6-dicarboxylic acid (0.5 mmol), NaOH (1 mmol), 4,4'-bipyridine (0.5 mmol), H_2O (8 ml) and ethanol (8 ml) were placed in a 25 ml Teflon-lined stainless steel autoclave and heated at 433 K for two days. On cooling to room temperature, pale pink crystals were obtained with a yield of 12%. Elemental analysis calculated: C 47.89, H 5.17, N 10.35%; found: C 47.87, H 5.21, N 10.33%.

Refinement

H atoms bound to C atoms were placed geometrically and refined as riding with C—H= 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of the water molecules were located from difference Fourier maps and were refined with distance restraints of O—H = 0.82 (1) Å and H···H = 1.35 (2) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$. The $[Mn(C_{10}H_8N_2)_2(H_2O)_4]^{2+}$ cations exhibit non-crystallographic inversion symmetry. The refined Flack parameter (Flack, 1983) from 530 Freidel pairs is 0.39 (3).

Figures

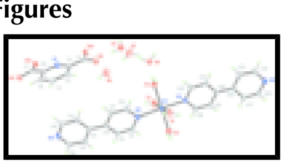


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids for non-H atoms.

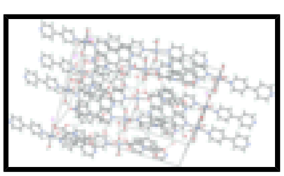


Fig. 2. Packing diagram showing hydrogen bonds as dashed lines.

Tetraaquabis(4,4'-bipyridine)manganese(II) pyridine-2,6-dicarboxylate tetrahydrate

Crystal data

$[Mn(C_{10}H_8N_2)_2(H_2O)_4](C_7H_3NO_4)\cdot 4H_2O$	F_{000} = 1412
M_r = 676.54	D_x = 1.434 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 3349 reflections
a = 18.407 (2) Å	θ = 1.6–25.2º
b = 6.8231 (10) Å	μ = 0.49 mm^{-1}
c = 25.2925 (10) Å	*T* = 293 (2) K
β = 99.40 (2)º	Cube, pink
V = 3133.9 (6) Å^3	0.15 × 0.15 × 0.15 mm
Z = 4	

Data collection

Bruker APEX II CCD diffractometer	3349 independent reflections
Radiation source: fine-focus sealed tube	2946 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
T = 293(2) K	θ_{max} = 25.2º
ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -19 \rightarrow 21$
T_{min} = 0.930, T_{max} = 0.930	$k = -8 \rightarrow 4$
5104 measured reflections	$l = -29 \rightarrow 12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.8622P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.091	$(\Delta/\sigma)_{max}$ < 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
3349 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
455 parameters	Extinction correction: none
26 restraints	Absolute structure: Flack (1983), 530 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.39 (3)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.82217 (6)	0.73736 (8)	0.62273 (5)	0.03257 (14)
C1	0.5731 (2)	0.1741 (6)	0.81919 (19)	0.0408 (10)
C2	0.5712 (5)	0.2656 (5)	0.8731 (3)	0.0358 (7)
C3	0.5691 (3)	0.4672 (5)	0.8799 (2)	0.0421 (10)
H3A	0.5680	0.5491	0.8504	0.050*
C4	0.5684 (2)	0.5490 (6)	0.93058 (18)	0.0434 (10)
H4A	0.5665	0.6844	0.9342	0.052*
C5	0.5706 (2)	0.4305 (6)	0.97556 (17)	0.0414 (9)
H5A	0.5704	0.4872	1.0090	0.050*
C6	0.5732 (3)	0.2276 (6)	0.9708 (2)	0.0363 (12)
C7	0.5791 (2)	0.0999 (5)	1.02024 (16)	0.0370 (8)
C8	0.8772 (3)	0.8253 (8)	0.74589 (18)	0.0497 (12)
H8A	0.9222	0.8122	0.7340	0.060*
C9	0.8771 (2)	0.8419 (7)	0.80050 (18)	0.0464 (11)
H9A	0.9216	0.8419	0.8240	0.056*
C10	0.8112 (2)	0.8586 (5)	0.82070 (16)	0.0301 (9)
C11	0.7466 (3)	0.8699 (8)	0.78146 (19)	0.0500 (12)
H11A	0.7010	0.8890	0.7919	0.060*
C12	0.7516 (3)	0.8527 (8)	0.72754 (19)	0.0520 (13)
H12A	0.7083	0.8591	0.7028	0.062*
C13	0.8082 (2)	0.8624 (5)	0.87922 (16)	0.0310 (9)
C14	0.8729 (3)	0.8650 (6)	0.91719 (16)	0.0396 (10)
H14A	0.9187	0.8655	0.9063	0.048*
C15	0.8674 (3)	0.8669 (6)	0.97181 (18)	0.0424 (11)
H15A	0.9108	0.8682	0.9965	0.051*
C16	0.7425 (3)	0.8638 (7)	0.95350 (18)	0.0474 (11)
H16A	0.6975	0.8623	0.9657	0.057*
C17	0.7411 (3)	0.8627 (6)	0.89898 (18)	0.0421 (10)
H17A	0.6965	0.8623	0.8756	0.051*
C18	0.8957 (2)	0.6419 (6)	0.51675 (17)	0.0412 (10)
H18A	0.9398	0.6410	0.5407	0.049*
C19	0.8986 (3)	0.6322 (7)	0.46217 (16)	0.0436 (11)
H19A	0.9437	0.6237	0.4503	0.052*

C20	0.8331 (2)	0.6353 (5)	0.42529 (16)	0.0309 (9)
C21	0.7675 (3)	0.6402 (7)	0.44593 (18)	0.0438 (11)
H21A	0.7225	0.6383	0.4230	0.053*
C22	0.7698 (3)	0.6477 (7)	0.50062 (19)	0.0473 (11)
H22A	0.7252	0.6496	0.5134	0.057*
C23	0.8328 (2)	0.6382 (5)	0.36570 (16)	0.0315 (9)
C24	0.7671 (3)	0.6310 (7)	0.32853 (19)	0.0495 (12)
H24A	0.7221	0.6229	0.3406	0.059*
C25	0.7691 (3)	0.6360 (7)	0.27403 (19)	0.0502 (12)
H25A	0.7247	0.6304	0.2505	0.060*
C26	0.8949 (3)	0.6552 (8)	0.2887 (2)	0.0598 (14)
H26A	0.9391	0.6630	0.2754	0.072*
C27	0.8980 (3)	0.6511 (7)	0.34413 (19)	0.0489 (12)
H27A	0.9432	0.6570	0.3667	0.059*
N1	0.5734 (2)	0.1475 (6)	0.91978 (18)	0.0500 (10)
N2	0.8152 (2)	0.8273 (5)	0.70905 (14)	0.0366 (8)
N3	0.8036 (2)	0.8668 (5)	0.99039 (14)	0.0402 (9)
N4	0.83172 (19)	0.6525 (5)	0.53679 (13)	0.0347 (8)
N5	0.8318 (2)	0.6486 (5)	0.25320 (15)	0.0449 (9)
O1	0.7849 (2)	1.0206 (4)	0.59321 (13)	0.0497 (8)
H11	0.760 (3)	1.104 (6)	0.6050 (19)	0.075*
H12	0.796 (3)	1.064 (7)	0.5654 (14)	0.075*
O2	0.93765 (18)	0.8415 (4)	0.63048 (14)	0.0485 (8)
H21	0.948 (3)	0.958 (2)	0.630 (2)	0.073*
H22	0.9748 (18)	0.785 (6)	0.645 (2)	0.073*
O3	0.8599 (2)	0.4530 (4)	0.65233 (13)	0.0515 (8)
H31	0.894 (2)	0.388 (7)	0.646 (2)	0.077*
H32	0.851 (3)	0.420 (8)	0.6814 (12)	0.077*
O4	0.70691 (17)	0.6294 (4)	0.61365 (13)	0.0436 (7)
H41	0.693 (2)	0.514 (2)	0.613 (2)	0.065*
H42	0.6709 (18)	0.694 (5)	0.600 (2)	0.065*
O5	0.4858 (3)	0.7285 (6)	0.6359 (2)	0.0613 (13)
H51	0.511 (3)	0.737 (9)	0.6122 (17)	0.092*
H52	0.514 (3)	0.722 (10)	0.6646 (12)	0.092*
O6	0.5642 (3)	0.6923 (6)	0.73882 (15)	0.0740 (10)
H61	0.566 (4)	0.769 (8)	0.7639 (18)	0.111*
H62	0.597 (3)	0.611 (8)	0.747 (3)	0.111*
O7	0.5641 (2)	0.1488 (5)	0.68155 (14)	0.0581 (10)
H71	0.571 (4)	0.179 (7)	0.7135 (7)	0.087*
H72	0.548 (3)	0.037 (4)	0.680 (2)	0.087*
O8	0.6591 (3)	0.2453 (4)	0.60733 (18)	0.0517 (12)
H81	0.638 (3)	0.222 (8)	0.6326 (14)	0.078*
H82	0.634 (3)	0.204 (8)	0.5802 (12)	0.078*
O9	0.5725 (3)	0.2894 (6)	0.77983 (15)	0.0566 (11)
O10	0.57394 (19)	−0.0066 (4)	0.81609 (12)	0.0498 (8)
O11	0.58120 (19)	0.1830 (5)	1.06520 (12)	0.0499 (8)
O12	0.58386 (18)	−0.0786 (4)	1.01351 (12)	0.0484 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0349 (2)	0.0397 (3)	0.0231 (2)	0.0010 (3)	0.00508 (16)	0.0010 (2)
C1	0.030 (2)	0.050 (2)	0.041 (2)	0.0043 (19)	0.0021 (18)	−0.001 (2)
C2	0.0228 (13)	0.0455 (16)	0.0374 (15)	0.002 (2)	0.0003 (11)	0.005 (2)
C3	0.0371 (18)	0.0439 (17)	0.043 (3)	0.002 (2)	−0.0005 (18)	0.0038 (19)
C4	0.042 (2)	0.0342 (19)	0.052 (3)	0.0047 (18)	0.0020 (19)	−0.0038 (18)
C5	0.038 (2)	0.044 (2)	0.040 (2)	0.0005 (18)	0.0026 (17)	−0.0120 (19)
C6	0.029 (2)	0.043 (2)	0.037 (3)	−0.0019 (18)	0.006 (2)	−0.0073 (18)
C7	0.0320 (19)	0.046 (2)	0.034 (2)	−0.0036 (17)	0.0075 (16)	−0.0073 (17)
C8	0.034 (3)	0.087 (3)	0.031 (2)	−0.004 (2)	0.011 (2)	−0.007 (2)
C9	0.026 (2)	0.081 (3)	0.029 (2)	−0.001 (2)	−0.001 (2)	−0.005 (2)
C10	0.033 (2)	0.0304 (17)	0.027 (2)	0.0008 (16)	0.0053 (18)	−0.0010 (15)
C11	0.032 (3)	0.081 (3)	0.040 (3)	0.008 (2)	0.012 (2)	−0.009 (2)
C12	0.041 (3)	0.082 (3)	0.031 (3)	0.014 (2)	0.001 (2)	−0.005 (2)
C13	0.036 (3)	0.0260 (16)	0.030 (2)	0.0016 (16)	0.0035 (19)	−0.0032 (15)
C14	0.038 (3)	0.059 (2)	0.023 (2)	0.000 (2)	0.007 (2)	−0.0020 (18)
C15	0.040 (3)	0.052 (2)	0.031 (2)	−0.004 (2)	−0.005 (2)	−0.0027 (18)
C16	0.046 (3)	0.060 (3)	0.039 (3)	0.003 (2)	0.016 (2)	0.001 (2)
C17	0.037 (3)	0.058 (2)	0.033 (2)	0.003 (2)	0.008 (2)	−0.0036 (19)
C18	0.033 (2)	0.061 (3)	0.028 (2)	0.009 (2)	−0.0001 (19)	−0.0049 (19)
C19	0.036 (3)	0.070 (3)	0.024 (2)	0.005 (2)	0.004 (2)	−0.004 (2)
C20	0.038 (2)	0.0291 (17)	0.025 (2)	0.0008 (16)	0.0048 (18)	−0.0019 (15)
C21	0.033 (3)	0.069 (3)	0.029 (2)	−0.007 (2)	0.003 (2)	−0.007 (2)
C22	0.035 (3)	0.074 (3)	0.033 (2)	−0.007 (2)	0.008 (2)	−0.007 (2)
C23	0.039 (2)	0.0308 (17)	0.027 (2)	0.0023 (17)	0.0116 (18)	−0.0018 (15)
C24	0.036 (3)	0.074 (3)	0.039 (3)	0.003 (2)	0.008 (2)	0.001 (2)
C25	0.050 (3)	0.070 (3)	0.031 (3)	0.003 (2)	0.008 (2)	0.000 (2)
C26	0.057 (3)	0.091 (4)	0.036 (3)	−0.007 (3)	0.022 (3)	−0.008 (3)
C27	0.037 (3)	0.074 (3)	0.036 (3)	−0.004 (2)	0.007 (2)	−0.005 (2)
N1	0.039 (2)	0.058 (2)	0.052 (2)	0.0024 (19)	0.0071 (18)	−0.0018 (19)
N2	0.038 (2)	0.0420 (18)	0.030 (2)	0.0026 (16)	0.0047 (16)	−0.0013 (15)
N3	0.053 (2)	0.0439 (18)	0.0256 (19)	0.0023 (16)	0.0104 (17)	−0.0004 (15)
N4	0.037 (2)	0.0417 (19)	0.0257 (19)	−0.0023 (15)	0.0047 (16)	−0.0021 (15)
N5	0.058 (3)	0.0468 (19)	0.031 (2)	−0.0045 (18)	0.0106 (18)	−0.0048 (16)
O1	0.067 (2)	0.0500 (17)	0.0366 (18)	0.0176 (16)	0.0209 (16)	0.0105 (14)
O2	0.0414 (19)	0.0535 (16)	0.050 (2)	−0.0056 (15)	0.0066 (16)	−0.0030 (15)
O3	0.075 (3)	0.0473 (16)	0.0361 (17)	0.0218 (16)	0.0209 (17)	0.0117 (14)
O4	0.0395 (19)	0.0456 (15)	0.0449 (18)	−0.0041 (13)	0.0041 (15)	0.0012 (14)
O5	0.059 (3)	0.068 (2)	0.062 (3)	0.0074 (19)	0.026 (3)	0.0148 (19)
O6	0.088 (3)	0.084 (3)	0.050 (2)	−0.005 (2)	0.0095 (19)	−0.011 (2)
O7	0.074 (3)	0.053 (2)	0.048 (2)	−0.0077 (18)	0.015 (2)	−0.0040 (16)
O8	0.054 (3)	0.055 (2)	0.047 (3)	−0.0064 (15)	0.012 (2)	−0.0069 (15)
O9	0.072 (3)	0.0643 (19)	0.033 (2)	0.007 (2)	0.0086 (19)	0.0020 (18)
O10	0.061 (2)	0.0491 (17)	0.0388 (16)	0.0013 (15)	0.0053 (14)	−0.0098 (14)
O11	0.056 (2)	0.0596 (18)	0.0355 (18)	−0.0070 (16)	0.0117 (15)	−0.0124 (15)

O12	0.0629 (19)	0.0427 (15)	0.0390 (16)	0.0005 (15)	0.0065 (14)	0.0000 (13)

Geometric parameters (Å, °)

Mn1—O1	2.144 (3)	C16—H16A	0.930
Mn1—O3	2.153 (3)	C17—H17A	0.930
Mn1—O2	2.219 (4)	C18—N4	1.357 (6)
Mn1—O4	2.222 (3)	C18—C19	1.392 (6)
Mn1—N4	2.284 (4)	C18—H18A	0.930
Mn1—N2	2.291 (4)	C19—C20	1.399 (6)
C1—O10	1.236 (5)	C19—H19A	0.930
C1—O9	1.267 (6)	C20—C21	1.392 (6)
C1—C2	1.504 (9)	C20—C23	1.506 (5)
C2—C3	1.388 (5)	C21—C22	1.378 (6)
C2—N1	1.425 (8)	C21—H21A	0.930
C3—C4	1.400 (7)	C22—N4	1.340 (6)
C3—H3A	0.930	C22—H22A	0.930
C4—C5	1.391 (6)	C23—C27	1.399 (7)
C4—H4A	0.930	C23—C24	1.407 (7)
C5—C6	1.391 (5)	C24—C25	1.385 (7)
C5—H5A	0.930	C24—H24A	0.930
C6—N1	1.402 (6)	C25—N5	1.349 (7)
C6—C7	1.514 (6)	C25—H25A	0.930
C7—O12	1.235 (4)	C26—N5	1.347 (7)
C7—O11	1.265 (5)	C26—C27	1.395 (7)
C8—N2	1.350 (6)	C26—H26A	0.930
C8—C9	1.386 (6)	C27—H27A	0.930
C8—H8A	0.930	O1—H11	0.82 (1)
C9—C10	1.396 (6)	O1—H12	0.82 (1)
C9—H9A	0.930	O2—H21	0.82 (1)
C10—C11	1.421 (6)	O2—H22	0.82 (1)
C10—C13	1.490 (5)	O3—H31	0.82 (1)
C11—C12	1.387 (7)	O3—H32	0.81 (1)
C11—H11A	0.930	O4—H41	0.83 (1)
C12—N2	1.341 (6)	O4—H42	0.82 (1)
C12—H12A	0.930	O5—H51	0.82 (1)
C13—C14	1.402 (6)	O5—H52	0.82 (1)
C13—C17	1.406 (6)	O6—H61	0.82 (1)
C14—C15	1.401 (6)	O6—H62	0.82 (1)
C14—H14A	0.930	O7—H71	0.82 (1)
C15—N3	1.334 (7)	O7—H72	0.82 (1)
C15—H15A	0.930	O8—H81	0.82 (1)
C16—N3	1.340 (6)	O8—H82	0.82 (1)
C16—C17	1.375 (6)		
O1—Mn1—O3	179.8 (2)	N3—C16—H16A	117.5
O1—Mn1—O2	89.39 (13)	C17—C16—H16A	117.5
O3—Mn1—O2	90.46 (15)	C16—C17—C13	118.9 (4)
O1—Mn1—O4	90.98 (14)	C16—C17—H17A	120.6
O3—Mn1—O4	89.17 (14)	C13—C17—H17A	120.6

O2—Mn1—O4	178.88 (16)	N4—C18—C19	123.3 (4)
O1—Mn1—N4	88.12 (13)	N4—C18—H18A	118.4
O3—Mn1—N4	91.82 (12)	C19—C18—H18A	118.4
O2—Mn1—N4	86.78 (14)	C18—C19—C20	119.5 (4)
O4—Mn1—N4	92.18 (14)	C18—C19—H19A	120.3
O1—Mn1—N2	91.49 (13)	C20—C19—H19A	120.3
O3—Mn1—N2	88.57 (13)	C21—C20—C19	117.1 (4)
O2—Mn1—N2	91.84 (14)	C21—C20—C23	120.9 (4)
O4—Mn1—N2	89.20 (14)	C19—C20—C23	121.9 (4)
N4—Mn1—N2	178.57 (17)	C22—C21—C20	119.4 (4)
O10—C1—O9	124.6 (5)	C22—C21—H21A	120.3
O10—C1—C2	118.3 (4)	C20—C21—H21A	120.3
O9—C1—C2	117.1 (4)	N4—C22—C21	124.8 (5)
C3—C2—N1	117.0 (6)	N4—C22—H22A	117.6
C3—C2—C1	122.0 (6)	C21—C22—H22A	117.6
N1—C2—C1	121.0 (3)	C27—C23—C24	116.1 (4)
C2—C3—C4	120.9 (5)	C27—C23—C20	121.9 (4)
C2—C3—H3A	119.5	C24—C23—C20	122.0 (4)
C4—C3—H3A	119.5	C25—C24—C23	120.3 (5)
C5—C4—C3	120.9 (4)	C25—C24—H24A	119.9
C5—C4—H4A	119.5	C23—C24—H24A	119.9
C3—C4—H4A	119.5	N5—C25—C24	123.6 (5)
C4—C5—C6	120.3 (4)	N5—C25—H25A	118.2
C4—C5—H5A	119.9	C24—C25—H25A	118.2
C6—C5—H5A	119.9	N5—C26—C27	123.9 (5)
C5—C6—N1	118.3 (4)	N5—C26—H26A	118.1
C5—C6—C7	120.0 (4)	C27—C26—H26A	118.1
N1—C6—C7	121.7 (3)	C26—C27—C23	119.8 (5)
O12—C7—O11	125.0 (4)	C26—C27—H27A	120.1
O12—C7—C6	116.8 (3)	C23—C27—H27A	120.1
O11—C7—C6	118.2 (4)	C6—N1—C2	122.6 (4)
N2—C8—C9	123.3 (4)	C12—N2—C8	116.6 (4)
N2—C8—H8A	118.4	C12—N2—Mn1	123.7 (3)
C9—C8—H8A	118.4	C8—N2—Mn1	118.8 (3)
C8—C9—C10	120.9 (4)	C15—N3—C16	116.3 (4)
C8—C9—H9A	119.5	C22—N4—C18	115.9 (4)
C10—C9—H9A	119.5	C22—N4—Mn1	117.8 (3)
C9—C10—C11	115.3 (4)	C18—N4—Mn1	125.1 (3)
C9—C10—C13	122.7 (4)	C26—N5—C25	116.3 (4)
C11—C10—C13	122.0 (4)	Mn1—O1—H11	132 (3)
C12—C11—C10	120.0 (4)	Mn1—O1—H12	121 (3)
C12—C11—H11A	120.0	H11—O1—H12	107 (2)
C10—C11—H11A	120.0	Mn1—O2—H21	122 (3)
N2—C12—C11	123.8 (4)	Mn1—O2—H22	127 (4)
N2—C12—H12A	118.1	H21—O2—H22	107 (2)
C11—C12—H12A	118.1	Mn1—O3—H31	130 (4)
C14—C13—C17	116.9 (4)	Mn1—O3—H32	117 (3)
C14—C13—C10	121.0 (4)	H31—O3—H32	109 (2)
C17—C13—C10	122.0 (4)	Mn1—O4—H41	127 (3)

C15—C14—C13	119.1 (4)	Mn1—O4—H42	124 (3)
C15—C14—H14A	120.5	H41—O4—H42	103 (2)
C13—C14—H14A	120.5	H51—O5—H52	107 (2)
N3—C15—C14	123.8 (4)	H61—O6—H62	107 (2)
N3—C15—H15A	118.1	H71—O7—H72	107 (2)
C14—C15—H15A	118.1	H81—O8—H82	108 (2)
N3—C16—C17	125.0 (5)		

O10—C1—C2—C3	−179.0 (6)	C19—C20—C23—C24	176.6 (4)
O9—C1—C2—C3	−0.1 (10)	C27—C23—C24—C25	0.3 (7)
O10—C1—C2—N1	2.4 (10)	C20—C23—C24—C25	179.4 (4)
O9—C1—C2—N1	−178.6 (5)	C23—C24—C25—N5	−0.3 (8)
N1—C2—C3—C4	−0.5 (10)	N5—C26—C27—C23	0.4 (8)
C1—C2—C3—C4	−179.1 (5)	C24—C23—C27—C26	−0.3 (7)
C2—C3—C4—C5	0.6 (8)	C20—C23—C27—C26	−179.4 (4)
C3—C4—C5—C6	−0.3 (7)	C5—C6—N1—C2	0.2 (8)
C4—C5—C6—N1	−0.1 (7)	C7—C6—N1—C2	−177.1 (5)
C4—C5—C6—C7	177.2 (4)	C3—C2—N1—C6	0.1 (10)
C5—C6—C7—O12	−177.5 (4)	C1—C2—N1—C6	178.7 (5)
N1—C6—C7—O12	−0.3 (6)	C11—C12—N2—C8	−2.2 (7)
C5—C6—C7—O11	0.4 (7)	C11—C12—N2—Mn1	167.2 (4)
N1—C6—C7—O11	177.6 (4)	C9—C8—N2—C12	2.1 (7)
N2—C8—C9—C10	1.1 (8)	C9—C8—N2—Mn1	−167.9 (4)
C8—C9—C10—C11	−3.9 (7)	O1—Mn1—N2—C12	72.0 (4)
C8—C9—C10—C13	175.5 (4)	O3—Mn1—N2—C12	−108.2 (4)
C9—C10—C11—C12	3.8 (7)	O2—Mn1—N2—C12	161.4 (4)
C13—C10—C11—C12	−175.7 (4)	O4—Mn1—N2—C12	−19.0 (4)
C10—C11—C12—N2	−0.8 (8)	O1—Mn1—N2—C8	−118.9 (4)
C9—C10—C13—C14	5.2 (6)	O3—Mn1—N2—C8	61.0 (4)
C11—C10—C13—C14	−175.4 (4)	O2—Mn1—N2—C8	−29.4 (4)
C9—C10—C13—C17	−174.6 (4)	O4—Mn1—N2—C8	150.2 (4)
C11—C10—C13—C17	4.8 (6)	C14—C15—N3—C16	0.3 (6)
C17—C13—C14—C15	0.3 (6)	C17—C16—N3—C15	−0.7 (7)
C10—C13—C14—C15	−179.5 (4)	C21—C22—N4—C18	−2.4 (7)
C13—C14—C15—N3	−0.2 (7)	C21—C22—N4—Mn1	165.7 (4)
N3—C16—C17—C13	0.8 (7)	C19—C18—N4—C22	1.8 (6)
C14—C13—C17—C16	−0.6 (6)	C19—C18—N4—Mn1	−165.4 (3)
C10—C13—C17—C16	179.2 (4)	O1—Mn1—N4—C22	−63.9 (3)
N4—C18—C19—C20	0.7 (7)	O3—Mn1—N4—C22	116.2 (3)
C18—C19—C20—C21	−2.5 (6)	O2—Mn1—N4—C22	−153.4 (3)
C18—C19—C20—C23	176.0 (4)	O4—Mn1—N4—C22	27.0 (3)
C19—C20—C21—C22	2.0 (6)	O1—Mn1—N4—C18	103.0 (3)
C23—C20—C21—C22	−176.6 (4)	O3—Mn1—N4—C18	−76.8 (3)
C20—C21—C22—N4	0.6 (7)	O2—Mn1—N4—C18	13.6 (3)
C21—C20—C23—C27	174.2 (4)	O4—Mn1—N4—C18	−166.0 (3)
C19—C20—C23—C27	−4.3 (6)	C27—C26—N5—C25	−0.4 (8)
C21—C20—C23—C24	−4.9 (6)	C24—C25—N5—C26	0.4 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···O8^{i}	0.82 (1)	2.10 (3)	2.848 (6)	152 (6)
O1—H12···N3^{ii}	0.82 (1)	1.98 (2)	2.787 (5)	167 (6)
O2—H21···O5^{iii}	0.82 (1)	1.97 (1)	2.781 (5)	171 (5)
O2—H22···O7^{iii}	0.82 (1)	1.98 (1)	2.799 (5)	179 (7)
O3—H31···O5^{iv}	0.82 (1)	2.05 (1)	2.864 (6)	175 (6)
O3—H32···N5^{v}	0.81 (1)	1.96 (1)	2.772 (5)	177 (7)
O4—H41···O8	0.83 (1)	1.93 (1)	2.760 (4)	177 (5)
O4—H42···O11^{vi}	0.82 (1)	1.93 (1)	2.751 (4)	173 (5)
O5—H52···O6	0.82 (1)	1.96 (2)	2.773 (7)	169 (6)
O5—H51···O11^{vi}	0.82 (1)	1.97 (2)	2.770 (6)	165 (6)
O6—H62···O9	0.82 (1)	2.41 (7)	2.933 (6)	123 (7)
O6—H61···O10^{i}	0.82 (1)	2.01 (2)	2.821 (5)	169 (7)
O7—H72···O5^{vii}	0.82 (1)	2.56 (2)	3.330 (6)	158 (5)
O7—H71···O9	0.82 (1)	1.84 (2)	2.645 (5)	168 (6)
O8—H81···O7	0.82 (1)	2.04 (2)	2.844 (6)	166 (6)
O8—H82···O12^{viii}	0.82 (1)	1.98 (1)	2.787 (5)	172 (6)

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

Fig. 1

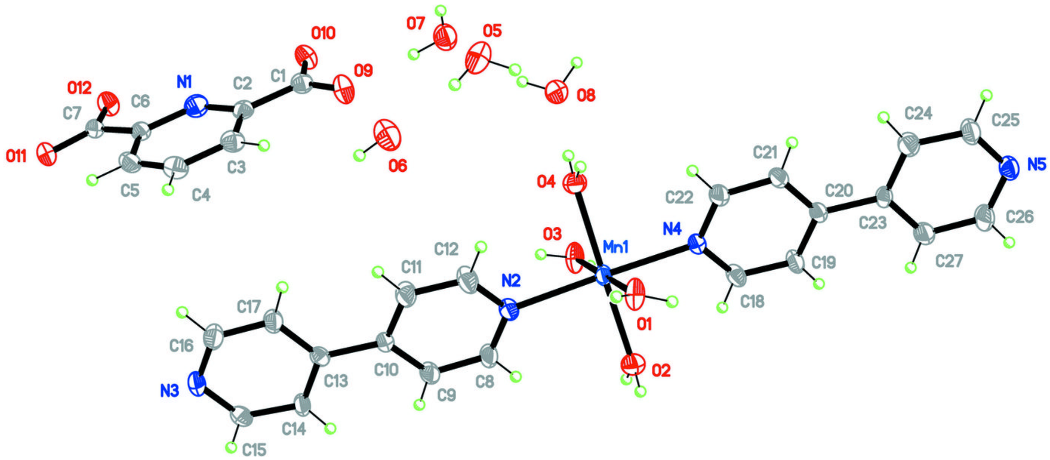

O10
O9
C1
C2
N1
C6
O12
C7
O11
C5
C4
C3
O6
O7
O5
O8
C24
C25
N5
C21
C20
C23
C26
C22
C27
C19
C18
N4
O4
O3
Mn1
O1
O2
N2
C12
C11
C10
C9
C8
C17
C16
N3
C13
C14
C15

Fig. 2