Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[aqua(4,4′-bipyridine-κN)-manganese(II)]-μ-imidazole-4,5-dicarboxylato-$\kappa^4N^3,O^4:O^{4'},O^5$]

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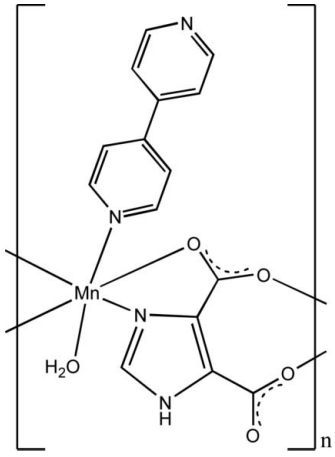
Received 29 October 2007; accepted 29 October 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.074; data-to-parameter ratio = 15.7.

In the crystal structure of the title compound, $[Mn(C_5H_2N_2O_4)(C_{10}H_8N_2)(H_2O)]_n$, the Mn atom is coordinated by three O atoms, two N atoms and one water molecule in a distorted octahedral geometry. Mn atoms are connected *via* the imidazole-4,5-dicarboxylate anions into chains, which are further connected by intermolecular N—H···O, O—H···N and O—H···O hydrogen bonding.

Related literature

For general background, see: Wang *et al.* (2005). For related structures, see: Hao *et al.* (2005).



Experimental

Crystal data

$[Mn(C_5H_2N_2O_4)(C_{10}H_8N_2)(H_2O)]$
M_r = 383.23
Monoclinic, $P2_1/c$
a = 14.051 (3) Å
b = 8.2084 (16) Å
c = 13.979 (3) Å
β = 103.80 (3)°
V = 1565.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 298 (2) K
0.24 × 0.18 × 0.17 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.817, T_{max} = 0.865
14768 measured reflections
3585 independent reflections
3170 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.08
3585 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.86	1.99	2.8002 (17)	156
N2—H2A···O2^{i}	0.86	2.65	3.2305 (18)	126
O1W—H1···N4^{ii}	0.85	1.91	2.7513 (19)	173
O1W—H2···O4^{iii}	0.85	1.85	2.6972 (17)	171

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

This work was financially supported by the National Natural Science Foundation of China (No. 20701006), the Foundation for Excellent Youth of Jilin, China (Grant No. 20070103), and the Science Foundation for Young Teachers of Northeast Normal University (No. 20070303).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2070).

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  doi:10.1107/S1600536807054141

supplementary materials

Acta Cryst. (2007). E**63**, m2876 [**doi:10.1107/S1600536807054141**]

catena-Poly[[aqua(4,4'-bipyridine-κ*N*)manganese(II)]-μ-imidazole-4,5-dicarboxylato-$\kappa^4N^3,O^4:O^{4'},O^5$]

C. Qin and E.-B. Wang

Comment

Investigations on metal carboxylate coordination polymers have become of increasing interest in the past few years Wang *et al.* 2005; Hao *et al.* 2005). As a part of our ongoing investigations in this field we report here the crystal structure of the title compound. In the crystal structure of the title compound the Mn atoms are coordinated by one oxygen atom of a water molecule, one nitrogen atom of a 4,4'-bipyridine ligand, one N and one O atom of an imidazole-4,5-dicarboxylate anion and one carboxylate group of a symmetry related imidazole-4,5-dicarboxylate anion within a distorted octahedral coordination geometry (Figure 1). The manganese atoms are linked by the anions into chains that elongate in the direction of the crystallographic *b* axis. These chains are further connected by N—H···O, O—H···N and O—H···O hydrogen bonding into a three-dimensional network (Tab. 1).

Experimental

A mixture of $MnCl_2$ (0.5 mmol), imidazole-4,5-dicarboxylic acid (0.5 mmol), 4,4'-bipyridine (0.8 mmol), and water (10 ml) was stirred for 20 min and then transferred into a 23 ml Teflon reactor. The reactor was kept at 433 K for 120 h under autogenous pressure. Single crystals of (I) were obtained after cooling to room temperature.

Refinement

H atoms were placed in calculated positions with C—H = 0.93 Å and N—H = 0.86 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,*N*). The H atoms of the water molecule were located in difference map, their bond lengths were set to 0.85 Å and afterwards they were refined using a riding model with U_{iso}(H) = 1.5U_{eq}(O).

Figures

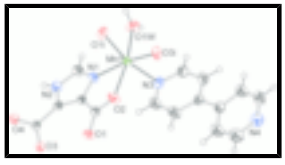

Fig. 1. Crystal structure of (I) with labeling and displacement ellipsoids drawn at the 50% probability level.

catena-Poly[[aqua(4,4'-bipyridine-κ*N*)manganese(II)]-μ-imidazole-4,5- dicarboxylato-$\kappa^4N^3,O^4:O^{4'},O^5$]

Crystal data

$[Mn(C_5H_2N_2O_4)(C_{10}H_8N_2)(H_2O_1)]$	F_{000} = 780
M_r = 383.23	D_x = 1.626 Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 14768 reflections
$a = 14.051$ (3) Å	$\theta = 3.0$–27.5º
$b = 8.2084$ (16) Å	$\mu = 0.88$ mm^{-1}
$c = 13.979$ (3) Å	$T = 298$ (2) K
$\beta = 103.80$ (3)º	Block, colorless
$V = 1565.8$ (5) Å^3	0.24 × 0.18 × 0.17 mm
$Z = 4$	

Data collection

Bruker APEX CCD area-detector diffractometer	3585 independent reflections
Radiation source: fine-focus sealed tube	3170 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 298$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -18 \rightarrow 18$
$T_{min} = 0.817$, $T_{max} = 0.865$	$k = -10 \rightarrow 10$
14768 measured reflections	$l = -18 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	H-atom parameters constrained
$wR(F^2) = 0.074$	$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 0.4434P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
3585 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
228 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.655818 (15)	0.01342 (3)	0.319366 (15)	0.01988 (8)
C1	0.54650 (12)	0.1764 (2)	0.48789 (11)	0.0298 (3)
H1A	0.5925	0.1506	0.5456	0.036*
C2	0.47557 (10)	0.21157 (17)	0.33523 (10)	0.0205 (3)
C3	0.41124 (11)	0.26685 (17)	0.38842 (10)	0.0218 (3)
C4	0.47212 (10)	0.20023 (17)	0.22797 (10)	0.0211 (3)
C5	0.30854 (11)	0.33264 (18)	0.36474 (11)	0.0240 (3)
C6	0.84725 (13)	0.2004 (2)	0.31644 (14)	0.0353 (4)
H6A	0.8634	0.0935	0.3049	0.042*
C7	0.92054 (13)	0.3157 (2)	0.33212 (14)	0.0349 (4)
H7A	0.9844	0.2855	0.3322	0.042*
C8	0.89897 (12)	0.47683 (18)	0.34779 (12)	0.0280 (3)
C9	0.80176 (14)	0.5129 (2)	0.34472 (18)	0.0451 (5)
H9A	0.7829	0.6197	0.3523	0.054*
C10	0.73332 (13)	0.3891 (2)	0.33030 (17)	0.0432 (5)
H10A	0.6689	0.4156	0.3299	0.052*
C11	1.14620 (13)	0.6796 (2)	0.42065 (14)	0.0407 (4)
H11A	1.2117	0.6482	0.4351	0.049*
C12	1.07570 (13)	0.5603 (2)	0.39433 (14)	0.0383 (4)
H12A	1.0941	0.4518	0.3922	0.046*
C13	0.97745 (12)	0.60229 (19)	0.37104 (12)	0.0292 (3)
C14	0.95562 (14)	0.7667 (2)	0.37459 (17)	0.0446 (5)
H14A	0.8909	0.8023	0.3585	0.054*
C15	1.03154 (15)	0.8763 (2)	0.40235 (17)	0.0497 (5)
H15A	1.0156	0.9860	0.4043	0.060*
N1	0.55941 (9)	0.15294 (16)	0.39850 (9)	0.0250 (3)
N2	0.45860 (10)	0.24189 (17)	0.48485 (9)	0.0277 (3)
H2A	0.4357	0.2645	0.5351	0.033*
N3	0.75455 (10)	0.23313 (16)	0.31690 (10)	0.0302 (3)
N4	1.12591 (11)	0.83635 (19)	0.42656 (12)	0.0411 (4)
O1	0.40748 (8)	0.27583 (13)	0.16630 (7)	0.0267 (2)
O2	0.53640 (9)	0.11390 (15)	0.20466 (7)	0.0329 (3)
O3	0.27564 (8)	0.39872 (14)	0.28237 (8)	0.0289 (2)
O4	0.26300 (9)	0.31810 (17)	0.43017 (9)	0.0432 (3)
O1W	0.75594 (8)	−0.06111 (14)	0.45556 (8)	0.0335 (3)
H1	0.7967	0.0042	0.4908	0.050*
H2	0.7548	−0.1473	0.4890	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.01936 (12)	0.02130 (12)	0.01915 (11)	0.00103 (8)	0.00493 (8)	−0.00106 (8)
C1	0.0283 (8)	0.0426 (9)	0.0173 (6)	0.0069 (7)	0.0032 (6)	0.0028 (6)
C2	0.0214 (7)	0.0234 (6)	0.0165 (6)	0.0028 (5)	0.0045 (5)	0.0016 (5)

C3	0.0250 (7)	0.0238 (7)	0.0175 (6)	0.0029 (6)	0.0071 (5)	0.0026 (5)
C4	0.0232 (7)	0.0232 (6)	0.0172 (6)	0.0005 (6)	0.0054 (5)	−0.0007 (5)
C5	0.0251 (7)	0.0238 (7)	0.0258 (7)	0.0045 (6)	0.0115 (6)	0.0046 (6)
C6	0.0365 (9)	0.0250 (7)	0.0482 (10)	−0.0016 (7)	0.0178 (8)	−0.0051 (7)
C7	0.0284 (8)	0.0289 (8)	0.0512 (10)	−0.0011 (7)	0.0171 (7)	−0.0053 (7)
C8	0.0280 (8)	0.0244 (7)	0.0313 (8)	−0.0023 (6)	0.0066 (6)	0.0003 (6)
C9	0.0313 (9)	0.0234 (8)	0.0796 (15)	0.0017 (7)	0.0110 (9)	−0.0024 (8)
C10	0.0252 (8)	0.0297 (8)	0.0738 (13)	0.0008 (7)	0.0100 (8)	−0.0002 (9)
C11	0.0272 (8)	0.0425 (10)	0.0492 (10)	−0.0043 (7)	0.0030 (8)	−0.0037 (8)
C12	0.0318 (9)	0.0300 (8)	0.0515 (10)	−0.0002 (7)	0.0068 (8)	−0.0035 (8)
C13	0.0291 (8)	0.0259 (7)	0.0318 (8)	−0.0026 (6)	0.0061 (6)	−0.0022 (6)
C14	0.0314 (9)	0.0280 (8)	0.0699 (13)	−0.0004 (7)	0.0030 (9)	−0.0051 (9)
C15	0.0438 (11)	0.0262 (8)	0.0734 (14)	−0.0043 (8)	0.0023 (10)	−0.0076 (9)
N1	0.0230 (6)	0.0341 (7)	0.0177 (5)	0.0055 (5)	0.0043 (5)	0.0017 (5)
N2	0.0314 (7)	0.0376 (7)	0.0157 (5)	0.0069 (6)	0.0087 (5)	0.0009 (5)
N3	0.0291 (7)	0.0265 (6)	0.0355 (7)	−0.0035 (5)	0.0084 (6)	0.0009 (6)
N4	0.0371 (8)	0.0382 (8)	0.0434 (8)	−0.0112 (7)	0.0003 (7)	−0.0048 (7)
O1	0.0304 (6)	0.0332 (6)	0.0159 (4)	0.0109 (5)	0.0044 (4)	0.0028 (4)
O2	0.0347 (6)	0.0458 (7)	0.0185 (5)	0.0190 (5)	0.0069 (4)	0.0000 (5)
O3	0.0235 (5)	0.0364 (6)	0.0282 (5)	0.0051 (5)	0.0090 (4)	0.0116 (5)
O4	0.0412 (7)	0.0554 (8)	0.0424 (7)	0.0229 (6)	0.0284 (6)	0.0240 (6)
O1W	0.0351 (6)	0.0305 (6)	0.0281 (5)	−0.0091 (5)	−0.0060 (5)	0.0048 (5)

Geometric parameters (Å, °)

Mn1—O3^{i}	2.1190 (11)	C7—H7A	0.9300
Mn1—O1W	2.1680 (13)	C8—C9	1.388 (2)
Mn1—O1^{i}	2.1725 (11)	C8—C13	1.487 (2)
Mn1—O2	2.1870 (13)	C9—C10	1.380 (3)
Mn1—N1	2.2550 (13)	C9—H9A	0.9300
Mn1—N3	2.2805 (14)	C10—N3	1.338 (2)
C1—N1	1.3190 (19)	C10—H10A	0.9300
C1—N2	1.338 (2)	C11—N4	1.325 (3)
C1—H1A	0.9300	C11—C12	1.379 (3)
C2—C3	1.3772 (19)	C11—H11A	0.9300
C2—N1	1.3800 (18)	C12—C13	1.384 (2)
C2—C4	1.4915 (18)	C12—H12A	0.9300
C3—N2	1.3689 (18)	C13—C14	1.387 (2)
C3—C5	1.502 (2)	C14—C15	1.379 (3)
C4—O2	1.2509 (18)	C14—H14A	0.9300
C4—O1	1.2567 (18)	C15—N4	1.329 (3)
C5—O4	1.2409 (18)	C15—H15A	0.9300
C5—O3	1.2569 (18)	N2—H2A	0.8600
C6—N3	1.331 (2)	O1—Mn1^{ii}	2.1725 (11)
C6—C7	1.377 (2)	O3—Mn1^{ii}	2.1190 (11)
C6—H6A	0.9300	O1W—H1	0.8499
C7—C8	1.386 (2)	O1W—H2	0.8500
O3^{i}—Mn1—O1W	99.23 (5)	C9—C8—C13	122.15 (15)

O3^{i}—Mn1—O1^{i}	85.68 (4)	C10—C9—C8	119.60 (16)
O1W—Mn1—O1^{i}	81.94 (4)	C10—C9—H9A	120.2
O3^{i}—Mn1—O2	93.87 (4)	C8—C9—H9A	120.2
O1W—Mn1—O2	166.88 (5)	N3—C10—C9	123.64 (17)
O1^{i}—Mn1—O2	98.44 (5)	N3—C10—H10A	118.2
O3^{i}—Mn1—N1	167.76 (4)	C9—C10—H10A	118.2
O1W—Mn1—N1	93.00 (5)	N4—C11—C12	123.70 (17)
O1^{i}—Mn1—N1	95.95 (5)	N4—C11—H11A	118.2
O2—Mn1—N1	73.89 (4)	C12—C11—H11A	118.2
O3^{i}—Mn1—N3	88.03 (5)	C11—C12—C13	119.90 (17)
O1W—Mn1—N3	88.10 (5)	C11—C12—H12A	120.0
O1^{i}—Mn1—N3	167.21 (5)	C13—C12—H12A	120.0
O2—Mn1—N3	93.08 (5)	C12—C13—C14	116.77 (16)
N1—Mn1—N3	92.56 (5)	C12—C13—C8	121.66 (15)
N1—C1—N2	111.28 (13)	C14—C13—C8	121.52 (15)
N1—C1—H1A	124.4	C15—C14—C13	118.82 (17)
N2—C1—H1A	124.4	C15—C14—H14A	120.6
C3—C2—N1	109.80 (12)	C13—C14—H14A	120.6
C3—C2—C4	134.05 (13)	N4—C15—C14	124.66 (18)
N1—C2—C4	116.14 (12)	N4—C15—H15A	117.7
N2—C3—C2	104.77 (12)	C14—C15—H15A	117.7
N2—C3—C5	119.12 (13)	C1—N1—C2	105.49 (12)
C2—C3—C5	136.00 (13)	C1—N1—Mn1	140.65 (11)
O2—C4—O1	123.34 (13)	C2—N1—Mn1	112.55 (9)
O2—C4—C2	116.41 (12)	C1—N2—C3	108.64 (12)
O1—C4—C2	120.24 (13)	C1—N2—H2A	125.7
O4—C5—O3	125.12 (14)	C3—N2—H2A	125.7
O4—C5—C3	116.12 (13)	C6—N3—C10	116.42 (14)
O3—C5—C3	118.76 (13)	C6—N3—Mn1	116.08 (11)
N3—C6—C7	123.76 (15)	C10—N3—Mn1	126.72 (12)
N3—C6—H6A	118.1	C11—N4—C15	116.11 (16)
C7—C6—H6A	118.1	C4—O1—Mn1^{ii}	128.66 (9)
C6—C7—C8	119.84 (16)	C4—O2—Mn1	119.87 (9)
C6—C7—H7A	120.1	C5—O3—Mn1^{ii}	132.84 (10)
C8—C7—H7A	120.1	Mn1—O1W—H1	122.5
C7—C8—C9	116.69 (15)	Mn1—O1W—H2	128.7
C7—C8—C13	121.11 (15)	H1—O1W—H2	107.7

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1^{iii}	0.86	1.99	2.8002 (17)	156
N2—H2A···O2^{iii}	0.86	2.65	3.2305 (18)	126
O1W—H1···N4^{iv}	0.85	1.91	2.7513 (19)	173
O1W—H2···O4^{v}	0.85	1.85	2.6972 (17)	171

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

Fig. 1