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A dinuclear manganese(II) complex with a 4-aminoantipyrine-derived Schiff base ligand

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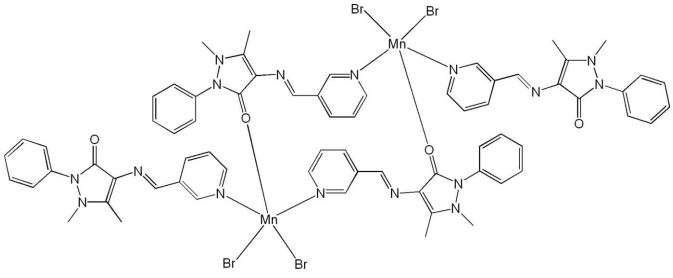
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.058; wR factor = 0.114; data-to-parameter ratio = 17.9.

In the crystal structure of the centrosymmetric title complex, bis[μ-(*E*)-1,5-dimethyl-2-phenyl-4-(3-pyridylmethyleneamino)pyrazol-3(2*H*)-one]bis{dibromido[(*E*)-1,5-dimethyl-2-phenyl-4-(3-pyridylmethyleneamino)pyrazol-3(2*H*)-one]manganese(II)}, $[Mn_2Br_4(C_{17}H_{16}N_4O)_4]$, the Mn atom adopts a trigonal–bipyramidal geometry and the ligand adopts two coordination modes, monodentate and bidentate bridging.

Related literature

For related literature, see: Liang *et al.* (2002, 2004); Montalvo-Gonzalez & Ariza-Castolo (2003); O'Donnell (2004); Rajendran & Sreeletha (2002); Raman *et al.* (2001); Wang *et al.* (2003).



Experimental

Crystal data

$[Mn_2Br_4(C_{17}H_{16}N_4O)_4]$
M_r = 1598.87
Triclinic, $P\overline{1}$
a = 10.052 (2) Å
b = 12.372 (3) Å
c = 15.257 (3) Å
α = 72.68 (3)°
β = 77.66 (3)°
γ = 71.09 (3)°
V = 1699.2 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.78 mm^{-1}
T = 298 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.555, T_{max} = 0.634
16756 measured reflections
7658 independent reflections
4058 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.114
S = 0.99
7658 reflections
428 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—Mn1	2.5441 (12)	Mn1—N5^{i}	2.341 (4)
Br2—Mn1	2.5387 (12)	Mn1—N1	2.360 (4)
Mn1—O2	2.080 (3)		
O2—Mn1—N5^{i}	87.27 (13)	N1—Mn1—Br2	93.63 (11)
O2—Mn1—N1	89.45 (14)	O2—Mn1—Br1	122.63 (10)
N5^{i}—Mn1—N1	171.60 (15)	N5^{i}—Mn1—Br1	86.76 (10)
O2—Mn1—Br2	109.22 (10)	N1—Mn1—Br1	88.51 (11)
N5^{i}—Mn1—Br2	94.75 (10)	Br2—Mn1—Br1	128.13 (4)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2058).

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supplementary materials

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A dinuclear manganese(II) complex with a 4-aminoantipyrine-derived Schiff base ligand

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Comment

Great effort is currently being devoted to the design and syntheses of metal Schiff base complexes due to their potential applications as functional materials (O'Donnell, 2004). The Schiff bases of 4-aminoantipyrine and their complexes have been extensively investigated because of their biological, clinical and pharmacological applications (Rajendran & Sreeletha, 2002; Raman *et al.*, 2001). However, only a few structurally characterized metal complexes with 4-aminoantipyrine Schiff base derived ligands have been reported, and its coordination chemistry remains largely unexplored (Liang *et al.*, 2004; Liang *et al.*, 2002; Wang *et al.*, 2003). Herein we report the synthesis and crystal structure of a new dinuclear manganese(II) complex with a 4-aminoantipyrine derived Schiff base ligand: $Mn_2(L_4)Br_4$ (*L* = (*E*)-1,5-dimethyl-2-phenyl-4-(pyridin-3-yl-methyleneamino)-1,2-dihydropyrazol-3-one) (**I**).

The ligand *L* was synthesized as reported previously by the base condensation of 4-aminoantipyrine with pyridine-3-carboxaldehyde (Montalvo-Gonzalez & Arisa-Castolo 2003). The title complex (**I**) was obtained under solvothermal conditions and characterized by X-ray crystallography. The molecular structure of (**I**) is shown in Fig. 1. Selected bond distances and bond angles are normal and listed in Table 1. (**I**) is a dinuclear Mn^{II} complex arranged around an inversion center. Each Mn atom is coordinated by two pyridine N atoms from two ligands, and one pyrazole O atom from another ligand, and two Br anions in a trigonal-bipyramidal geometry. There are two kinds of coordination modes of ligand *L*: one is monodentately linked to the Mn center through the N atom of the pyridine group, the other bidentately bridges two Mn centers by pyridine N atom and pyrazole O atom. The dimer Mn_2L_2 ring is formed with Mn···Mn separation of 8.878 (4) Å.

Experimental

A 25 ml Teflon-lined stainless steel autoclave was charged with 0.215 g (1 mmol) $MnBr_2$, 0.260 g (1 mmol) *L* and 15 ml CH_3OH and heated at 80 °C for 24 h in oven, then cooled to room temperature. Red crystals were obtained in 60% yield based on the initial $MnBr_2$.

Refinement

All H atoms on sp^2 C atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H = 0.93 and U_{iso}(H) = 1.2 U_{eq}(C); All H atoms on sp^3 C (Me groups) atoms were located and refined by using the hfix 137 command.

Figures

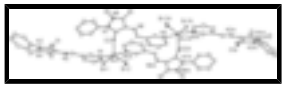


Fig. 1. The molecular structure of (**I**), with displacement ellipsoids drawn at the 30% probability level. H atoms were omitted for clarity. (Symmetry codes: (A) −*x* + 1, −*y* + 1, −*z* + 1.)

bis[μ-(*E*)-1,5-dimethyl-2-phenyl-4-(3-pyridylmethyleneamino)pyrazol-\ 3(2*H*)-one]bis{dibromido[(*E*)-1,5-dimethyl-2-phenyl-4-(3-\ pyridylmethyleneamino)pyrazol-3(2*H*)-one]manganese(II)}

Crystal data

$[Mn_2Br_4(C_{17}H_{16}N_4O)_4]$	V = 1699.2 (6) Å^3
M_r = 1598.87	Z = 1
Triclinic, $P\overline{1}$	F_{000} = 806
Hall symbol: -P 1	D_x = 1.563 Mg m^{-3}
a = 10.052 (2) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 12.372 (3) Å	θ = 3.1–27.5º
c = 15.257 (3) Å	μ = 2.78 mm^{-1}
α = 72.68 (3)º	T = 298 (2) K
β = 77.66 (3)º	Block, red
γ = 71.09 (3)º	0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX II CCD diffractometer	7658 independent reflections
Radiation source: fine-focus sealed tube	4058 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
Detector resolution: 8.40 pixels mm^{-1}	θ_{max} = 27.5º
T = 298(2) K	θ_{min} = 3.1º
ω scans	h = −13→12
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	k = −16→13
T_{min} = 0.555, T_{max} = 0.634	l = −19→19
16756 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: geom, Me from difmap
$R[F^2 > 2\sigma(F^2)]$ = 0.058	H-atom parameters constrained
$wR(F^2)$ = 0.114	$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 1.9264P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.001
7658 reflections	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
428 parameters	$\Delta\rho_{min}$ = −0.53 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.63805 (6)	0.05458 (5)	0.35815 (4)	0.04788 (16)
Br2	0.63104 (6)	0.44060 (5)	0.23134 (4)	0.05393 (18)
Mn1	0.51827 (8)	0.27528 (6)	0.31633 (5)	0.03622 (19)
C1	0.4160 (5)	0.1657 (5)	0.1809 (4)	0.0478 (14)
H1A	0.4031	0.1123	0.2373	0.057*
C2	0.3812 (5)	0.1489 (5)	0.1036 (3)	0.0441 (13)
C3	0.4052 (6)	0.2288 (5)	0.0195 (4)	0.0579 (16)
H3A	0.3857	0.2203	−0.0346	0.069*
C4	0.4569 (6)	0.3189 (5)	0.0165 (4)	0.0592 (16)
H4A	0.4725	0.3725	−0.0394	0.071*
C5	0.4861 (6)	0.3296 (5)	0.0976 (4)	0.0511 (14)
H5A	0.5204	0.3920	0.0951	0.061*
C6	0.3263 (5)	0.0506 (5)	0.1086 (4)	0.0503 (14)
H6A	0.3232	−0.0083	0.1631	0.060*
C7	0.2306 (5)	−0.0400 (5)	0.0312 (3)	0.0444 (13)
C8	0.2039 (6)	−0.1426 (5)	0.1000 (4)	0.0532 (15)
C9	0.1419 (7)	−0.1849 (6)	−0.1123 (4)	0.0653 (17)
H9A	0.1759	−0.1408	−0.1713	0.098*
H9B	0.0449	−0.1813	−0.1116	0.098*
H9C	0.1985	−0.2656	−0.1019	0.098*
C10	0.1982 (6)	−0.0416 (5)	−0.0504 (3)	0.0478 (14)
C11	0.2115 (7)	0.0452 (5)	−0.1417 (4)	0.0659 (17)
H11A	0.2774	0.0057	−0.1856	0.099*
H11B	0.2450	0.1061	−0.1346	0.099*
H11C	0.1205	0.0795	−0.1635	0.099*
C12	0.1099 (6)	−0.3036 (5)	0.0855 (3)	0.0456 (13)
C13	0.1934 (6)	−0.4053 (6)	0.1355 (4)	0.0611 (17)
H13A	0.2790	−0.4059	0.1498	0.073*
C14	0.1494 (7)	−0.5066 (6)	0.1643 (4)	0.0684 (19)
H14A	0.2055	−0.5752	0.1988	0.082*
C15	0.0245 (8)	−0.5076 (6)	0.1429 (4)	0.0716 (19)
H15A	−0.0033	−0.5766	0.1614	0.086*
C16	−0.0588 (7)	−0.4060 (5)	0.0940 (4)	0.0633 (17)

H16A	−0.1443	−0.4059	0.0798	0.076*
C17	−0.0176 (6)	−0.3035 (5)	0.0656 (4)	0.0537 (15)
H17A	−0.0757	−0.2345	0.0331	0.064*
C18	0.5023 (5)	0.7949 (4)	0.4609 (4)	0.0428 (13)
H18A	0.5413	0.8495	0.4687	0.051*
C19	0.5012 (6)	0.7883 (5)	0.3727 (4)	0.0475 (13)
H19A	0.5408	0.8370	0.3221	0.057*
C20	0.4414 (5)	0.7093 (4)	0.3593 (4)	0.0464 (13)
H20A	0.4409	0.7036	0.2999	0.056*
C21	0.3823 (5)	0.6389 (4)	0.4360 (3)	0.0379 (12)
C22	0.3906 (5)	0.6490 (4)	0.5229 (3)	0.0388 (12)
H22A	0.3535	0.6000	0.5746	0.047*
C23	0.3187 (5)	0.5523 (4)	0.4278 (4)	0.0415 (12)
H23A	0.3280	0.5357	0.3709	0.050*
C24	0.1985 (5)	0.4090 (4)	0.4968 (3)	0.0350 (11)
C25	0.2266 (5)	0.3429 (4)	0.4310 (3)	0.0342 (11)
C26	0.1086 (5)	0.3641 (4)	0.5703 (3)	0.0405 (12)
C27	0.0579 (6)	0.3964 (5)	0.6601 (4)	0.0620 (16)
H27A	−0.0420	0.4352	0.6639	0.093*
H27B	0.1074	0.4485	0.6650	0.093*
H27C	0.0755	0.3265	0.7098	0.093*
C28	0.0008 (6)	0.1944 (5)	0.6100 (4)	0.0629 (17)
H28A	0.0684	0.1202	0.6311	0.094*
H28B	−0.0619	0.1841	0.5757	0.094*
H28C	−0.0531	0.2236	0.6624	0.094*
C29	0.1161 (5)	0.1969 (4)	0.4157 (3)	0.0371 (11)
C30	0.2016 (5)	0.0863 (4)	0.4116 (4)	0.0475 (14)
H30A	0.2800	0.0520	0.4437	0.057*
C31	0.1695 (6)	0.0269 (5)	0.3593 (4)	0.0592 (16)
H31A	0.2277	−0.0476	0.3549	0.071*
C32	0.0524 (6)	0.0767 (5)	0.3135 (4)	0.0578 (16)
H32A	0.0318	0.0360	0.2781	0.069*
C33	−0.0341 (6)	0.1856 (5)	0.3195 (4)	0.0664 (18)
H33A	−0.1144	0.2184	0.2893	0.080*
C34	−0.0025 (6)	0.2472 (5)	0.3706 (4)	0.0548 (15)
H34A	−0.0606	0.3218	0.3745	0.066*
N1	0.4672 (4)	0.2542 (4)	0.1794 (3)	0.0422 (10)
N2	0.2830 (4)	0.0471 (4)	0.0375 (3)	0.0460 (11)
N3	0.1569 (5)	−0.2006 (4)	0.0520 (3)	0.0510 (12)
N4	0.1516 (5)	−0.1351 (4)	−0.0398 (3)	0.0498 (12)
N5	0.4485 (4)	0.7247 (3)	0.5364 (3)	0.0376 (10)
N6	0.2502 (4)	0.4994 (3)	0.4991 (3)	0.0408 (10)
N7	0.1511 (4)	0.2608 (3)	0.4669 (3)	0.0390 (10)
N8	0.0750 (4)	0.2783 (4)	0.5509 (3)	0.0434 (10)
O1	0.2122 (5)	−0.1777 (4)	0.1843 (3)	0.0763 (13)
O2	0.3029 (3)	0.3472 (3)	0.3532 (2)	0.0402 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0660 (4)	0.0392 (3)	0.0413 (3)	−0.0147 (3)	−0.0104 (3)	−0.0116 (2)
Br2	0.0723 (4)	0.0535 (3)	0.0454 (3)	−0.0370 (3)	−0.0010 (3)	−0.0092 (3)
Mn1	0.0430 (4)	0.0372 (4)	0.0343 (4)	−0.0177 (4)	−0.0038 (3)	−0.0111 (3)
C1	0.054 (3)	0.048 (3)	0.043 (3)	−0.015 (3)	−0.015 (3)	−0.008 (3)
C2	0.046 (3)	0.053 (3)	0.039 (3)	−0.013 (3)	−0.009 (3)	−0.018 (3)
C3	0.069 (4)	0.073 (4)	0.032 (3)	−0.022 (3)	−0.011 (3)	−0.009 (3)
C4	0.071 (4)	0.069 (4)	0.036 (3)	−0.027 (3)	−0.009 (3)	−0.002 (3)
C5	0.058 (4)	0.052 (3)	0.045 (3)	−0.021 (3)	−0.008 (3)	−0.006 (3)
C6	0.056 (3)	0.061 (4)	0.040 (3)	−0.015 (3)	−0.015 (3)	−0.017 (3)
C7	0.037 (3)	0.063 (4)	0.036 (3)	−0.011 (3)	−0.006 (2)	−0.020 (3)
C8	0.057 (4)	0.078 (4)	0.035 (3)	−0.023 (3)	−0.006 (3)	−0.023 (3)
C9	0.083 (4)	0.086 (5)	0.046 (4)	−0.039 (4)	−0.010 (3)	−0.027 (3)
C10	0.051 (3)	0.056 (3)	0.037 (3)	−0.008 (3)	−0.007 (3)	−0.020 (3)
C11	0.098 (5)	0.063 (4)	0.041 (3)	−0.023 (4)	−0.014 (3)	−0.016 (3)
C12	0.051 (3)	0.056 (3)	0.033 (3)	−0.016 (3)	−0.005 (3)	−0.014 (3)
C13	0.048 (3)	0.086 (5)	0.042 (3)	−0.002 (4)	−0.007 (3)	−0.022 (3)
C14	0.074 (5)	0.062 (4)	0.049 (4)	0.007 (4)	−0.009 (3)	−0.013 (3)
C15	0.096 (5)	0.054 (4)	0.062 (4)	−0.025 (4)	0.000 (4)	−0.014 (3)
C16	0.067 (4)	0.064 (4)	0.069 (4)	−0.024 (3)	−0.013 (3)	−0.022 (3)
C17	0.054 (3)	0.056 (4)	0.052 (3)	−0.010 (3)	−0.017 (3)	−0.012 (3)
C18	0.052 (3)	0.039 (3)	0.047 (3)	−0.019 (3)	−0.013 (3)	−0.013 (2)
C19	0.059 (3)	0.049 (3)	0.038 (3)	−0.022 (3)	−0.009 (3)	−0.006 (2)
C20	0.057 (3)	0.045 (3)	0.039 (3)	−0.013 (3)	−0.011 (3)	−0.011 (2)
C21	0.040 (3)	0.039 (3)	0.042 (3)	−0.013 (2)	−0.009 (2)	−0.015 (2)
C22	0.043 (3)	0.039 (3)	0.040 (3)	−0.015 (2)	−0.010 (2)	−0.012 (2)
C23	0.050 (3)	0.040 (3)	0.042 (3)	−0.015 (3)	−0.014 (3)	−0.014 (2)
C24	0.036 (3)	0.038 (3)	0.035 (3)	−0.013 (2)	−0.008 (2)	−0.011 (2)
C25	0.037 (3)	0.038 (3)	0.033 (3)	−0.014 (2)	−0.006 (2)	−0.011 (2)
C26	0.040 (3)	0.044 (3)	0.039 (3)	−0.012 (2)	−0.002 (2)	−0.016 (2)
C27	0.076 (4)	0.067 (4)	0.047 (3)	−0.021 (3)	0.004 (3)	−0.026 (3)
C28	0.059 (4)	0.061 (4)	0.062 (4)	−0.032 (3)	0.010 (3)	−0.002 (3)
C29	0.040 (3)	0.038 (3)	0.043 (3)	−0.020 (2)	−0.005 (2)	−0.013 (2)
C30	0.048 (3)	0.044 (3)	0.060 (4)	−0.013 (3)	−0.019 (3)	−0.019 (3)
C31	0.065 (4)	0.041 (3)	0.080 (4)	−0.016 (3)	−0.021 (4)	−0.017 (3)
C32	0.079 (4)	0.053 (4)	0.057 (4)	−0.034 (3)	−0.020 (3)	−0.012 (3)
C33	0.065 (4)	0.056 (4)	0.090 (5)	−0.019 (3)	−0.044 (4)	−0.010 (4)
C34	0.051 (3)	0.043 (3)	0.074 (4)	−0.008 (3)	−0.028 (3)	−0.013 (3)
N1	0.047 (3)	0.047 (2)	0.035 (2)	−0.013 (2)	−0.006 (2)	−0.014 (2)
N2	0.045 (3)	0.061 (3)	0.041 (3)	−0.014 (2)	−0.005 (2)	−0.026 (2)
N3	0.057 (3)	0.074 (3)	0.033 (2)	−0.028 (3)	−0.007 (2)	−0.017 (2)
N4	0.062 (3)	0.060 (3)	0.033 (2)	−0.011 (2)	−0.013 (2)	−0.021 (2)
N5	0.045 (2)	0.032 (2)	0.042 (2)	−0.0137 (19)	−0.012 (2)	−0.0093 (18)
N6	0.044 (2)	0.043 (2)	0.044 (3)	−0.016 (2)	−0.009 (2)	−0.017 (2)
N7	0.043 (2)	0.043 (2)	0.038 (2)	−0.017 (2)	−0.003 (2)	−0.0165 (19)

N8	0.051 (3)	0.050 (3)	0.035 (2)	−0.025 (2)	0.004 (2)	−0.012 (2)
O1	0.114 (4)	0.101 (3)	0.035 (2)	−0.056 (3)	−0.019 (2)	−0.013 (2)
O2	0.0418 (19)	0.054 (2)	0.0354 (19)	−0.0218 (17)	−0.0022 (16)	−0.0186 (16)

Geometric parameters (Å, °)

Br1—Mn1	2.5441 (12)	C17—H17A	0.9300
Br2—Mn1	2.5387 (12)	C18—N5	1.348 (6)
Mn1—O2	2.080 (3)	C18—C19	1.374 (7)
Mn1—N5^{i}	2.341 (4)	C18—H18A	0.9300
Mn1—N1	2.360 (4)	C19—C20	1.384 (7)
C1—N1	1.345 (6)	C19—H19A	0.9300
C1—C2	1.386 (7)	C20—C21	1.383 (7)
C1—H1A	0.9300	C20—H20A	0.9300
C2—C3	1.395 (7)	C21—C22	1.389 (6)
C2—C6	1.467 (7)	C21—C23	1.459 (6)
C3—C4	1.360 (8)	C22—N5	1.334 (6)
C3—H3A	0.9300	C22—H22A	0.9300
C4—C5	1.384 (7)	C23—N6	1.279 (6)
C4—H4A	0.9300	C23—H23A	0.9300
C5—N1	1.336 (6)	C24—C26	1.380 (7)
C5—H5A	0.9300	C24—N6	1.389 (6)
C6—N2	1.270 (6)	C24—C25	1.405 (7)
C6—H6A	0.9300	C25—O2	1.265 (5)
C7—C10	1.361 (7)	C25—N7	1.378 (6)
C7—N2	1.378 (7)	C26—N8	1.337 (6)
C7—C8	1.446 (8)	C26—C27	1.482 (7)
C8—O1	1.241 (6)	C27—H27A	0.9600
C8—N3	1.399 (7)	C27—H27B	0.9600
C9—N4	1.450 (7)	C27—H27C	0.9600
C9—H9A	0.9600	C28—N8	1.450 (6)
C9—H9B	0.9600	C28—H28A	0.9600
C9—H9C	0.9600	C28—H28B	0.9600
C10—N4	1.339 (7)	C28—H28C	0.9600
C10—C11	1.494 (7)	C29—C30	1.371 (7)
C11—H11A	0.9600	C29—C34	1.378 (6)
C11—H11B	0.9600	C29—N7	1.423 (6)
C11—H11C	0.9600	C30—C31	1.377 (7)
C12—C13	1.374 (7)	C30—H30A	0.9300
C12—C17	1.378 (7)	C31—C32	1.370 (7)
C12—N3	1.418 (7)	C31—H31A	0.9300
C13—C14	1.381 (9)	C32—C33	1.364 (8)
C13—H13A	0.9300	C32—H32A	0.9300
C14—C15	1.368 (9)	C33—C34	1.379 (8)
C14—H14A	0.9300	C33—H33A	0.9300
C15—C16	1.365 (8)	C34—H34A	0.9300
C15—H15A	0.9300	N3—N4	1.395 (5)
C16—C17	1.380 (8)	N5—Mn1^{i}	2.341 (4)
C16—H16A	0.9300	N7—N8	1.383 (5)

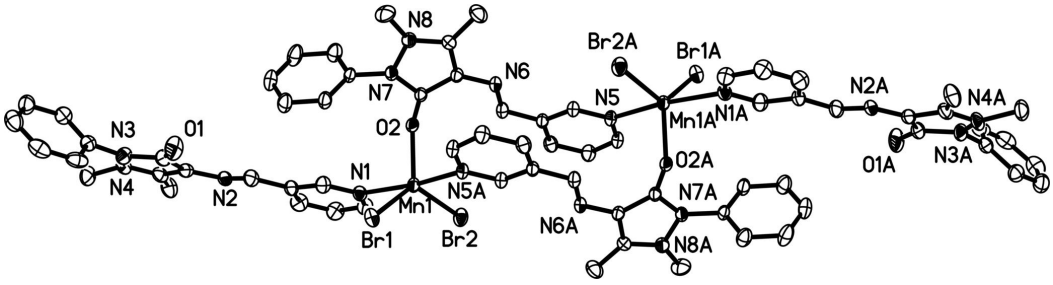
O2—Mn1—N5^{i}	87.27 (13)	C21—C20—C19	118.5 (5)
O2—Mn1—N1	89.45 (14)	C21—C20—H20A	120.7
N5^{i}—Mn1—N1	171.60 (15)	C19—C20—H20A	120.7
O2—Mn1—Br2	109.22 (10)	C20—C21—C22	117.9 (5)
N5^{i}—Mn1—Br2	94.75 (10)	C20—C21—C23	121.9 (5)
N1—Mn1—Br2	93.63 (11)	C22—C21—C23	120.1 (5)
O2—Mn1—Br1	122.63 (10)	N5—C22—C21	123.9 (5)
N5^{i}—Mn1—Br1	86.76 (10)	N5—C22—H22A	118.1
N1—Mn1—Br1	88.51 (11)	C21—C22—H22A	118.1
Br2—Mn1—Br1	128.13 (4)	N6—C23—C21	119.8 (5)
N1—C1—C2	124.3 (5)	N6—C23—H23A	120.1
N1—C1—H1A	117.9	C21—C23—H23A	120.1
C2—C1—H1A	117.9	C26—C24—N6	121.0 (4)
C1—C2—C3	116.5 (5)	C26—C24—C25	107.5 (4)
C1—C2—C6	122.2 (5)	N6—C24—C25	131.4 (5)
C3—C2—C6	121.3 (5)	O2—C25—N7	121.1 (4)
C4—C3—C2	120.2 (5)	O2—C25—C24	132.7 (5)
C4—C3—H3A	119.9	N7—C25—C24	106.2 (4)
C2—C3—H3A	119.9	N8—C26—C24	109.2 (4)
C3—C4—C5	119.1 (5)	N8—C26—C27	122.4 (5)
C3—C4—H4A	120.4	C24—C26—C27	128.3 (5)
C5—C4—H4A	120.4	C26—C27—H27A	109.5
N1—C5—C4	122.7 (5)	C26—C27—H27B	109.5
N1—C5—H5A	118.6	H27A—C27—H27B	109.5
C4—C5—H5A	118.6	C26—C27—H27C	109.5
N2—C6—C2	119.0 (5)	H27A—C27—H27C	109.5
N2—C6—H6A	120.5	H27B—C27—H27C	109.5
C2—C6—H6A	120.5	N8—C28—H28A	109.5
C10—C7—N2	121.4 (5)	N8—C28—H28B	109.5
C10—C7—C8	107.6 (5)	H28A—C28—H28B	109.5
N2—C7—C8	131.0 (5)	N8—C28—H28C	109.5
O1—C8—N3	123.0 (5)	H28A—C28—H28C	109.5
O1—C8—C7	132.3 (5)	H28B—C28—H28C	109.5
N3—C8—C7	104.7 (4)	C30—C29—C34	121.0 (5)
N4—C9—H9A	109.5	C30—C29—N7	119.4 (4)
N4—C9—H9B	109.5	C34—C29—N7	119.6 (5)
H9A—C9—H9B	109.5	C29—C30—C31	118.9 (5)
N4—C9—H9C	109.5	C29—C30—H30A	120.5
H9A—C9—H9C	109.5	C31—C30—H30A	120.5
H9B—C9—H9C	109.5	C32—C31—C30	120.4 (5)
N4—C10—C7	110.6 (5)	C32—C31—H31A	119.8
N4—C10—C11	122.3 (5)	C30—C31—H31A	119.8
C7—C10—C11	127.2 (6)	C33—C32—C31	120.4 (5)
C10—C11—H11A	109.5	C33—C32—H32A	119.8
C10—C11—H11B	109.5	C31—C32—H32A	119.8
H11A—C11—H11B	109.5	C32—C33—C34	120.0 (5)
C10—C11—H11C	109.5	C32—C33—H33A	120.0
H11A—C11—H11C	109.5	C34—C33—H33A	120.0

H11B—C11—H11C	109.5	C29—C34—C33	119.2 (5)
C13—C12—C17	119.6 (6)	C29—C34—H34A	120.4
C13—C12—N3	120.1 (5)	C33—C34—H34A	120.4
C17—C12—N3	120.2 (5)	C5—N1—C1	117.2 (4)
C12—C13—C14	119.6 (6)	C5—N1—Mn1	121.8 (4)
C12—C13—H13A	120.2	C1—N1—Mn1	121.0 (3)
C14—C13—H13A	120.2	C6—N2—C7	125.6 (5)
C15—C14—C13	120.9 (6)	N4—N3—C8	108.8 (4)
C15—C14—H14A	119.5	N4—N3—C12	121.6 (4)
C13—C14—H14A	119.5	C8—N3—C12	129.4 (4)
C16—C15—C14	119.2 (6)	C10—N4—N3	108.2 (4)
C16—C15—H15A	120.4	C10—N4—C9	127.0 (5)
C14—C15—H15A	120.4	N3—N4—C9	122.0 (5)
C15—C16—C17	120.7 (6)	C22—N5—C18	117.5 (4)
C15—C16—H16A	119.6	C22—N5—Mn1^{i}	122.6 (3)
C17—C16—H16A	119.6	C18—N5—Mn1^{i}	119.5 (3)
C12—C17—C16	119.8 (5)	C23—N6—C24	122.0 (4)
C12—C17—H17A	120.1	C25—N7—N8	108.7 (4)
C16—C17—H17A	120.1	C25—N7—C29	125.7 (4)
N5—C18—C19	122.1 (5)	N8—N7—C29	122.4 (4)
N5—C18—H18A	118.9	C26—N8—N7	108.3 (4)
C19—C18—H18A	118.9	C26—N8—C28	129.9 (5)
C18—C19—C20	120.0 (5)	N7—N8—C28	120.4 (5)
C18—C19—H19A	120.0	C25—O2—Mn1	132.0 (3)
C20—C19—H19A	120.0		
N1—C1—C2—C3	1.6 (8)	Br2—Mn1—N1—C5	−7.7 (4)
N1—C1—C2—C6	179.7 (5)	Br1—Mn1—N1—C5	−135.8 (4)
C1—C2—C3—C4	−1.5 (8)	O2—Mn1—N1—C1	−77.7 (4)
C6—C2—C3—C4	−179.6 (5)	N5^{i}—Mn1—N1—C1	−10.8 (12)
C2—C3—C4—C5	0.4 (9)	Br2—Mn1—N1—C1	173.1 (4)
C3—C4—C5—N1	0.8 (9)	Br1—Mn1—N1—C1	44.9 (4)
C1—C2—C6—N2	172.9 (5)	C2—C6—N2—C7	179.1 (5)
C3—C2—C6—N2	−9.1 (8)	C10—C7—N2—C6	−174.2 (5)
C10—C7—C8—O1	−177.1 (6)	C8—C7—N2—C6	3.6 (9)
N2—C7—C8—O1	4.8 (11)	O1—C8—N3—N4	176.4 (5)
C10—C7—C8—N3	0.6 (6)	C7—C8—N3—N4	−1.6 (6)
N2—C7—C8—N3	−177.5 (5)	O1—C8—N3—C12	0.9 (9)
N2—C7—C10—N4	179.0 (4)	C7—C8—N3—C12	−177.1 (5)
C8—C7—C10—N4	0.7 (6)	C13—C12—N3—N4	131.6 (5)
N2—C7—C10—C11	−0.5 (9)	C17—C12—N3—N4	−46.3 (7)
C8—C7—C10—C11	−178.8 (5)	C13—C12—N3—C8	−53.4 (8)
C17—C12—C13—C14	0.7 (8)	C17—C12—N3—C8	128.7 (6)
N3—C12—C13—C14	−177.2 (5)	C7—C10—N4—N3	−1.8 (6)
C12—C13—C14—C15	0.8 (9)	C11—C10—N4—N3	177.8 (5)
C13—C14—C15—C16	−1.4 (10)	C7—C10—N4—C9	−162.7 (5)
C14—C15—C16—C17	0.6 (10)	C11—C10—N4—C9	16.9 (8)
C13—C12—C17—C16	−1.5 (9)	C8—N3—N4—C10	2.1 (6)
N3—C12—C17—C16	176.4 (5)	C12—N3—N4—C10	178.1 (5)

C15—C16—C17—C12	0.9 (9)	C8—N3—N4—C9	164.2 (5)
N5—C18—C19—C20	1.2 (8)	C12—N3—N4—C9	−19.9 (7)
C18—C19—C20—C21	0.6 (8)	C21—C22—N5—C18	−0.2 (7)
C19—C20—C21—C22	−2.1 (7)	C21—C22—N5—Mn1^{i}	−173.3 (4)
C19—C20—C21—C23	−179.2 (4)	C19—C18—N5—C22	−1.4 (7)
C20—C21—C22—N5	1.9 (7)	C19—C18—N5—Mn1^{i}	172.0 (4)
C23—C21—C22—N5	179.2 (4)	C21—C23—N6—C24	−174.2 (4)
C20—C21—C23—N6	−171.5 (5)	C26—C24—N6—C23	−171.0 (4)
C22—C21—C23—N6	11.4 (7)	C25—C24—N6—C23	13.1 (7)
C26—C24—C25—O2	−179.0 (5)	O2—C25—N7—N8	−178.5 (4)
N6—C24—C25—O2	−2.6 (8)	C24—C25—N7—N8	1.9 (5)
C26—C24—C25—N7	0.6 (5)	O2—C25—N7—C29	−18.5 (7)
N6—C24—C25—N7	176.9 (4)	C24—C25—N7—C29	161.9 (4)
N6—C24—C26—N8	−179.8 (4)	C30—C29—N7—C25	95.3 (6)
C25—C24—C26—N8	−3.0 (5)	C34—C29—N7—C25	−84.4 (6)
N6—C24—C26—C27	−2.6 (8)	C30—C29—N7—N8	−107.3 (5)
C25—C24—C26—C27	174.2 (5)	C34—C29—N7—N8	72.9 (6)
C34—C29—C30—C31	1.9 (8)	C24—C26—N8—N7	4.2 (5)
N7—C29—C30—C31	−177.8 (5)	C27—C26—N8—N7	−173.2 (4)
C29—C30—C31—C32	−1.3 (9)	C24—C26—N8—C28	170.5 (5)
C30—C31—C32—C33	−0.3 (9)	C27—C26—N8—C28	−6.9 (8)
C31—C32—C33—C34	1.2 (10)	C25—N7—N8—C26	−3.8 (5)
C30—C29—C34—C33	−1.0 (8)	C29—N7—N8—C26	−164.6 (4)
N7—C29—C34—C33	178.8 (5)	C25—N7—N8—C28	−171.7 (4)
C32—C33—C34—C29	−0.6 (9)	C29—N7—N8—C28	27.6 (6)
C4—C5—N1—C1	−0.7 (8)	N7—C25—O2—Mn1	−95.7 (5)
C4—C5—N1—Mn1	180.0 (4)	C24—C25—O2—Mn1	83.8 (6)
C2—C1—N1—C5	−0.5 (8)	N5^{i}—Mn1—O2—C25	−24.9 (4)
C2—C1—N1—Mn1	178.8 (4)	N1—Mn1—O2—C25	147.3 (4)
O2—Mn1—N1—C5	101.5 (4)	Br2—Mn1—O2—C25	−119.0 (4)
N5^{i}—Mn1—N1—C5	168.5 (8)	Br1—Mn1—O2—C25	59.4 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


N8
Br2A
Br1A
N6
N7
N5
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N1A
N2A
N4A
N3
O1
O2
O2A
N1
N5A
N7A
O1A
N3A
N4
N2
Mn1
N6A
Br1
Br2
N8A