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Diaquabis[2-(2-pyridylmethoxy)-pyrazine-κN^4]bis(thiocyanato-κN)-manganese(II)

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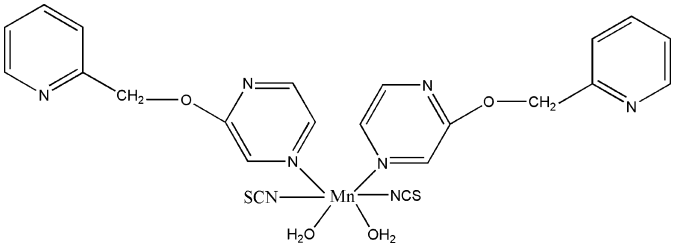
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.083; data-to-parameter ratio = 13.7.

In the title complex, $[Mn(NCS)_2(C_{10}H_9N_3O)_2(H_2O)_2]$, the Mn^{II} ion lies on a twofold rotation axis and assumes a distorted octahedral MnN_4O_2 coordination geometry. There is a weak π–π stacking interaction between adjacent pyridyl and pyrazine rings [centroid-to-centroid distance 3.7457 (13) Å]. The mononuclear complexes are connected to each other by O—H···N and O—H···S hydrogen bonds. The dihedral angle between the pyridyl and pyrazine rings is 85.82 (9)°.

Related literature

For related structures, see: McMorran *et al.* (2002); Zhao *et al.* (2007*a*,*b*).



Experimental

Crystal data

$[Mn(NCS)_2(C_{10}H_9N_3O)_2(H_2O)_2]$
M_r = 581.54
Monoclinic, $C2/c$
a = 20.060 (3) Å
b = 10.1381 (12) Å
c = 13.7285 (17) Å
β = 110.844 (2)°
V = 2609.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.71 mm^{-1}
T = 298 (2) K
0.26 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.837, T_{max} = 0.895
5374 measured reflections
2317 independent reflections
2133 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
S = 1.04
2317 reflections
169 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H6···S1^{i}	0.89	2.49	3.3776 (16)	171
O2—H1···N4^{ii}	0.89	1.90	2.793 (2)	176

Symmetry codes: (i) $-x+2, -y+2, -z+2$; (ii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+2$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2445).

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Zhao, H.-Y., Shi, J.-M. & Liu, L.-D. (2007*b*). *Acta Cryst.* E**63**, m824–m825.

  doi:10.1107/S1600536807037166

supplementary materials

Acta Cryst. (2007). E**63**, m2266 [**doi:10.1107/S1600536807037166**]

Diaquabis[2-(2-pyridylmethoxy)pyrazine-κN^4]bis(thiocyanato-κN)manganese(II)

J.-M. Li

Comment

Metal complexes containing N-heterocyclic ligands play a pivotal role in the area of coordination chemistry, but the ligand molecules that consist of pyridyl and pyrazyl groups are very limited (McMorran *et al.* 2002; Zhao *et al.*, 2007*a*,b).

The title compound is shown in Fig. 1. In the mono-nuclear complex atom Mn1 is in a distorted octahedral geometry and is located on a twofold ratation axis. Between adjacent complexes there is a weak π-π stacking interaction between pyrazyl and pyridyl rings; the relevant distances are $Cg1\cdots Cg2^{i}$ = 3.7457 (13) Å and $Cg1\cdots Cg2^{i}_{perp}$ = 3.222 Å [symmetry codes: (i) *X*, 1-Y, 1/2+*Z*; *Cg*1 and *Cg*2 are the centroids of the N2,N3,C2,C3,C4,C5 and N4,C7,C8,C9,C10,C11 rings, respectively; $Cg1\cdots Cg2_{perp}$ is the perpendicular distance from ring *Cg*1 to ring *Cg*2]. Fig. 2 shows the O—H···N and O—H···S hydrogen bonds and Table 1 lists the geometric parameters. The dihedral angle between the pyridyl ring and the pyrazyl ring in 2-[(pyridin-2-yl)methoxy]pyrazine is 85.82 (9)°.

Experimental

5 ml me thanol solution of 2-[(pyridin-2-yl)methoxy]pyrazine (0.0468 g, 0.250 mmol) was added into 10 ml H_2O solution containing $Mn(ClO_4)_2\cdot 6H_2O$ (0.1021 g, 0.282 mmol) and NaSCN (0.0459 g, 0.566 mmol), and the mixed soulution was stirred for a few minutes. Colourless single crystals were obtained after the solution had been allowed to stand at room temperature for two weeks.

Refinement

The H atoms from H_2O were found in a difference Fourier map, and placed in idealized positions with O—H = 0.894–0.895 Å. The C-bound H atom were placed in calculated positions, C—H = 0.93–0.97 Å. All H atoms were refined as riding, with U_{iso}(H) = 1.2–1.5U_{eq}(C,*O*).

Figures

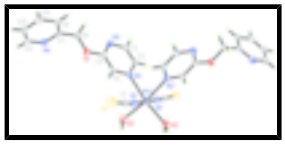

Fig. 1. View of the title complex, showing the the atom numbering scheme with thermal ellipsoids drawn at the 30% probability level [symmetry code: (i) −*x* + 2, *y*, −*z* + 5/2].

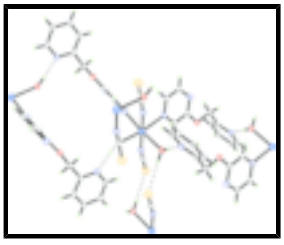

Fig. 2. Hydrogen bonds (dashed lines) between complexes.

Diaquabis[2-(2-pyridylmethoxy)pyrazine-κN^4]bis(thiocyanato-κ*N*)manganese(II)

Crystal data

$[Mn(NCS)_2(C_{10}H_9N_3O)_2(H_2O)_2]$	F_{000} = 1196
M_r = 581.54	D_x = 1.480 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4687 reflections
a = 20.060 (3) Å	θ = 2.2–28.3º
b = 10.1381 (12) Å	μ = 0.71 mm^{-1}
c = 13.7285 (17) Å	*T* = 298 (2) K
β = 110.844 (2)º	Block, colourless
V = 2609.3 (6) Å^3	0.26 × 0.18 × 0.16 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	2317 independent reflections
Radiation source: fine-focus sealed tube	2133 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −23→22
T_{min} = 0.837, T_{max} = 0.895	*k* = −12→11
5374 measured reflections	*l* = −9→16

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 1.6969P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.083	$(\Delta/\sigma)_{max}$ = 0.010
S = 1.04	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
2317 reflections	$\Delta\rho_{min}$ = −0.45 e Å^{-3}

169 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXTL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0033 (4)

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	1.0000	0.79418 (3)	1.2500	0.03392 (15)
S1	1.03076 (5)	0.77723 (7)	0.91123 (5)	0.0820 (2)
N2	0.92253 (7)	0.61791 (14)	1.18728 (11)	0.0387 (3)
O1	0.80883 (7)	0.47898 (12)	0.94850 (9)	0.0490 (3)
N4	0.67814 (8)	0.44033 (15)	0.74592 (11)	0.0435 (4)
O2	0.91697 (7)	0.94209 (13)	1.17325 (9)	0.0493 (3)
H1	0.8847	0.9782	1.1964	0.074*
H6	0.9331	1.0103	1.1468	0.074*
N1	1.02389 (9)	0.79825 (16)	1.10881 (13)	0.0492 (4)
C5	0.84117 (9)	0.49147 (17)	1.05252 (13)	0.0387 (4)
C8	0.76848 (10)	0.28795 (18)	0.74656 (16)	0.0459 (4)
H8	0.8078	0.2371	0.7843	0.055*
N3	0.82651 (8)	0.40955 (15)	1.11682 (11)	0.0429 (4)
C1	1.02672 (10)	0.79049 (17)	1.02685 (15)	0.0423 (4)
C9	0.74294 (11)	0.28611 (19)	0.63920 (17)	0.0515 (5)
H9	0.7643	0.2330	0.6034	0.062*
C7	0.73497 (9)	0.36634 (16)	0.79734 (13)	0.0374 (4)
C3	0.86224 (10)	0.43152 (19)	1.21803 (14)	0.0472 (4)
H3	0.8549	0.3748	1.2664	0.057*
C4	0.88960 (9)	0.59529 (17)	1.08683 (13)	0.0385 (4)
H4	0.8988	0.6493	1.0383	0.046*
C6	0.76005 (10)	0.36903 (18)	0.91382 (14)	0.0467 (4)
H6A	0.7199	0.3801	0.9367	0.056*
H6B	0.7840	0.2871	0.9424	0.056*
C2	0.90920 (10)	0.53366 (19)	1.25373 (14)	0.0453 (4)
H2	0.9323	0.5450	1.3251	0.054*
C11	0.65489 (11)	0.4379 (2)	0.64193 (15)	0.0511 (5)
H11	0.6156	0.4895	0.6054	0.061*

C10	0.68574 (11)	0.3634 (2)	0.58593 (15)	0.0520 (5)
H10	0.6682	0.3655	0.5135	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0365 (2)	0.0357 (2)	0.0277 (2)	0.000	0.00914 (15)	0.000
S1	0.1351 (6)	0.0759 (5)	0.0542 (4)	0.0111 (4)	0.0571 (4)	0.0012 (3)
N2	0.0368 (7)	0.0388 (8)	0.0357 (7)	−0.0029 (6)	0.0070 (6)	0.0008 (6)
O1	0.0611 (8)	0.0431 (7)	0.0324 (6)	−0.0182 (6)	0.0040 (6)	0.0015 (5)
N4	0.0454 (8)	0.0435 (8)	0.0391 (8)	0.0011 (6)	0.0120 (7)	−0.0035 (6)
O2	0.0534 (7)	0.0538 (8)	0.0419 (7)	0.0150 (6)	0.0185 (6)	0.0082 (6)
N1	0.0614 (10)	0.0511 (10)	0.0407 (9)	−0.0029 (7)	0.0251 (8)	0.0007 (7)
C5	0.0408 (9)	0.0359 (9)	0.0345 (9)	−0.0011 (7)	0.0076 (7)	0.0002 (7)
C8	0.0418 (10)	0.0402 (10)	0.0536 (11)	−0.0006 (7)	0.0145 (8)	0.0000 (8)
N3	0.0469 (8)	0.0399 (8)	0.0380 (8)	−0.0081 (6)	0.0103 (6)	0.0010 (6)
C1	0.0465 (10)	0.0377 (10)	0.0454 (11)	0.0019 (7)	0.0197 (8)	0.0021 (7)
C9	0.0604 (12)	0.0501 (11)	0.0518 (11)	−0.0081 (9)	0.0295 (10)	−0.0130 (9)
C7	0.0403 (9)	0.0337 (9)	0.0356 (9)	−0.0101 (7)	0.0103 (7)	−0.0020 (7)
C3	0.0535 (10)	0.0476 (10)	0.0371 (9)	−0.0105 (8)	0.0119 (8)	0.0050 (8)
C4	0.0408 (9)	0.0363 (9)	0.0346 (9)	−0.0030 (7)	0.0087 (7)	0.0027 (7)
C6	0.0537 (10)	0.0423 (10)	0.0377 (9)	−0.0153 (8)	0.0083 (8)	−0.0003 (8)
C2	0.0477 (10)	0.0492 (11)	0.0334 (9)	−0.0076 (8)	0.0077 (8)	0.0010 (8)
C11	0.0512 (10)	0.0523 (11)	0.0411 (10)	0.0046 (9)	0.0058 (8)	0.0026 (8)
C10	0.0637 (12)	0.0551 (12)	0.0350 (9)	−0.0123 (10)	0.0151 (9)	−0.0059 (8)

Geometric parameters (Å, °)

Mn1—N1^{i}	2.1564 (16)	C5—C4	1.396 (2)
Mn1—N1	2.1564 (16)	C8—C9	1.378 (3)
Mn1—O2^{i}	2.2100 (13)	C8—C7	1.380 (3)
Mn1—O2	2.2100 (12)	C8—H8	0.9300
Mn1—N2	2.3233 (14)	N3—C3	1.336 (2)
Mn1—N2^{i}	2.3233 (14)	C9—C10	1.367 (3)
S1—C1	1.623 (2)	C9—H9	0.9300
N2—C4	1.320 (2)	C7—C6	1.496 (2)
N2—C2	1.344 (2)	C3—C2	1.368 (3)
O1—C5	1.348 (2)	C3—H3	0.9300
O1—C6	1.448 (2)	C4—H4	0.9300
N4—C11	1.335 (2)	C6—H6A	0.9700
N4—C7	1.337 (2)	C6—H6B	0.9700
O2—H1	0.8947	C2—H2	0.9300
O2—H6	0.8938	C11—C10	1.372 (3)
N1—C1	1.149 (3)	C11—H11	0.9300
C5—N3	1.319 (2)	C10—H10	0.9300
N1^{i}—Mn1—N1	177.81 (9)	C5—N3—C3	115.22 (15)
N1^{i}—Mn1—O2^{i}	85.95 (6)	N1—C1—S1	179.17 (17)

N1—Mn1—O2^{i}	92.56 (6)	C10—C9—C8	119.12 (18)
N1^{i}—Mn1—O2	92.56 (6)	C10—C9—H9	120.4
N1—Mn1—O2	85.95 (6)	C8—C9—H9	120.4
O2^{i}—Mn1—O2	94.55 (7)	N4—C7—C8	122.25 (16)
N1^{i}—Mn1—N2	90.83 (6)	N4—C7—C6	116.96 (16)
N1—Mn1—N2	90.85 (6)	C8—C7—C6	120.77 (17)
O2^{i}—Mn1—N2	171.83 (5)	N3—C3—C2	123.03 (17)
O2—Mn1—N2	93.09 (5)	N3—C3—H3	118.5
N1^{i}—Mn1—N2^{i}	90.85 (6)	C2—C3—H3	118.5
N1—Mn1—N2^{i}	90.83 (6)	N2—C4—C5	120.88 (16)
O2^{i}—Mn1—N2^{i}	93.09 (5)	N2—C4—H4	119.6
O2—Mn1—N2^{i}	171.83 (5)	C5—C4—H4	119.6
N2—Mn1—N2^{i}	79.44 (7)	O1—C6—C7	107.25 (14)
C4—N2—C2	116.88 (15)	O1—C6—H6A	110.3
C4—N2—Mn1	122.75 (11)	C7—C6—H6A	110.3
C2—N2—Mn1	120.37 (11)	O1—C6—H6B	110.3
C5—O1—C6	115.79 (13)	C7—C6—H6B	110.3
C11—N4—C7	117.52 (16)	H6A—C6—H6B	108.5
Mn1—O2—H1	128.8	N2—C2—C3	121.05 (16)
Mn1—O2—H6	113.5	N2—C2—H2	119.5
H1—O2—H6	103.9	C3—C2—H2	119.5
C1—N1—Mn1	169.40 (16)	N4—C11—C10	123.61 (18)
N3—C5—O1	120.80 (15)	N4—C11—H11	118.2
N3—C5—C4	122.89 (15)	C10—C11—H11	118.2
O1—C5—C4	116.31 (15)	C9—C10—C11	118.41 (18)
C9—C8—C7	119.06 (17)	C9—C10—H10	120.8
C9—C8—H8	120.5	C11—C10—H10	120.8
C7—C8—H8	120.5		
N1^{i}—Mn1—N2—C4	152.48 (14)	C11—N4—C7—C6	−179.46 (16)
N1—Mn1—N2—C4	−26.12 (14)	C9—C8—C7—N4	0.4 (3)
O2—Mn1—N2—C4	59.87 (14)	C9—C8—C7—C6	178.70 (16)
N2^{i}—Mn1—N2—C4	−116.80 (15)	C5—N3—C3—C2	1.9 (3)
N1^{i}—Mn1—N2—C2	−27.27 (14)	C2—N2—C4—C5	2.5 (2)
N1—Mn1—N2—C2	154.13 (14)	Mn1—N2—C4—C5	−177.28 (12)
O2—Mn1—N2—C2	−119.88 (13)	N3—C5—C4—N2	−1.3 (3)
N2^{i}—Mn1—N2—C2	63.44 (12)	O1—C5—C4—N2	178.14 (15)
O2^{i}—Mn1—N1—C1	−165.5 (8)	C5—O1—C6—C7	−175.36 (15)
O2—Mn1—N1—C1	−71.1 (8)	N4—C7—C6—O1	−87.09 (19)
N2—Mn1—N1—C1	22.0 (8)	C8—C7—C6—O1	94.48 (19)
N2^{i}—Mn1—N1—C1	101.4 (8)	C4—N2—C2—C3	−1.6 (3)
C6—O1—C5—N3	−2.0 (2)	Mn1—N2—C2—C3	178.21 (14)
C6—O1—C5—C4	178.54 (15)	N3—C3—C2—N2	−0.7 (3)
O1—C5—N3—C3	179.65 (16)	C7—N4—C11—C10	0.5 (3)
C4—C5—N3—C3	−1.0 (3)	C8—C9—C10—C11	−1.5 (3)
C7—C8—C9—C10	0.9 (3)	N4—C11—C10—C9	0.8 (3)

C11—N4—C7—C8	−1.1 (3)

Symmetry codes: (i) −*x*+2, *y*, −*z*+5/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H6···S1^{ii}	0.89	2.49	3.3776 (16)	171
O2—H1···N4^{iii}	0.89	1.90	2.793 (2)	176

Symmetry codes: (ii) −*x*+2, −*y*+2, −*z*+2; (iii) −*x*+3/2, −*y*+3/2, −*z*+2.

Fig. 1

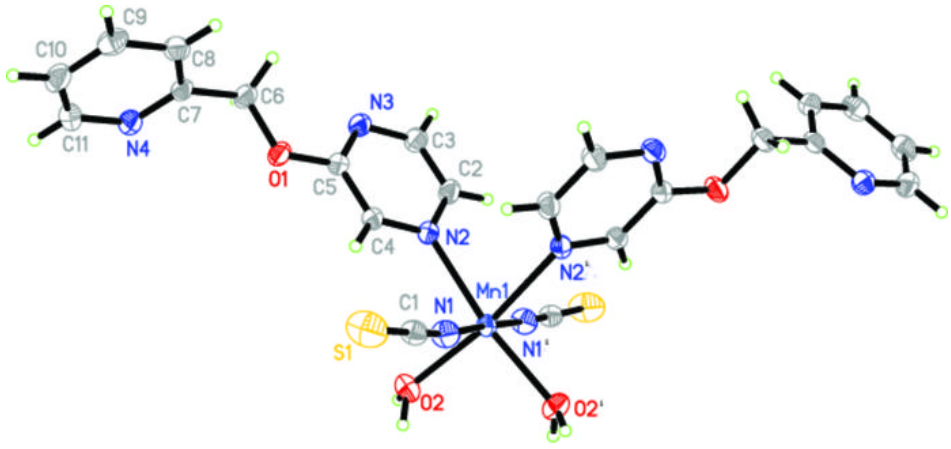

Fig. 2