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Crystal structure of bis(2,2′-bipyridine-κ^2N,N')bis(thiocyanato-κN)manganese(II) 2,2′-bipyridine monosolvate

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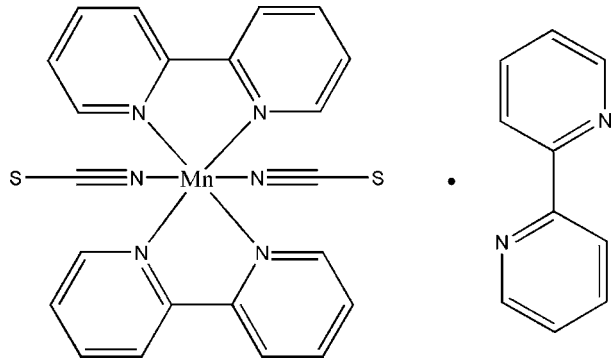
In the crystal structure of the mononuclear title compound, $[Mn(NCS)_2(C_{10}H_8N_2)_2]\cdot C_{10}H_8N_2$, the Mn^{II} cation is coordinated in an all-*cis* configuration by two N-bound thiocyanate anions and two 2,2′-bipyridine ligands within a slightly distorted octahedral environment. The asymmetric unit consists of one Mn^{II} cation, two thiocyanate anions and two 2,2′-bipyridine ligands, as well as two non-coordinating 2,2′-bipyridine ligands that are each located on centres of inversion. In the crystal structure, the discrete $[Mn(NCS)_2(C_{10}H_8N_2)_2]$ complex molecules are arranged in such a way that cavities are formed, in which the solvent 2,2′-bipyridine molecules are located. Apart from van der Waals forces, there are no remarkable intermolecular interactions present in the crystal structure.

Keywords: crystal structure; coordination polymer; octahedral manganese(II) coordination.

CCDC reference: 1034429

1. Related literature

For similar crystal structures with thiocyanate anions in *cis*-coordination to a manganese(II) cation, see: Małecki *et al.* (2011).



2. Experimental

2.1. Crystal data

$[Mn(NCS)_2(C_{10}H_8N_2)_2]\cdot C_{10}H_8N_2$
M_r = 639.65
Monoclinic, $P2_1/c$
a = 14.5263 (6) Å
b = 13.5383 (4) Å
c = 16.0726 (7) Å
β = 105.535 (3)°
V = 3045.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 293 K
0.32 × 0.19 × 0.07 mm

2.2. Data collection

Stoe IPDS-2 diffractometer
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2008)
T_{min} = 0.820, T_{max} = 0.919
41565 measured reflections
6630 independent reflections
5766 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.094
S = 1.08
6630 reflections
389 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2008); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5090).

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supporting information

Acta Cryst. (2015). E**71**, m3–m4 [https://doi.org/10.1107/S205698901402516X]

Crystal structure of bis(2,2′-bipyridine-κ^2N,N')bis(thiocyanato-κN)manganese(II) 2,2′-bipyridine monosolvate

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S1. Synthesis and crystallization

$MnSO_4·H_2O$ was purchased from Merck and 2,2′-bipyridine and $Ba(NCS)_2·3H_2O$ were purchased from Alfa Aesar. $Mn(NCS)_2$ was synthesized by stirring 17.97 g (58.44 mmol) $Ba(NCS)_2·3H_2O$ and 9.88 g (58.44 mmol) $MnSO_4·H_2O$ in 300 ml water at room temperature for three hours. The white residue of $BaSO_4$ was filtered off and the solvent removed with a rotary evaporator. The homogeneity of the product was investigated by X-ray powder diffraction and elemental analysis. The title compound was prepared by the reaction of 25.7 mg (0.15 mmol) $Mn(NCS)_2$ and 93.7 mg (0.60 mmol) 2,2′-bipyridine in 1.0 ml water at room temperature. After few days, yellow plates of the title compound were obtained.

S2. Refinement

The hydrogen atoms were positioned with idealized geometry and were refined with C—H = 0.93 Å and U_{eq}(H) = 1.2 U_{eq}(C) using a riding model approximation.

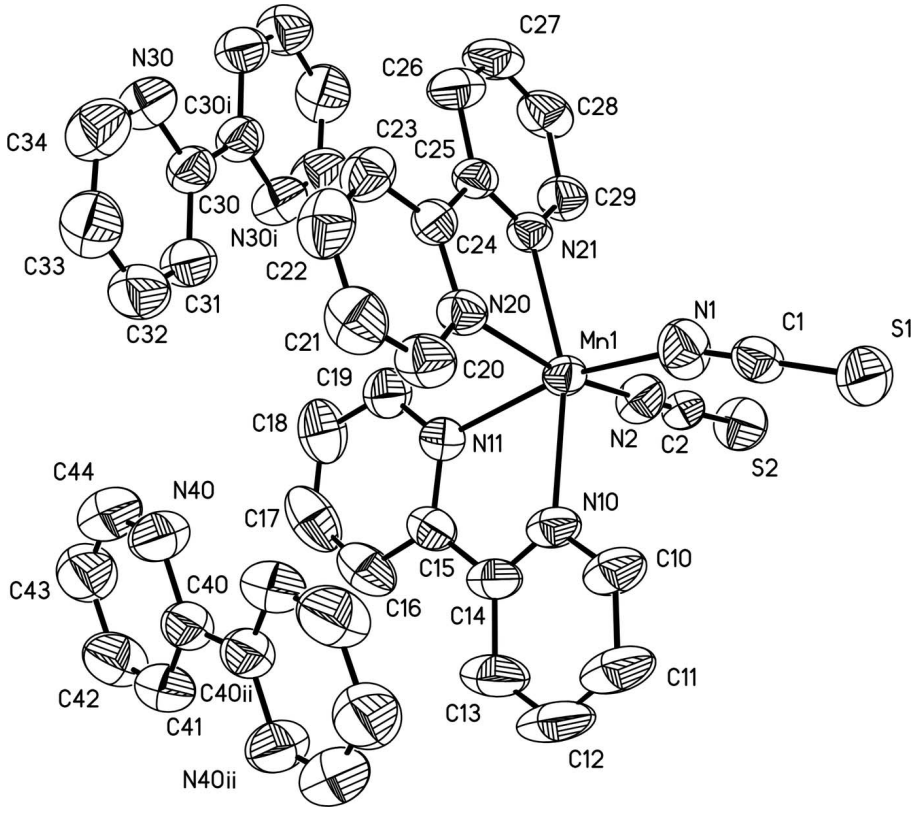

Figure 1

The molecular components of the title compound with labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) -x+1,-y+1,-z+1; (ii) -x+2,-y+1,-z+1.]

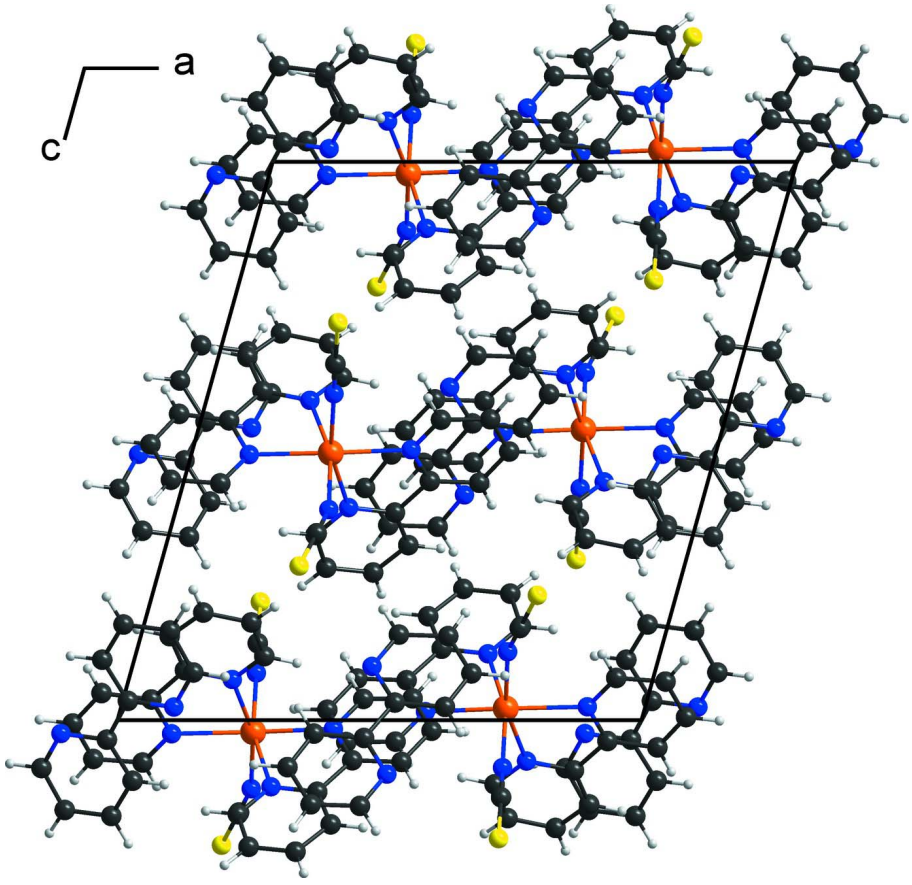

Figure 2

The packing of the molecules in the crystal structure of the title compound in a view along [010].

Bis(2,2′-bipyridine-κ^2N,N')bis(thiocyanato-κN)manganese(II) 2,2′-bipyridine monosolvate

Crystal data

$[Mn(NCS)_2(C_{10}H_8N_2)_2]\cdot C_{10}H_8N_2$
$M_r = 639.65$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.5263$ (6) Å
$b = 13.5383$ (4) Å
$c = 16.0726$ (7) Å
$\beta = 105.535$ (3)°
$V = 3045.4$ (2) Å^3
$Z = 4$
$F(000) = 1316$
$D_x = 1.395$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 1.5$–27.0°
$\mu = 0.61$ mm^{-1}
$T = 293$ K
Plate, yellow
0.32 × 0.19 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2008)
$T_{min} = 0.820$, $T_{max} = 0.919$
41565 measured reflections
6630 independent reflections
5766 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.5°$
$h = -18\rightarrow18$
$k = -17\rightarrow17$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.094$
$S = 1.08$
6630 reflections
389 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
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.9654P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0025 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
Mn1	0.734793 (17)	0.128336 (19)	0.478914 (17)	0.04106 (9)
N1	0.70830 (14)	0.02009 (14)	0.37737 (12)	0.0665 (5)
C1	0.71894 (13)	−0.04547 (14)	0.33491 (12)	0.0502 (4)
S1	0.73507 (5)	−0.13676 (5)	0.27623 (4)	0.0792 (2)
N2	0.75999 (12)	0.02533 (13)	0.58481 (11)	0.0583 (4)
C2	0.77308 (12)	−0.03438 (13)	0.63794 (12)	0.0453 (4)
S2	0.79008 (5)	−0.11880 (5)	0.71196 (4)	0.07089 (17)
N10	0.88949 (10)	0.14680 (12)	0.47586 (10)	0.0513 (4)
C10	0.92943 (15)	0.09366 (18)	0.42424 (15)	0.0652 (6)
H10	0.8898	0.0546	0.3818	0.078*
C11	1.02539 (17)	0.0938 (2)	0.43073 (19)	0.0824 (8)
H11	1.0502	0.0572	0.3928	0.099*
C12	1.08341 (17)	0.1492 (2)	0.4943 (2)	0.0908 (9)
H12	1.1490	0.1497	0.5010	0.109*
C13	1.04482 (15)	0.2043 (2)	0.54863 (18)	0.0792 (7)
H13	1.0840	0.2420	0.5924	0.095*
C14	0.94611 (13)	0.20298 (15)	0.53718 (13)	0.0541 (5)
C15	0.89768 (13)	0.26359 (14)	0.58963 (12)	0.0517 (4)
C16	0.94487 (18)	0.33141 (19)	0.65064 (15)	0.0728 (6)
H16	1.0108	0.3385	0.6629	0.087*
C17	0.8933 (2)	0.3882 (2)	0.69288 (16)	0.0852 (8)
H17	0.9244	0.4343	0.7337	0.102*
C18	0.7964 (2)	0.37728 (17)	0.67522 (16)	0.0771 (7)

H18	0.7605	0.4157	0.7030	0.092*
C19	0.75380 (16)	0.30723 (16)	0.61475 (13)	0.0607 (5)
H19	0.6880	0.2987	0.6025	0.073*
N11	0.80238 (10)	0.25125 (11)	0.57302 (10)	0.0488 (3)
N20	0.67171 (10)	0.24892 (11)	0.38090 (9)	0.0470 (3)
C20	0.72036 (15)	0.29317 (17)	0.33176 (14)	0.0624 (5)
H20	0.7831	0.2736	0.3374	0.075*
C21	0.68249 (19)	0.36615 (18)	0.27327 (15)	0.0726 (6)
H21	0.7188	0.3955	0.2404	0.087*
C22	0.59047 (19)	0.39454 (17)	0.26467 (14)	0.0713 (6)
H22	0.5632	0.4443	0.2260	0.086*
C24	0.58074 (12)	0.27636 (13)	0.37188 (11)	0.0446 (4)
C25	0.53069 (12)	0.22504 (13)	0.42834 (11)	0.0438 (4)
C26	0.43568 (13)	0.24294 (17)	0.42531 (14)	0.0613 (5)
H26	0.4000	0.2878	0.3858	0.074*
C27	0.39498 (14)	0.19383 (19)	0.48122 (15)	0.0689 (6)
H27	0.3314	0.2050	0.4797	0.083*
C28	0.44834 (15)	0.12849 (17)	0.53914 (15)	0.0652 (6)
H28	0.4223	0.0955	0.5782	0.078*
C29	0.54214 (14)	0.11259 (15)	0.53824 (13)	0.0538 (4)
H29	0.5782	0.0671	0.5768	0.065*
N21	0.58328 (10)	0.15956 (11)	0.48459 (9)	0.0427 (3)
N30	0.45727 (13)	0.57292 (15)	0.40356 (13)	0.0690 (5)
C30	0.52000 (14)	0.52678 (15)	0.46832 (13)	0.0557 (5)
C31	0.61789 (15)	0.52953 (17)	0.47611 (15)	0.0654 (5)
H31	0.6605	0.4974	0.5216	0.078*
C23	0.53780 (16)	0.34899 (15)	0.31364 (13)	0.0597 (5)
H23	0.4745	0.3668	0.3076	0.072*
C32	0.65066 (18)	0.5801 (2)	0.41603 (18)	0.0766 (6)
H32	0.7158	0.5826	0.4203	0.092*
C33	0.5866 (2)	0.6271 (2)	0.34934 (19)	0.0813 (7)
H33	0.6069	0.6617	0.3075	0.098*
C34	0.4917 (2)	0.6212 (2)	0.34664 (18)	0.0822 (7)
H34	0.4483	0.6533	0.3017	0.099*
N40	0.89931 (14)	0.56056 (16)	0.52370 (14)	0.0753 (5)
C40	0.99023 (15)	0.53074 (16)	0.53470 (14)	0.0617 (5)
C41	1.06105 (17)	0.55483 (19)	0.60838 (17)	0.0756 (6)
H41	1.1234	0.5332	0.6150	0.091*
C42	1.0391 (2)	0.6106 (2)	0.67145 (19)	0.0877 (8)
H42	1.0863	0.6269	0.7212	0.105*
C43	0.9471 (2)	0.6423 (2)	0.6607 (2)	0.0887 (8)
H43	0.9301	0.6808	0.7022	0.106*
C44	0.8805 (2)	0.6148 (2)	0.5856 (2)	0.0891 (8)
H44	0.8179	0.6360	0.5779	0.107*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.03601 (14)	0.04340 (15)	0.04746 (15)	0.00108 (10)	0.01753 (10)	0.00063 (11)
N1	0.0761 (12)	0.0621 (10)	0.0701 (11)	−0.0069 (9)	0.0350 (9)	−0.0150 (9)
C1	0.0426 (9)	0.0562 (11)	0.0537 (10)	−0.0084 (8)	0.0160 (8)	−0.0048 (9)
S1	0.0676 (4)	0.0790 (4)	0.0828 (4)	0.0061 (3)	0.0057 (3)	−0.0377 (3)
N2	0.0596 (10)	0.0556 (9)	0.0651 (10)	0.0078 (8)	0.0263 (8)	0.0123 (8)
C2	0.0384 (9)	0.0475 (9)	0.0520 (10)	0.0034 (7)	0.0156 (7)	−0.0024 (8)
S2	0.0751 (4)	0.0693 (4)	0.0641 (3)	0.0054 (3)	0.0114 (3)	0.0214 (3)
N10	0.0365 (7)	0.0616 (9)	0.0595 (9)	0.0044 (7)	0.0193 (7)	0.0112 (7)
C10	0.0494 (11)	0.0803 (14)	0.0749 (14)	0.0122 (10)	0.0322 (10)	0.0105 (11)
C11	0.0504 (13)	0.110 (2)	0.0989 (19)	0.0219 (13)	0.0401 (13)	0.0237 (16)
C12	0.0393 (12)	0.122 (2)	0.118 (2)	0.0176 (13)	0.0336 (14)	0.0357 (19)
C13	0.0369 (10)	0.1010 (19)	0.0934 (17)	−0.0024 (11)	0.0064 (11)	0.0213 (15)
C14	0.0358 (9)	0.0635 (11)	0.0622 (11)	0.0022 (8)	0.0118 (8)	0.0231 (9)
C15	0.0438 (10)	0.0546 (10)	0.0511 (10)	−0.0077 (8)	0.0028 (8)	0.0144 (8)
C16	0.0667 (14)	0.0834 (16)	0.0601 (13)	−0.0265 (12)	0.0026 (11)	0.0038 (12)
C17	0.107 (2)	0.0806 (17)	0.0594 (13)	−0.0404 (15)	0.0067 (13)	−0.0107 (12)
C18	0.105 (2)	0.0623 (13)	0.0658 (14)	−0.0101 (13)	0.0267 (13)	−0.0163 (11)
C19	0.0612 (12)	0.0589 (12)	0.0613 (12)	0.0014 (9)	0.0152 (10)	−0.0102 (9)
N11	0.0435 (8)	0.0482 (8)	0.0525 (8)	−0.0004 (6)	0.0092 (6)	−0.0006 (7)
N20	0.0417 (8)	0.0520 (8)	0.0484 (8)	−0.0029 (6)	0.0138 (6)	0.0047 (6)
C20	0.0565 (12)	0.0711 (13)	0.0632 (12)	−0.0047 (10)	0.0224 (10)	0.0149 (10)
C21	0.0851 (17)	0.0725 (14)	0.0640 (13)	−0.0082 (12)	0.0263 (12)	0.0184 (11)
C22	0.0941 (18)	0.0619 (13)	0.0537 (12)	0.0076 (12)	0.0124 (11)	0.0127 (10)
C24	0.0443 (9)	0.0451 (9)	0.0416 (8)	−0.0004 (7)	0.0067 (7)	−0.0065 (7)
C25	0.0356 (8)	0.0490 (9)	0.0449 (9)	−0.0015 (7)	0.0074 (7)	−0.0106 (7)
C26	0.0382 (10)	0.0787 (14)	0.0643 (12)	0.0056 (9)	0.0092 (9)	−0.0058 (10)
C27	0.0356 (10)	0.0932 (17)	0.0808 (15)	−0.0046 (10)	0.0204 (10)	−0.0164 (13)
C28	0.0515 (11)	0.0793 (14)	0.0750 (14)	−0.0152 (11)	0.0347 (10)	−0.0095 (11)
C29	0.0471 (10)	0.0600 (11)	0.0604 (11)	−0.0049 (8)	0.0252 (9)	0.0006 (9)
N21	0.0356 (7)	0.0481 (8)	0.0470 (7)	−0.0026 (6)	0.0156 (6)	−0.0036 (6)
N30	0.0588 (11)	0.0760 (12)	0.0703 (11)	0.0131 (9)	0.0142 (9)	0.0083 (10)
C30	0.0503 (10)	0.0544 (11)	0.0604 (11)	0.0062 (8)	0.0114 (9)	−0.0080 (9)
C31	0.0506 (11)	0.0706 (13)	0.0729 (13)	0.0050 (10)	0.0130 (10)	−0.0043 (11)
C23	0.0614 (12)	0.0612 (12)	0.0510 (10)	0.0114 (9)	0.0057 (9)	0.0024 (9)
C32	0.0615 (14)	0.0809 (16)	0.0920 (17)	−0.0015 (12)	0.0284 (13)	−0.0054 (14)
C33	0.0883 (18)	0.0790 (16)	0.0859 (17)	0.0012 (14)	0.0393 (15)	0.0057 (13)
C34	0.0789 (17)	0.0874 (18)	0.0802 (16)	0.0168 (14)	0.0213 (13)	0.0194 (14)
N40	0.0546 (11)	0.0821 (13)	0.0871 (14)	0.0114 (9)	0.0154 (10)	0.0058 (11)
C40	0.0504 (11)	0.0597 (12)	0.0739 (13)	−0.0028 (9)	0.0149 (10)	0.0118 (10)
C41	0.0511 (12)	0.0830 (16)	0.0892 (17)	−0.0076 (11)	0.0129 (11)	−0.0039 (13)
C42	0.0705 (16)	0.101 (2)	0.0909 (19)	−0.0179 (14)	0.0202 (14)	−0.0150 (16)
C43	0.0837 (18)	0.0873 (18)	0.102 (2)	−0.0051 (14)	0.0361 (16)	−0.0132 (15)
C44	0.0668 (16)	0.095 (2)	0.106 (2)	0.0150 (14)	0.0247 (15)	−0.0003 (17)

Geometric parameters (Å, º)

Mn1—N1	2.1501 (18)	C22—C23	1.381 (3)
Mn1—N2	2.1546 (17)	C22—H22	0.9300
Mn1—N21	2.2669 (13)	C24—C23	1.386 (3)
Mn1—N10	2.2746 (14)	C24—C25	1.479 (2)
Mn1—N20	2.2833 (15)	C25—N21	1.348 (2)
Mn1—N11	2.2859 (15)	C25—C26	1.389 (2)
N1—C1	1.155 (2)	C26—C27	1.372 (3)
C1—S1	1.609 (2)	C26—H26	0.9300
N2—C2	1.154 (2)	C27—C28	1.365 (3)
C2—S2	1.6203 (19)	C27—H27	0.9300
N10—C14	1.339 (3)	C28—C29	1.383 (3)
N10—C10	1.342 (3)	C28—H28	0.9300
C10—C11	1.370 (3)	C29—N21	1.335 (2)
C10—H10	0.9300	C29—H29	0.9300
C11—C12	1.362 (4)	N30—C34	1.326 (3)
C11—H11	0.9300	N30—C30	1.340 (3)
C12—C13	1.377 (4)	C30—C31	1.394 (3)
C12—H12	0.9300	C30—C30^{i}	1.489 (4)
C13—C14	1.396 (3)	C31—C32	1.369 (3)
C13—H13	0.9300	C31—H31	0.9300
C14—C15	1.482 (3)	C23—H23	0.9300
C15—N11	1.348 (2)	C32—C33	1.373 (4)
C15—C16	1.384 (3)	C32—H32	0.9300
C16—C17	1.373 (4)	C33—C34	1.370 (4)
C16—H16	0.9300	C33—H33	0.9300
C17—C18	1.367 (4)	C34—H34	0.9300
C17—H17	0.9300	N40—C44	1.322 (3)
C18—C19	1.380 (3)	N40—C40	1.347 (3)
C18—H18	0.9300	C40—C41	1.384 (3)
C19—N11	1.333 (2)	C40—C40^{ii}	1.479 (5)
C19—H19	0.9300	C41—C42	1.368 (4)
N20—C20	1.335 (2)	C41—H41	0.9300
N20—C24	1.343 (2)	C42—C43	1.371 (4)
C20—C21	1.373 (3)	C42—H42	0.9300
C20—H20	0.9300	C43—C44	1.380 (4)
C21—C22	1.362 (4)	C43—H43	0.9300
C21—H21	0.9300	C44—H44	0.9300
N1—Mn1—N2	96.69 (7)	C22—C21—H21	120.8
N1—Mn1—N21	100.33 (6)	C20—C21—H21	120.8
N2—Mn1—N21	92.88 (6)	C21—C22—C23	119.6 (2)
N1—Mn1—N10	92.04 (7)	C21—C22—H22	120.2
N2—Mn1—N10	97.38 (6)	C23—C22—H22	120.2
N21—Mn1—N10	162.91 (6)	N20—C24—C23	121.42 (18)
N1—Mn1—N20	90.37 (7)	N20—C24—C25	115.79 (15)
N2—Mn1—N20	163.68 (6)	C23—C24—C25	122.79 (17)

N21—Mn1—N20	71.33 (5)	N21—C25—C26	121.16 (18)
N10—Mn1—N20	97.05 (5)	N21—C25—C24	115.91 (14)
N1—Mn1—N11	163.00 (6)	C26—C25—C24	122.92 (17)
N2—Mn1—N11	89.80 (6)	C27—C26—C25	119.4 (2)
N21—Mn1—N11	95.00 (5)	C27—C26—H26	120.3
N10—Mn1—N11	71.49 (6)	C25—C26—H26	120.3
N20—Mn1—N11	87.59 (5)	C28—C27—C26	119.67 (19)
C1—N1—Mn1	161.31 (18)	C28—C27—H27	120.2
N1—C1—S1	179.3 (2)	C26—C27—H27	120.2
C2—N2—Mn1	175.86 (16)	C27—C28—C29	118.3 (2)
N2—C2—S2	179.25 (19)	C27—C28—H28	120.8
C14—N10—C10	118.54 (17)	C29—C28—H28	120.8
C14—N10—Mn1	117.53 (12)	N21—C29—C28	123.0 (2)
C10—N10—Mn1	123.21 (14)	N21—C29—H29	118.5
N10—C10—C11	123.5 (2)	C28—C29—H29	118.5
N10—C10—H10	118.3	C29—N21—C25	118.38 (15)
C11—C10—H10	118.3	C29—N21—Mn1	123.00 (12)
C12—C11—C10	118.1 (3)	C25—N21—Mn1	118.53 (11)
C12—C11—H11	121.0	C34—N30—C30	117.5 (2)
C10—C11—H11	121.0	N30—C30—C31	121.5 (2)
C11—C12—C13	119.9 (2)	N30—C30—C30^{i}	116.7 (2)
C11—C12—H12	120.0	C31—C30—C30^{i}	121.8 (2)
C13—C12—H12	120.0	C32—C31—C30	119.3 (2)
C12—C13—C14	119.2 (3)	C32—C31—H31	120.4
C12—C13—H13	120.4	C30—C31—H31	120.4
C14—C13—H13	120.4	C22—C23—C24	119.0 (2)
N10—C14—C13	120.7 (2)	C22—C23—H23	120.5
N10—C14—C15	116.21 (15)	C24—C23—H23	120.5
C13—C14—C15	123.0 (2)	C31—C32—C33	119.4 (2)
N11—C15—C16	120.7 (2)	C31—C32—H32	120.3
N11—C15—C14	115.93 (16)	C33—C32—H32	120.3
C16—C15—C14	123.36 (19)	C34—C33—C32	117.6 (2)
C17—C16—C15	119.3 (2)	C34—C33—H33	121.2
C17—C16—H16	120.3	C32—C33—H33	121.2
C15—C16—H16	120.3	N30—C34—C33	124.7 (2)
C18—C17—C16	120.3 (2)	N30—C34—H34	117.7
C18—C17—H17	119.9	C33—C34—H34	117.7
C16—C17—H17	119.9	C44—N40—C40	117.4 (2)
C17—C18—C19	117.6 (2)	N40—C40—C41	121.3 (2)
C17—C18—H18	121.2	N40—C40—C40^{ii}	116.7 (2)
C19—C18—H18	121.2	C41—C40—C40^{ii}	122.0 (3)
N11—C19—C18	123.2 (2)	C42—C41—C40	119.8 (2)
N11—C19—H19	118.4	C42—C41—H41	120.1
C18—C19—H19	118.4	C40—C41—H41	120.1
C19—N11—C15	118.94 (17)	C41—C42—C43	119.5 (3)
C19—N11—Mn1	123.75 (13)	C41—C42—H42	120.3
C15—N11—Mn1	117.23 (13)	C43—C42—H42	120.3
C20—N20—C24	118.28 (17)	C42—C43—C44	117.2 (3)

C20—N20—Mn1	123.43 (13)	C42—C43—H43	121.4
C24—N20—Mn1	118.28 (11)	C44—C43—H43	121.4
N20—C20—C21	123.3 (2)	N40—C44—C43	124.8 (3)
N20—C20—H20	118.3	N40—C44—H44	117.6
C21—C20—H20	118.3	C43—C44—H44	117.6
C22—C21—C20	118.4 (2)		

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