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Hexakis(dimethylformamide-κO)-manganese(II) (dimethylformamide-κO)-pentakis(thiocyanato-κN)chromate(III)

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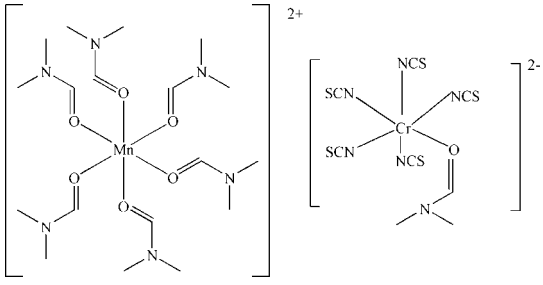
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(N–C) = 0.007 Å; R factor = 0.053; wR factor = 0.100; data-to-parameter ratio = 20.8.

The title compound, $[Mn(C_3H_7NO)_6][Cr(NCS)_5(C_3H_7NO)]$, was obtained unintentionally as a product of an attempted synthesis of heterometallic complexes based on Reineckes anion using manganese powder, Reineckes salt and 1-(2-hydroxyethyl)tetrazole as starting materials. The crystal structure of the complex consists of an $[Mn(dmf)_6]^{2+}$ cation and a $[Cr(NCS)_5(dmf)]^{2-}$ anion (dmf = dimethylformamide). The Mn^{II} and Cr^{III} atoms show a slightly distorted octahedral MnO_6 and CrN_5O coordination geometries with adjacent angles in the range 85.29 (13)–95.96 (14)°.

Related literature

For structures including $[Mn(dmf)_6]^{2+}$ cations, see: Khutornoi *et al.* (2002); Bencini *et al.* (1992). For background to direct synthesis, see: Makhankova (2011).



Experimental

Crystal data

$[Mn(C_3H_7NO)_6][Cr(NCS)_5(C_3H_7NO)]$
M_r = 909.01
Monoclinic, $P2_1/c$
a = 15.327 (3) Å
b = 17.742 (2) Å
c = 17.278 (2) Å
β = 110.36 (2)°
V = 4404.9 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 294 K
0.40 × 0.20 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.735, T_{max} = 0.922
20206 measured reflections
9620 independent reflections
2863 reflections with $I > 2\sigma(I)$
R_{int} = 0.092

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.100
S = 0.67
9620 reflections
463 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cr1—N8	1.969 (4)	Mn1—O4	2.133 (4)
Cr1—N9	1.977 (4)	Mn1—O3	2.140 (4)
Cr1—N11	1.996 (4)	Mn1—O1	2.140 (3)
Cr1—O7	1.999 (3)	Mn1—O6	2.143 (3)
Cr1—N7	2.002 (4)	Mn1—O5	2.167 (3)
Cr1—N12	2.006 (4)	Mn1—O2	2.171 (3)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2010); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2010); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XP* in *SHELXTL*; software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Viktoriya V. Dyakonenko for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2065).

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supporting information

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Hexakis(dimethylformamide-κO)manganese(II) (dimethylformamide-κO)pentakis(thiocyanato-κN)chromate(III)

Valentyna V. Semenaka, Oksana V. Nesterova, Vladimir N. Kokozay, Irina V. Omelchenko and Oleg V. Shishkin

S1. Comment

Continuing our research on direct synthesis of heterometallic complexes using Reineckes salt, $(NH)_4[Cr(NCS)_4(NH_3)_2].H_2O$, as a source of building blocks or metalloligands (Makhankova, 2011), we present here a new Mn^{II}/Cr^{III} complex, which was obtained unintentionally as a product of an attempted reaction of manganese powder, Reineckes salt and 1-(2-hydroxyethyl)tetrazole in dmf (dimethylformamide). The crystal structure of the complex consists of a slightly distorted octahedral $[Mn(dmf)_6]^{2+}$ cation and $[Cr(NCS)_5(dmf)]^{+}$ anion blocks (Fig. 1). Manganese centers have octahedral coordination environment of six oxygen atoms of dmf ligands. The Mn–O bond lengths vary in the range of 2.133 (4) – 2.171 (3) Å that is in good agreement with those in $[Mn(dmf)_6][Mo_6Br_8(NCS)_6]$ [2.152 Å (Khutornoi *et al.*, 2002)]. The *cis* and *trans* O–Mn–O bond angles vary from 85.29 (13)° to 95.96 (14)° and from 173.81 (14)° to 175.64 (13)°, respectively. The Cr(III) ions have ON_5 environment formed by N atoms of NCS groups and O atom of dmf that replace NH_3 groups of initial complex anion of Reineckes salt. The Cr–N(O) bond lengths vary from 1.969 (4) to 2.006 (4) Å. The *cis* and *trans* N–Cr–N(O) bond angles vary from 86.51 (13)° to 92.83 (16)° and from 175.62 (12)° to 179.24 (17)°, respectively.

S2. Experimental

Manganese powder (0.069 g, 1.25 mmol), $NH_4[Cr(NCS)_4(NH_3)_2]\cdot H_2O$ (0.443 g, 1.25 mmol), NH_4NCS (0.095 g, 1.25 mmol), 1-(2-hydroxyethyl)tetrazole (0.5 g, 2.5 mmol) and dmf (20 ml) were heated to 50–60° and stirred magnetically until total dissolution of the manganese was observed (4.2 h). Dark blue crystals suitable for the X-ray crystallographic study were deposited after successive addition of Pr^iOH into the resulting blue solution. The crystals were filtered off, washed with dry Pr^iOH and finally dried *in vacuo* at room temperature. Yield: 0.17 g. Anal. Calc. for $C_{26}H_{49}MnCrN_{12}O_7S_5$: Mn, 6.04; Cr, 5.72; C, 34.35; H, 2.86; N, 18.49; S, 17.63. Found: Mn, 6.0; Cr, 5.9; C, 34.5; H, 3.0; N, 18.6; S, 17.7% IR (KBr, cm^{-1}): 3420(w, br), 2964(sh), 2930(w or m), 2807(w), 2116(sh), 2081(*vs*), 1688(sh), 1653(*vs*), 1556(sh), 1496(sh), 1425(sh), 1373(*m*), 1241(m or sh), 1111(*m*), 1058(sh), 971(w), 865(w), 708(sh), 673(*m*), 481(w). The compound is sparingly soluble in dmso and dmf, insoluble in water.

S3. Refinement

Structure was solved by direct methods and refined against F^2 within anisotropic approximation for all non-hydrogen atoms. All hydrogen atoms were located geometrically and refined within riding model approximation with C—H = 0.96 (1) Å and U_{iso}(H)= 1.5Ueq(C) for methyl group H atoms, and C—H = 0.93 (1) Å and U_{iso}(H)= 1.2Ueq(C) for carbonyl H atoms. O3—C7 bond length was restrained to 1.250 (2) Å value, N3—C7 to 1.330 (3) Å, N3—C8 and N3—C9 to 1.450 (2) Å. Some pairs of atoms (C1 and C7, C3 and C8, C5 and C9) were constrained to have the same

anisotropic displacement parameters.

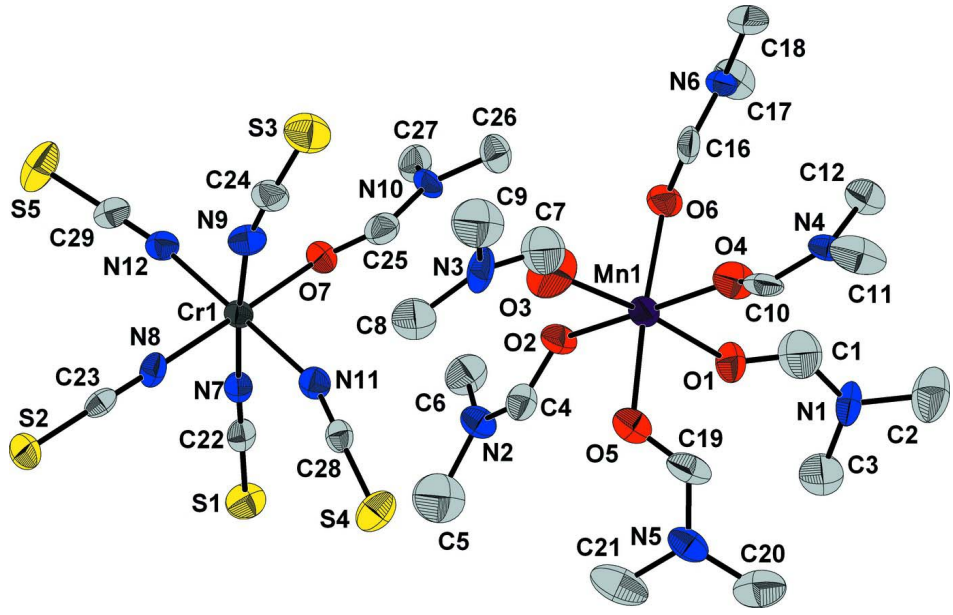

Figure 1

Crystal structure of the complex, showing the atom numbering, with 45% probability displacement ellipsoids

Hexakis(dimethylformamide-*κO*)manganese(II) (dimethylformamide-*κO*)pentakis(thiocyanato-*κN*)chromate(III)

Crystal data

$[Mn(C_3H_7NO)_6][Cr(NCS)_5(C_3H_7NO)]$
M_r = 909.01
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.327 (3) Å
b = 17.742 (2) Å
c = 17.278 (2) Å
β = 110.36 (2)°
V = 4404.9 (11) Å^3
Z = 4
$F(000)$ = 1896
D_x = 1.371 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 300 reflections
θ = 3.2–28.5°
μ = 0.82 mm^{-1}
T = 294 K
Block, blue
0.40 × 0.20 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1827 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.735, T_{max} = 0.922
20206 measured reflections
9620 independent reflections
2863 reflections with $I > 2\sigma(I)$
R_{int} = 0.092
θ_{max} = 27.5°, θ_{min} = 2.7°
h = −19→19
k = −23→22
l = −12→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.100
S = 0.67
9620 reflections
463 parameters
4 restraints

104 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.85$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}

Special details

Experimental. Absorption correction: *CrysAlis RED* (Oxford Diffraction, 2010) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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}
Cr1	0.22880 (5)	0.21566 (4)	0.23165 (5)	0.0298 (2)
Mn1	0.70617 (5)	0.21884 (4)	0.26170 (5)	0.0372 (2)
N1	0.8824 (3)	0.0894 (2)	0.1622 (2)	0.0450 (12)
N2	0.4621 (3)	0.0800 (2)	0.1678 (3)	0.0393 (11)
N3	0.6171 (3)	0.3210 (2)	0.4454 (3)	0.0520 (13)
N4	0.9826 (3)	0.3188 (2)	0.3868 (2)	0.0329 (10)
N6	0.7430 (3)	0.4134 (2)	0.1329 (3)	0.0361 (10)
N7	0.1901 (3)	0.1206 (2)	0.1662 (2)	0.0315 (10)
N8	0.1676 (3)	0.1834 (2)	0.3092 (2)	0.0340 (10)
N9	0.2747 (3)	0.3103 (2)	0.2927 (3)	0.0423 (12)
N10	0.3868 (3)	0.3073 (2)	0.1029 (2)	0.0329 (10)
N11	0.3458 (3)	0.1635 (2)	0.2994 (2)	0.0357 (11)
N12	0.1107 (3)	0.2669 (2)	0.1626 (2)	0.0353 (11)
O1	0.7688 (2)	0.14527 (17)	0.1978 (2)	0.0477 (10)
O2	0.5714 (2)	0.17089 (17)	0.1918 (2)	0.0441 (9)
O3	0.6391 (3)	0.2817 (2)	0.3308 (3)	0.0773 (13)
O4	0.8408 (2)	0.2668 (2)	0.3198 (2)	0.0544 (11)
O5	0.7315 (2)	0.12866 (18)	0.35140 (19)	0.0438 (9)
O6	0.6900 (2)	0.30489 (18)	0.1707 (2)	0.0447 (9)
O7	0.2835 (2)	0.24700 (16)	0.14712 (19)	0.0387 (9)
S1	0.15171 (9)	−0.02018 (7)	0.08949 (9)	0.0478 (4)
S2	0.06542 (10)	0.13086 (8)	0.40395 (9)	0.0548 (4)
S3	0.38322 (11)	0.43885 (8)	0.35746 (10)	0.0648 (5)
S4	0.46635 (9)	0.06510 (8)	0.41462 (9)	0.0527 (4)
S5	−0.06415 (10)	0.32690 (9)	0.08380 (9)	0.0639 (5)
C1	0.8415 (5)	0.1480 (4)	0.1847 (4)	0.0816 (15)
H1A	0.8712	0.1944	0.1908	0.098*

C2	0.9712 (4)	0.0939 (3)	0.1524 (4)	0.077 (2)
H2A	0.9950	0.1443	0.1642	0.115*
H2B	0.9647	0.0811	0.0967	0.115*
H2C	1.0136	0.0594	0.1898	0.115*
C3	0.8435 (4)	0.0154 (3)	0.1565 (4)	0.1045 (19)
H3A	0.7820	0.0187	0.1591	0.157*
H3B	0.8820	−0.0149	0.2014	0.157*
H3C	0.8402	−0.0072	0.1051	0.157*
C4	0.5363 (4)	0.1137 (3)	0.2144 (3)	0.0405 (13)
H4A	0.5658	0.0952	0.2675	0.049*
C5	0.4271 (4)	0.0114 (3)	0.1972 (4)	0.0868 (15)
H5A	0.4554	0.0077	0.2561	0.130*
H5B	0.4426	−0.0325	0.1720	0.130*
H5C	0.3608	0.0146	0.1823	0.130*
C6	0.4090 (4)	0.1043 (3)	0.0861 (3)	0.0569 (16)
H6A	0.4339	0.1509	0.0747	0.085*
H6B	0.3454	0.1116	0.0818	0.085*
H6C	0.4119	0.0668	0.0471	0.085*
N5	0.8034 (3)	0.0143 (3)	0.3822 (2)	0.0483 (12)
C7	0.6621 (4)	0.3234 (3)	0.3923 (3)	0.0816 (15)
H7A	0.7114	0.3568	0.4012	0.098*
C8	0.5470 (4)	0.2770 (3)	0.4630 (5)	0.1045 (19)
H8A	0.5281	0.2358	0.4248	0.157*
H8B	0.4941	0.3083	0.4578	0.157*
H8C	0.5721	0.2577	0.5183	0.157*
C9	0.6448 (4)	0.3856 (3)	0.5001 (3)	0.0868 (15)
H9A	0.6959	0.4108	0.4912	0.130*
H9B	0.6634	0.3689	0.5564	0.130*
H9C	0.5933	0.4198	0.4888	0.130*
C10	0.9062 (4)	0.2806 (3)	0.3830 (3)	0.0426 (14)
H10A	0.9024	0.2632	0.4325	0.051*
C11	1.0567 (4)	0.3337 (3)	0.4630 (3)	0.0706 (19)
H11A	1.0388	0.3172	0.5083	0.106*
H11B	1.0694	0.3868	0.4679	0.106*
H11C	1.1116	0.3070	0.4639	0.106*
C12	0.9917 (4)	0.3480 (3)	0.3130 (3)	0.0528 (15)
H12A	0.9434	0.3277	0.2659	0.079*
H12B	1.0513	0.3341	0.3107	0.079*
H12C	0.9867	0.4020	0.3127	0.079*
C16	0.7301 (3)	0.3674 (3)	0.1886 (3)	0.0398 (14)
H16A	0.7518	0.3824	0.2436	0.048*
C17	0.7130 (3)	0.3912 (3)	0.0463 (3)	0.0555 (16)
H17A	0.6964	0.3388	0.0413	0.083*
H17B	0.7628	0.3994	0.0257	0.083*
H17C	0.6601	0.4208	0.0150	0.083*
C18	0.7886 (4)	0.4847 (2)	0.1548 (3)	0.0536 (15)
H18A	0.8060	0.4923	0.2132	0.080*
H18B	0.7471	0.5242	0.1260	0.080*

H18C	0.8433	0.4855	0.1397	0.080*
C19	0.8004 (4)	0.0875 (3)	0.3649 (3)	0.0493 (15)
H19A	0.8545	0.1096	0.3629	0.059*
C20	0.8854 (4)	−0.0308 (3)	0.3888 (3)	0.0727 (19)
H20A	0.9328	0.0012	0.3823	0.109*
H20B	0.8689	−0.0686	0.3465	0.109*
H20C	0.9082	−0.0546	0.4420	0.109*
C21	0.7238 (4)	−0.0250 (3)	0.3849 (3)	0.074 (2)
H21A	0.6763	0.0106	0.3842	0.110*
H21B	0.7404	−0.0545	0.4345	0.110*
H21C	0.7008	−0.0576	0.3378	0.110*
C22	0.1741 (3)	0.0613 (3)	0.1342 (3)	0.0325 (12)
C23	0.1256 (3)	0.1623 (2)	0.3479 (3)	0.0297 (12)
C24	0.3185 (4)	0.3642 (3)	0.3215 (3)	0.0420 (14)
C25	0.3606 (4)	0.2789 (3)	0.1597 (3)	0.0421 (13)
H25A	0.4015	0.2822	0.2139	0.050*
C26	0.4764 (3)	0.3431 (3)	0.1240 (3)	0.0424 (13)
H26A	0.5055	0.3450	0.1830	0.064*
H26B	0.4685	0.3935	0.1022	0.064*
H26C	0.5148	0.3149	0.1009	0.064*
C27	0.3291 (3)	0.3023 (3)	0.0172 (3)	0.0440 (14)
H27A	0.2659	0.2927	0.0128	0.066*
H27B	0.3508	0.2619	−0.0085	0.066*
H27C	0.3322	0.3489	−0.0100	0.066*
C28	0.3953 (3)	0.1229 (3)	0.3477 (3)	0.0314 (12)
C29	0.0390 (4)	0.2920 (3)	0.1304 (3)	0.0383 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0311 (4)	0.0319 (4)	0.0270 (5)	0.0015 (4)	0.0110 (4)	0.0068 (4)
Mn1	0.0416 (5)	0.0327 (4)	0.0430 (5)	−0.0013 (4)	0.0221 (4)	−0.0004 (5)
N1	0.026 (2)	0.060 (3)	0.051 (3)	0.000 (2)	0.016 (2)	−0.020 (3)
N2	0.043 (3)	0.038 (3)	0.034 (3)	−0.010 (2)	0.011 (2)	−0.001 (2)
N3	0.041 (3)	0.088 (3)	0.036 (3)	0.024 (3)	0.025 (2)	0.012 (3)
N4	0.042 (3)	0.023 (2)	0.028 (3)	−0.009 (2)	0.006 (2)	−0.002 (2)
N6	0.033 (2)	0.029 (2)	0.045 (3)	−0.001 (2)	0.012 (2)	0.011 (2)
N7	0.028 (2)	0.041 (2)	0.026 (3)	0.004 (2)	0.009 (2)	0.009 (2)
N8	0.029 (2)	0.045 (3)	0.028 (3)	0.009 (2)	0.012 (2)	0.001 (2)
N9	0.049 (3)	0.037 (3)	0.037 (3)	0.004 (2)	0.010 (2)	0.006 (2)
N10	0.036 (3)	0.039 (3)	0.030 (3)	−0.002 (2)	0.018 (2)	0.013 (2)
N11	0.038 (3)	0.041 (3)	0.030 (3)	0.001 (2)	0.014 (2)	0.004 (2)
N12	0.042 (3)	0.032 (3)	0.033 (3)	0.002 (2)	0.014 (2)	0.003 (2)
O1	0.043 (2)	0.057 (2)	0.051 (3)	0.001 (2)	0.027 (2)	−0.004 (2)
O2	0.049 (2)	0.0298 (18)	0.055 (3)	−0.0079 (19)	0.021 (2)	0.0002 (19)
O3	0.082 (3)	0.059 (2)	0.083 (3)	−0.003 (2)	0.018 (3)	−0.047 (3)
O4	0.043 (2)	0.055 (3)	0.050 (3)	−0.011 (2)	−0.004 (2)	0.007 (2)
O5	0.047 (2)	0.048 (2)	0.031 (2)	−0.011 (2)	0.007 (2)	0.0022 (19)

O6	0.034 (2)	0.040 (2)	0.053 (3)	−0.0068 (18)	0.0061 (18)	0.0076 (19)
O7	0.040 (2)	0.0407 (19)	0.041 (2)	−0.0003 (18)	0.0208 (18)	0.0063 (17)
S1	0.0461 (9)	0.0402 (8)	0.0479 (10)	−0.0033 (8)	0.0047 (8)	−0.0079 (8)
S2	0.0556 (10)	0.0605 (9)	0.0643 (11)	0.0111 (8)	0.0410 (9)	0.0229 (9)
S3	0.0703 (11)	0.0513 (9)	0.0672 (12)	−0.0134 (9)	0.0169 (10)	−0.0068 (9)
S4	0.0452 (9)	0.0624 (9)	0.0395 (9)	0.0171 (8)	0.0008 (7)	0.0036 (8)
S5	0.0514 (10)	0.0932 (12)	0.0425 (10)	0.0329 (10)	0.0104 (8)	−0.0002 (9)
C1	0.059 (3)	0.084 (4)	0.095 (4)	−0.006 (3)	0.019 (3)	0.003 (3)
C2	0.061 (4)	0.088 (5)	0.088 (5)	−0.001 (4)	0.035 (4)	−0.036 (4)
C3	0.099 (4)	0.053 (3)	0.187 (6)	0.004 (3)	0.083 (4)	0.008 (3)
C4	0.035 (3)	0.043 (3)	0.043 (4)	0.001 (3)	0.014 (3)	−0.008 (3)
C5	0.073 (3)	0.087 (3)	0.082 (4)	−0.012 (3)	0.003 (3)	0.001 (3)
C6	0.054 (4)	0.058 (4)	0.052 (4)	0.004 (3)	0.009 (3)	−0.002 (3)
N5	0.060 (3)	0.051 (3)	0.036 (3)	−0.011 (3)	0.019 (3)	0.009 (3)
C7	0.059 (3)	0.084 (4)	0.095 (4)	−0.006 (3)	0.019 (3)	0.003 (3)
C8	0.099 (4)	0.053 (3)	0.187 (6)	0.004 (3)	0.083 (4)	0.008 (3)
C9	0.073 (3)	0.087 (3)	0.082 (4)	−0.012 (3)	0.003 (3)	0.001 (3)
C10	0.072 (4)	0.024 (3)	0.041 (4)	0.003 (3)	0.030 (3)	0.012 (3)
C11	0.074 (4)	0.061 (4)	0.046 (4)	−0.032 (4)	−0.019 (3)	0.008 (3)
C12	0.056 (4)	0.046 (3)	0.056 (4)	−0.009 (3)	0.019 (3)	0.001 (3)
C16	0.028 (3)	0.055 (4)	0.043 (4)	0.010 (3)	0.022 (3)	0.005 (3)
C17	0.042 (3)	0.068 (4)	0.042 (4)	−0.012 (3)	−0.004 (3)	0.010 (3)
C18	0.061 (4)	0.029 (3)	0.072 (4)	−0.002 (3)	0.024 (3)	0.004 (3)
C19	0.055 (4)	0.041 (4)	0.040 (4)	−0.019 (3)	0.002 (3)	0.008 (3)
C20	0.101 (5)	0.055 (4)	0.060 (5)	0.010 (4)	0.026 (4)	0.009 (4)
C21	0.111 (6)	0.062 (4)	0.042 (4)	−0.035 (4)	0.019 (4)	−0.001 (3)
C22	0.023 (3)	0.048 (3)	0.022 (3)	0.006 (3)	0.002 (2)	0.011 (3)
C23	0.028 (3)	0.029 (3)	0.024 (3)	0.009 (2)	−0.001 (2)	−0.002 (2)
C24	0.054 (4)	0.041 (3)	0.035 (4)	0.003 (3)	0.019 (3)	0.010 (3)
C25	0.041 (3)	0.031 (3)	0.053 (4)	0.003 (3)	0.014 (3)	−0.004 (3)
C26	0.030 (3)	0.055 (3)	0.038 (3)	−0.007 (3)	0.008 (3)	−0.001 (3)
C27	0.035 (3)	0.056 (3)	0.038 (4)	0.006 (3)	0.009 (3)	0.008 (3)
C28	0.031 (3)	0.036 (3)	0.031 (3)	−0.002 (3)	0.015 (3)	−0.005 (3)
C29	0.054 (4)	0.035 (3)	0.029 (3)	0.011 (3)	0.019 (3)	0.002 (3)

Geometric parameters (Å, º)

Cr1—N8	1.969 (4)	C2—H2C	0.9600
Cr1—N9	1.977 (4)	C3—H3A	0.9600
Cr1—N11	1.996 (4)	C3—H3B	0.9600
Cr1—O7	1.999 (3)	C3—H3C	0.9600
Cr1—N7	2.002 (4)	C4—H4A	0.9300
Cr1—N12	2.006 (4)	C5—H5A	0.9600
Mn1—O4	2.133 (4)	C5—H5B	0.9600
Mn1—O3	2.140 (4)	C5—H5C	0.9600
Mn1—O1	2.140 (3)	C6—H6A	0.9600
Mn1—O6	2.143 (3)	C6—H6B	0.9600
Mn1—O5	2.167 (3)	C6—H6C	0.9600

Mn1—O2	2.171 (3)	N5—C19	1.329 (6)
N1—C1	1.340 (7)	N5—C21	1.421 (6)
N1—C2	1.430 (6)	N5—C20	1.460 (6)
N1—C3	1.432 (6)	C7—H7A	0.9300
N2—C4	1.290 (6)	C8—H8A	0.9600
N2—C6	1.428 (6)	C8—H8B	0.9600
N2—C5	1.488 (6)	C8—H8C	0.9600
N3—C7	1.326 (2)	C9—H9A	0.9600
N3—C8	1.444 (2)	C9—H9B	0.9600
N3—C9	1.451 (2)	C9—H9C	0.9600
N4—C10	1.334 (6)	C10—H10A	0.9300
N4—C12	1.428 (5)	C11—H11A	0.9600
N4—C11	1.434 (6)	C11—H11B	0.9600
N6—C16	1.328 (5)	C11—H11C	0.9600
N6—C18	1.432 (5)	C12—H12A	0.9600
N6—C17	1.457 (5)	C12—H12B	0.9600
N7—C22	1.174 (5)	C12—H12C	0.9600
N8—C23	1.142 (5)	C16—H16A	0.9300
N9—C24	1.174 (5)	C17—H17A	0.9600
N10—C25	1.284 (5)	C17—H17B	0.9600
N10—C27	1.440 (5)	C17—H17C	0.9600
N10—C26	1.441 (5)	C18—H18A	0.9600
N11—C28	1.162 (5)	C18—H18B	0.9600
N12—C29	1.136 (5)	C18—H18C	0.9600
O1—C1	1.213 (6)	C19—H19A	0.9300
O2—C4	1.270 (5)	C20—H20A	0.9600
O3—C7	1.242 (2)	C20—H20B	0.9600
O4—C10	1.223 (6)	C20—H20C	0.9600
O5—C19	1.238 (6)	C21—H21A	0.9600
O6—C16	1.254 (5)	C21—H21B	0.9600
O7—C25	1.260 (5)	C21—H21C	0.9600
S1—C22	1.618 (5)	C25—H25A	0.9300
S2—C23	1.649 (5)	C26—H26A	0.9600
S3—C24	1.642 (6)	C26—H26B	0.9600
S4—C28	1.642 (5)	C26—H26C	0.9600
S5—C29	1.626 (6)	C27—H27A	0.9600
C1—H1A	0.9300	C27—H27B	0.9600
C2—H2A	0.9600	C27—H27C	0.9600
C2—H2B	0.9600		

N8—Cr1—N9	92.83 (16)	N2—C6—H6C	109.5
N8—Cr1—N11	90.52 (15)	H6A—C6—H6C	109.5
N9—Cr1—N11	90.03 (16)	H6B—C6—H6C	109.5
N8—Cr1—O7	176.41 (15)	C19—N5—C21	121.6 (5)
N9—Cr1—O7	89.51 (14)	C19—N5—C20	121.0 (5)
N11—Cr1—O7	92.20 (14)	C21—N5—C20	117.0 (5)
N8—Cr1—N7	91.22 (15)	O3—C7—N3	120.8 (5)
N9—Cr1—N7	175.62 (15)	O3—C7—H7A	119.6

N11—Cr1—N7	88.27 (15)	N3—C7—H7A	119.6
O7—Cr1—N7	86.51 (13)	N3—C8—H8A	109.5
N8—Cr1—N12	89.55 (15)	N3—C8—H8B	109.5
N9—Cr1—N12	90.72 (16)	H8A—C8—H8B	109.5
N11—Cr1—N12	179.24 (17)	N3—C8—H8C	109.5
O7—Cr1—N12	87.70 (14)	H8A—C8—H8C	109.5
N7—Cr1—N12	90.97 (15)	H8B—C8—H8C	109.5
O4—Mn1—O3	95.96 (14)	N3—C9—H9A	109.5
O4—Mn1—O1	87.26 (14)	N3—C9—H9B	109.5
O3—Mn1—O1	173.81 (14)	H9A—C9—H9B	109.5
O4—Mn1—O6	84.69 (13)	N3—C9—H9C	109.5
O3—Mn1—O6	94.73 (14)	H9A—C9—H9C	109.5
O1—Mn1—O6	90.83 (12)	H9B—C9—H9C	109.5
O4—Mn1—O5	93.14 (13)	O4—C10—N4	125.3 (5)
O3—Mn1—O5	89.24 (15)	O4—C10—H10A	117.3
O1—Mn1—O5	85.29 (13)	N4—C10—H10A	117.3
O6—Mn1—O5	175.64 (13)	N4—C11—H11A	109.5
O4—Mn1—O2	174.71 (14)	N4—C11—H11B	109.5
O3—Mn1—O2	88.00 (13)	H11A—C11—H11B	109.5
O1—Mn1—O2	89.13 (12)	N4—C11—H11C	109.5
O6—Mn1—O2	91.51 (13)	H11A—C11—H11C	109.5
O5—Mn1—O2	90.41 (12)	H11B—C11—H11C	109.5
C1—N1—C2	123.5 (5)	N4—C12—H12A	109.5
C1—N1—C3	120.3 (4)	N4—C12—H12B	109.5
C2—N1—C3	115.8 (4)	H12A—C12—H12B	109.5
C4—N2—C6	123.5 (4)	N4—C12—H12C	109.5
C4—N2—C5	120.7 (5)	H12A—C12—H12C	109.5
C6—N2—C5	115.8 (4)	H12B—C12—H12C	109.5
C7—N3—C8	140.2 (5)	O6—C16—N6	123.2 (5)
C7—N3—C9	108.7 (4)	O6—C16—H16A	118.4
C8—N3—C9	111.1 (4)	N6—C16—H16A	118.4
C10—N4—C12	119.9 (4)	N6—C17—H17A	109.5
C10—N4—C11	122.7 (4)	N6—C17—H17B	109.5
C12—N4—C11	117.4 (4)	H17A—C17—H17B	109.5
C16—N6—C18	122.2 (5)	N6—C17—H17C	109.5
C16—N6—C17	120.4 (4)	H17A—C17—H17C	109.5
C18—N6—C17	117.4 (4)	H17B—C17—H17C	109.5
C22—N7—Cr1	173.3 (4)	N6—C18—H18A	109.5
C23—N8—Cr1	173.6 (4)	N6—C18—H18B	109.5
C24—N9—Cr1	164.1 (4)	H18A—C18—H18B	109.5
C25—N10—C27	121.2 (4)	N6—C18—H18C	109.5
C25—N10—C26	120.2 (4)	H18A—C18—H18C	109.5
C27—N10—C26	118.5 (4)	H18B—C18—H18C	109.5
C28—N11—Cr1	159.7 (4)	O5—C19—N5	125.4 (5)
C29—N12—Cr1	171.1 (4)	O5—C19—H19A	117.3
C1—O1—Mn1	132.7 (4)	N5—C19—H19A	117.3
C4—O2—Mn1	124.3 (3)	N5—C20—H20A	109.5
C7—O3—Mn1	137.7 (4)	N5—C20—H20B	109.5

C10—O4—Mn1	149.2 (4)	H20A—C20—H20B	109.5
C19—O5—Mn1	120.0 (3)	N5—C20—H20C	109.5
C16—O6—Mn1	121.9 (3)	H20A—C20—H20C	109.5
C25—O7—Cr1	127.3 (3)	H20B—C20—H20C	109.5
O1—C1—N1	125.3 (6)	N5—C21—H21A	109.5
O1—C1—H1A	117.4	N5—C21—H21B	109.5
N1—C1—H1A	117.4	H21A—C21—H21B	109.5
N1—C2—H2A	109.5	N5—C21—H21C	109.5
N1—C2—H2B	109.5	H21A—C21—H21C	109.5
H2A—C2—H2B	109.5	H21B—C21—H21C	109.5
N1—C2—H2C	109.5	N7—C22—S1	179.7 (6)
H2A—C2—H2C	109.5	N8—C23—S2	179.3 (4)
H2B—C2—H2C	109.5	N9—C24—S3	176.3 (5)
N1—C3—H3A	109.5	O7—C25—N10	124.6 (5)
N1—C3—H3B	109.5	O7—C25—H25A	117.7
H3A—C3—H3B	109.5	N10—C25—H25A	117.7
N1—C3—H3C	109.5	N10—C26—H26A	109.5
H3A—C3—H3C	109.5	N10—C26—H26B	109.5
H3B—C3—H3C	109.5	H26A—C26—H26B	109.5
O2—C4—N2	123.6 (5)	N10—C26—H26C	109.5
O2—C4—H4A	118.2	H26A—C26—H26C	109.5
N2—C4—H4A	118.2	H26B—C26—H26C	109.5
N2—C5—H5A	109.5	N10—C27—H27A	109.5
N2—C5—H5B	109.5	N10—C27—H27B	109.5
H5A—C5—H5B	109.5	H27A—C27—H27B	109.5
N2—C5—H5C	109.5	N10—C27—H27C	109.5
H5A—C5—H5C	109.5	H27A—C27—H27C	109.5
H5B—C5—H5C	109.5	H27B—C27—H27C	109.5
N2—C6—H6A	109.5	N11—C28—S4	178.8 (4)
N2—C6—H6B	109.5	N12—C29—S5	179.3 (5)
H6A—C6—H6B	109.5		

N8—Cr1—N9—C24	150.7 (15)	O3—Mn1—O6—C16	65.4 (3)
N11—Cr1—N9—C24	60.1 (15)	O1—Mn1—O6—C16	−117.3 (3)
O7—Cr1—N9—C24	−32.1 (15)	O2—Mn1—O6—C16	153.5 (3)
N12—Cr1—N9—C24	−119.7 (15)	N9—Cr1—O7—C25	40.3 (4)
N8—Cr1—N11—C28	17.6 (11)	N11—Cr1—O7—C25	−49.7 (4)
N9—Cr1—N11—C28	110.4 (11)	N7—Cr1—O7—C25	−137.9 (4)
O7—Cr1—N11—C28	−160.1 (11)	N12—Cr1—O7—C25	131.0 (4)
N7—Cr1—N11—C28	−73.6 (11)	Mn1—O1—C1—N1	162.0 (4)
O4—Mn1—O1—C1	−18.3 (5)	C2—N1—C1—O1	−175.8 (6)
O6—Mn1—O1—C1	66.3 (5)	C3—N1—C1—O1	−3.7 (10)
O5—Mn1—O1—C1	−111.7 (5)	Mn1—O2—C4—N2	−170.7 (3)
O2—Mn1—O1—C1	157.8 (5)	C6—N2—C4—O2	−2.0 (7)
O3—Mn1—O2—C4	−85.0 (3)	C5—N2—C4—O2	177.5 (4)
O1—Mn1—O2—C4	89.5 (3)	Mn1—O3—C7—N3	−142.2 (4)
O6—Mn1—O2—C4	−179.7 (3)	C8—N3—C7—O3	8.1 (11)
O5—Mn1—O2—C4	4.2 (3)	C9—N3—C7—O3	−168.0 (5)

O4—Mn1—O3—C7	−10.6 (6)	Mn1—O4—C10—N4	−177.5 (4)
O6—Mn1—O3—C7	−95.8 (6)	C12—N4—C10—O4	1.0 (7)
O5—Mn1—O3—C7	82.5 (6)	C11—N4—C10—O4	179.5 (5)
O2—Mn1—O3—C7	172.9 (6)	Mn1—O6—C16—N6	160.9 (3)
O3—Mn1—O4—C10	55.6 (7)	C18—N6—C16—O6	179.7 (4)
O1—Mn1—O4—C10	−119.1 (7)	C17—N6—C16—O6	−2.2 (6)
O6—Mn1—O4—C10	149.8 (7)	Mn1—O5—C19—N5	−144.6 (4)
O5—Mn1—O4—C10	−34.0 (7)	C21—N5—C19—O5	1.4 (8)
O4—Mn1—O5—C19	−54.4 (4)	C20—N5—C19—O5	173.6 (5)
O3—Mn1—O5—C19	−150.4 (4)	Cr1—O7—C25—N10	−169.8 (3)
O1—Mn1—O5—C19	32.6 (4)	C27—N10—C25—O7	−2.2 (7)
O2—Mn1—O5—C19	121.7 (4)	C26—N10—C25—O7	179.5 (4)
O4—Mn1—O6—C16	−30.2 (3)	Cr1—N12—C29—S5	−77 (43)