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trans-Bis[2-(4-ethyl-4,5-dihydro-1,3-oxazol-2-yl)phenolato-κ^2N,O](thiocyanato-κN)manganese(III)

Yan Zhang, Di Kong, Tian-Fu Liu* and Wen-Guo Xu

The Institute for Chemical Physics, Beijing Institute of Technology, Beijing 100081, People's Republic of China, and, Department of Chemistry, Beijing Institute of Technology, Beijing 100081, People's Republic of China
Correspondence e-mail: liutf@bit.edu.cn

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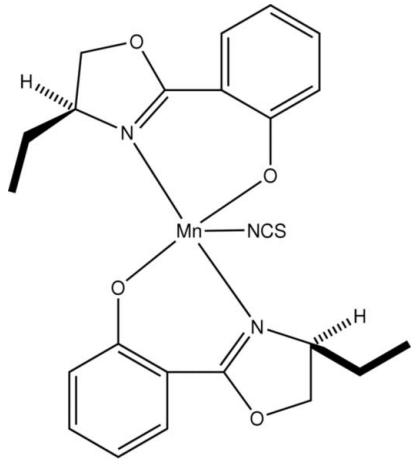
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.111; data-to-parameter ratio = 18.8.

In the title compound, $[Mn(C_{11}H_{12}NO_2)_2(NCS)]$, the coordination polyhedron of the Mn^{III} atom has a distorted square-pyramidal geometry, with the two phenolate ligands coordinated in the basal plane in *trans* positions and the thiocyanate ion coordinated at the apical position.

Related literature

For related literature, see: Addison *et al.* (1984); Braunstein & Naud (2001); Cozzi *et al.* (1995); Godbole *et al.* (2005); Hoogenraad *et al.* (1998); Kandasamy *et al.* (2004); Moreno *et al.* (2002); Serrano *et al.* (1995); Shyu *et al.* (1999).



Experimental

Crystal data

$[Mn(C_{11}H_{12}NO_2)_2(NCS)]$
M_r = 493.45
Triclinic, $P\overline{1}$
a = 9.6816 (13) Å
b = 9.9493 (13) Å
c = 12.5894 (17) Å
α = 91.116 (1)°
β = 97.550 (1)°
γ = 106.415 (1)°
V = 1151.1 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.70 mm^{-1}
T = 273 (2) K
0.49 × 0.42 × 0.42 mm

Data collection

Bruker CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.726, T_{max} = 0.758
10103 measured reflections
5463 independent reflections
4418 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.111
S = 1.03
5463 reflections
291 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Data collection: *SMART* (Bruker, 2003); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2015).

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supplementary materials

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trans-Bis[2-(4-ethyl-4,5-dihydro-1,3-oxazol-2-yl)phenolato-κ^2N,O](thiocyanato-κN)manganese(III)

Y. Zhang, D. Kong, T.-F. Liu and W.-G. Xu

Comment

The chemistry of oxazoline-based ligands continues to be an area of interest due to their use as chirality-transfer auxiliaries in combination with several transition metals in a wide range of asymmetric catalytic reactions (Moreno, *et al.*, 2002). Several metal complexes bearing 2-(2'-hydroxyphenyl)oxazolines have been reported in the literature (Cozzi, *et al.*, 1995; Braunstein, *et al.*, 2001; Kandasamy, *et al.*, 2004).

In the title compound, (I), the manganese(III) ion is coordinated to three nitrogen and two O atoms and has square-pyramidal geometry. The value of the τ parameter (0.131) indicates a square-pyramidal shape of the coordination polyhedron (ideal τ value for square-pyramidal is 0 and for trigonal bipyramid it is 1 (Addison, *et al.*, 1984)). The two ligands are coordinated in the basal plane in the *trans* configuration and involve no intercalation or stacking interactions. The Mn—O bond lengths are 1.8572 (14) and 1.8601 (14) Å, while the Mn—N bond lengths are 2.0156 (15) and 2.0296 (15) Å, respectively, typical for Mn^{III} distances (Hoogenraad, *et al.*, 1998; Shyu, *et al.*, 1999; Godbole, *et al.*, 2005). The manganese(III) ion is slightly above the plane formed by the phenoxo O atoms and oxazoline ring N atoms, as expected for a square-pyramidal geometry; the displacements of the manganese ion from the least-squares plane formed by O1—N1—O3—N2 is 0.2923 (2) Å. The thiocyano ion is coordinated at the apical position at 2.117 (2) Å on the Jahn-Teller axis. No classic hydrogen bonds are present.

Experimental

The racaemic ligand, 2-(4-ethyl-4,5-dihydrooxazol-2-yl)phenol was prepared from 2-hydroxybenzonitrile and 2-aminobutan-1-ol as reported in the literature. (Serrano, *et al.*, 1995).

A solution of 2-(4-ethyl-4,5-dihydrooxazol-2-yl)phenol (30.56 mg, 0.16 mmol) in methanol (1.60 ml) was added to a stirred solution of $Mn(CH_3COO)_2H_2O$ (39.93 mg, 0.2 mmol) in methanol(2.00 ml). A solution of KSCN (20 mg, 0.2 mmol) in methanol (2.0 ml) was added to the mixture after 30 min. The solution color changed slowly from yellow to dark-green. Crystals suitable for diffraction analysis were obtained after a few days.

Refinement

All non-hydrogen atoms were refined with anisotropic thermal parameters. All hydrogen atoms were included at calculated positions with isotropic thermal parameters derived from the attached atom.

Figures

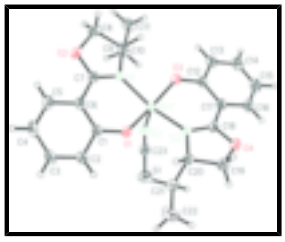


Fig. 1. *ORTEP* plot of (I) displacement ellipsoids are drawn at the 30% probability.

trans-Bis[2-(4-ethyl-4,5-dihydro-1,3-oxazol-2-yl)phenolato- κ^2N,O](thiocyanato-κ*N*)manganese(III)

Crystal data

$[Mn(C_{11}H_{12}NO_2)_2(NCS)]$	$Z = 2$
$M_r = 493.45$	$F_{000} = 512$
Triclinic, $P\overline{1}$	$D_x = 1.424$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.6816$ (13) Å	Cell parameters from 5529 reflections
$b = 9.9493$ (13) Å	$\theta = 2.6$–28.3º
$c = 12.5894$ (17) Å	$\mu = 0.70$ mm^{-1}
$\alpha = 91.116$ (1)º	$T = 273$ (2) K
$\beta = 97.550$ (1)º	Block, dark-green
$\gamma = 106.415$ (1)º	0.49 × 0.42 × 0.42 mm
$V = 1151.1$ (3) Å^3	

Data collection

Bruker CCD area-detector diffractometer	5463 independent reflections
Radiation source: fine-focus sealed tube	4418 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
$T = 291(2)$ K	$\theta_{max} = 28.4$º
φ and ω scans	$\theta_{min} = 2.6$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.726$, $T_{max} = 0.758$	$k = -13 \rightarrow 12$
10103 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.111$	$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 0.4703P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
5463 reflections	$\Delta\rho_{max} = 0.62$ e Å^{-3}
291 parameters	$\Delta\rho_{min} = -0.43$ 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	0.07783 (3)	0.80807 (3)	0.70819 (2)	0.03517 (10)
N3	0.2142 (2)	0.6748 (2)	0.72755 (17)	0.0555 (5)
C23	0.3268 (3)	0.6585 (2)	0.75531 (17)	0.0465 (5)
S1	0.48356 (8)	0.63184 (9)	0.79264 (6)	0.0734 (2)
C1	0.2035 (2)	0.9564 (2)	0.52856 (15)	0.0371 (4)
C6	0.0873 (2)	0.8892 (2)	0.44806 (15)	0.0365 (4)
C2	0.3288 (2)	1.0493 (2)	0.49754 (18)	0.0467 (5)
H2	0.4083	1.0913	0.5491	0.056*
C5	0.0955 (3)	0.9230 (2)	0.34030 (16)	0.0482 (5)
H5	0.0177	0.8806	0.2875	0.058*
C3	0.3348 (3)	1.0788 (2)	0.39084 (19)	0.0540 (6)
H3	0.4185	1.1400	0.3716	0.065*
C4	0.2172 (3)	1.0181 (3)	0.31225 (18)	0.0569 (6)
H4	0.2206	1.0414	0.2413	0.068*
C7	−0.0380 (2)	0.7834 (2)	0.47557 (15)	0.0359 (4)
C9	−0.1961 (2)	0.6198 (2)	0.55887 (16)	0.0399 (4)
H9	−0.2581	0.6408	0.6085	0.048*
C8	−0.2623 (3)	0.6300 (3)	0.44295 (19)	0.0548 (6)
H8A	−0.2934	0.5387	0.4045	0.066*
H8B	−0.3455	0.6665	0.4414	0.066*
O2	−0.14633 (17)	0.72584 (17)	0.39561 (11)	0.0497 (4)
N1	−0.05539 (17)	0.73434 (16)	0.56981 (12)	0.0357 (3)
O1	0.19958 (16)	0.93859 (16)	0.63258 (11)	0.0495 (4)
O3	−0.06990 (15)	0.70613 (16)	0.78009 (11)	0.0477 (4)
N2	0.16638 (17)	0.93136 (16)	0.84442 (12)	0.0353 (3)
O4	0.20307 (19)	0.99270 (17)	1.02044 (12)	0.0564 (4)

C18	0.1332 (2)	0.8983 (2)	0.93893 (15)	0.0383 (4)
C12	−0.0695 (2)	0.6824 (2)	0.88398 (15)	0.0373 (4)
C15	−0.0804 (3)	0.6240 (3)	1.10134 (19)	0.0592 (6)
H15	−0.0835	0.6034	1.1729	0.071*
C13	−0.1750 (2)	0.5662 (2)	0.91394 (19)	0.0482 (5)
H13	−0.2428	0.5077	0.8612	0.058*
C17	0.0289 (2)	0.7714 (2)	0.96596 (15)	0.0390 (4)
C20	0.2867 (2)	1.0670 (2)	0.85636 (16)	0.0428 (5)
H20	0.2608	1.1334	0.8066	0.051*
C19	0.2857 (3)	1.1175 (2)	0.97281 (19)	0.0540 (6)
H19A	0.3839	1.1520	1.0108	0.065*
H19B	0.2388	1.1916	0.9742	0.065*
C14	−0.1796 (3)	0.5374 (2)	1.0208 (2)	0.0550 (6)
H14	−0.2497	0.4593	1.0388	0.066*
C16	0.0218 (3)	0.7398 (3)	1.07457 (17)	0.0515 (5)
H16	0.0874	0.7984	1.1285	0.062*
C10	−0.1721 (2)	0.4775 (2)	0.5803 (2)	0.0511 (5)
H10A	−0.1122	0.4835	0.6493	0.061*
H10B	−0.1206	0.4522	0.5256	0.061*
C21	0.4293 (2)	1.0464 (3)	0.8374 (2)	0.0574 (6)
H21A	0.4179	0.9980	0.7677	0.069*
H21B	0.4598	0.9888	0.8917	0.069*
C11	−0.3165 (3)	0.3638 (3)	0.5801 (3)	0.0693 (8)
H11A	−0.3741	0.3548	0.5108	0.104*
H11B	−0.3682	0.3893	0.6336	0.104*
H11C	−0.2979	0.2760	0.5958	0.104*
C22	0.5469 (3)	1.1901 (4)	0.8417 (3)	0.0969 (12)
H22A	0.5058	1.2562	0.8044	0.145*
H22B	0.6269	1.1792	0.8081	0.145*
H22C	0.5808	1.2239	0.9151	0.145*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.03469 (16)	0.03693 (17)	0.02599 (15)	−0.00256 (11)	0.00502 (10)	−0.00057 (10)
N3	0.0557 (12)	0.0539 (11)	0.0572 (12)	0.0174 (9)	0.0061 (9)	−0.0002 (9)
C23	0.0549 (13)	0.0412 (11)	0.0376 (11)	0.0043 (9)	0.0079 (9)	−0.0037 (8)
S1	0.0523 (4)	0.0912 (5)	0.0715 (5)	0.0190 (4)	−0.0049 (3)	−0.0046 (4)
C1	0.0416 (10)	0.0361 (9)	0.0317 (9)	0.0060 (8)	0.0095 (7)	0.0027 (7)
C6	0.0430 (10)	0.0375 (10)	0.0299 (9)	0.0116 (8)	0.0088 (7)	−0.0009 (7)
C2	0.0451 (11)	0.0454 (11)	0.0429 (11)	−0.0001 (9)	0.0121 (9)	0.0038 (9)
C5	0.0589 (13)	0.0553 (13)	0.0305 (10)	0.0160 (10)	0.0079 (9)	0.0008 (9)
C3	0.0604 (14)	0.0502 (13)	0.0501 (13)	0.0043 (10)	0.0285 (11)	0.0091 (10)
C4	0.0781 (17)	0.0612 (14)	0.0348 (11)	0.0179 (12)	0.0239 (11)	0.0094 (10)
C7	0.0383 (9)	0.0372 (9)	0.0305 (9)	0.0102 (8)	0.0018 (7)	−0.0074 (7)
C9	0.0319 (9)	0.0388 (10)	0.0420 (10)	−0.0006 (7)	0.0058 (8)	−0.0104 (8)
C8	0.0444 (12)	0.0546 (13)	0.0503 (13)	−0.0038 (10)	−0.0057 (10)	−0.0108 (10)
O2	0.0470 (8)	0.0587 (9)	0.0334 (7)	0.0039 (7)	−0.0038 (6)	−0.0069 (6)

N1	0.0340 (8)	0.0344 (8)	0.0320 (8)	−0.0004 (6)	0.0046 (6)	−0.0046 (6)
O1	0.0470 (8)	0.0547 (9)	0.0289 (7)	−0.0132 (7)	0.0035 (6)	0.0031 (6)
O3	0.0438 (8)	0.0533 (9)	0.0316 (7)	−0.0100 (7)	0.0077 (6)	−0.0015 (6)
N2	0.0337 (8)	0.0353 (8)	0.0307 (8)	0.0001 (6)	0.0048 (6)	−0.0009 (6)
O4	0.0680 (10)	0.0535 (9)	0.0324 (7)	−0.0067 (8)	0.0077 (7)	−0.0097 (6)
C18	0.0402 (10)	0.0403 (10)	0.0303 (9)	0.0061 (8)	0.0032 (7)	−0.0035 (7)
C12	0.0398 (10)	0.0366 (10)	0.0345 (9)	0.0062 (8)	0.0126 (7)	0.0015 (7)
C15	0.0733 (16)	0.0631 (15)	0.0413 (12)	0.0130 (12)	0.0209 (11)	0.0170 (11)
C13	0.0478 (12)	0.0410 (11)	0.0499 (12)	−0.0005 (9)	0.0155 (9)	−0.0004 (9)
C17	0.0441 (10)	0.0382 (10)	0.0332 (9)	0.0073 (8)	0.0107 (8)	0.0024 (7)
C20	0.0407 (10)	0.0390 (10)	0.0387 (10)	−0.0031 (8)	0.0028 (8)	−0.0030 (8)
C19	0.0559 (13)	0.0448 (12)	0.0503 (13)	−0.0030 (10)	0.0094 (10)	−0.0107 (10)
C14	0.0633 (14)	0.0454 (12)	0.0548 (13)	0.0046 (10)	0.0262 (11)	0.0143 (10)
C16	0.0583 (13)	0.0580 (13)	0.0340 (10)	0.0083 (11)	0.0098 (9)	0.0049 (9)
C10	0.0401 (11)	0.0397 (11)	0.0682 (15)	0.0003 (9)	0.0149 (10)	−0.0041 (10)
C21	0.0431 (12)	0.0649 (15)	0.0561 (14)	0.0045 (11)	0.0041 (10)	−0.0079 (11)
C11	0.0548 (15)	0.0461 (13)	0.097 (2)	−0.0071 (11)	0.0247 (14)	−0.0018 (13)
C22	0.0528 (16)	0.109 (3)	0.104 (3)	−0.0217 (17)	0.0217 (17)	−0.004 (2)

Geometric parameters (Å, °)

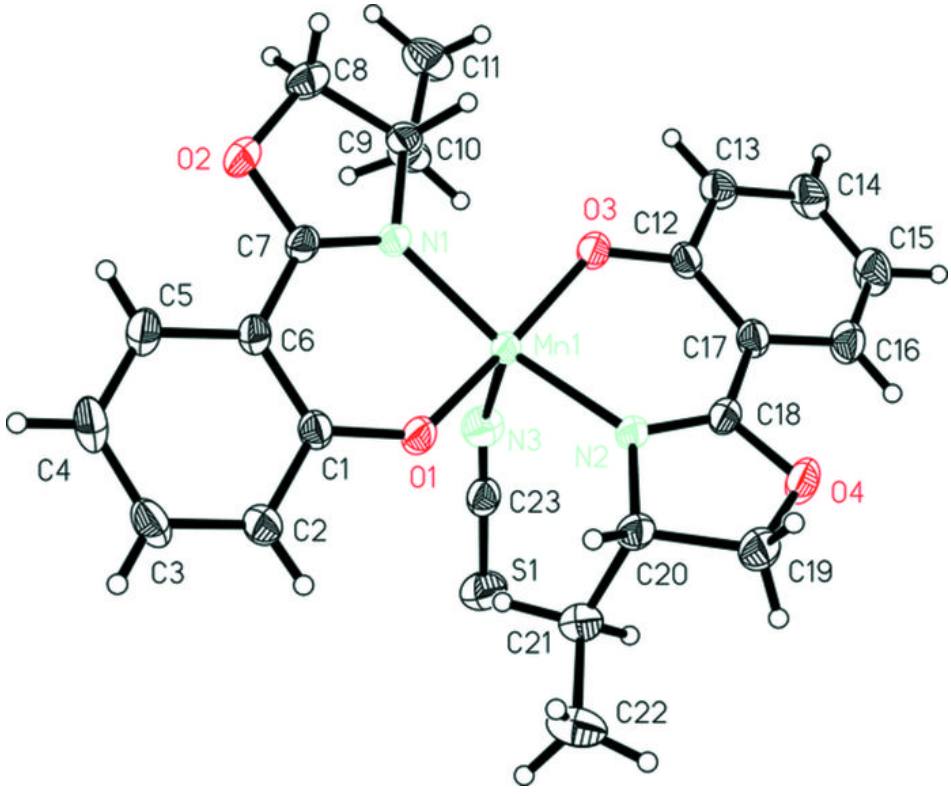
Mn1—O3	1.8573 (14)	O4—C18	1.347 (2)
Mn1—O1	1.8600 (14)	O4—C19	1.461 (3)
Mn1—N1	2.0153 (15)	C18—C17	1.455 (3)
Mn1—N2	2.0294 (15)	C12—C13	1.404 (3)
Mn1—N3	2.116 (2)	C12—C17	1.409 (3)
N3—C23	1.157 (3)	C15—C16	1.371 (3)
C23—S1	1.625 (3)	C15—C14	1.391 (4)
C1—O1	1.329 (2)	C15—H15	0.9300
C1—C2	1.408 (3)	C13—C14	1.384 (3)
C1—C6	1.411 (3)	C13—H13	0.9300
C6—C5	1.411 (3)	C17—C16	1.415 (3)
C6—C7	1.449 (3)	C20—C21	1.500 (3)
C2—C3	1.386 (3)	C20—C19	1.543 (3)
C2—H2	0.9300	C20—H20	0.9800
C5—C4	1.378 (3)	C19—H19A	0.9700
C5—H5	0.9300	C19—H19B	0.9700
C3—C4	1.390 (4)	C14—H14	0.9300
C3—H3	0.9300	C16—H16	0.9300
C4—H4	0.9300	C10—C11	1.530 (3)
C7—N1	1.305 (2)	C10—H10A	0.9700
C7—O2	1.343 (2)	C10—H10B	0.9700
C9—N1	1.497 (2)	C21—C22	1.551 (4)
C9—C10	1.521 (3)	C21—H21A	0.9700
C9—C8	1.533 (3)	C21—H21B	0.9700
C9—H9	0.9800	C11—H11A	0.9600
C8—O2	1.455 (3)	C11—H11B	0.9600
C8—H8A	0.9700	C11—H11C	0.9600
C8—H8B	0.9700	C22—H22A	0.9600

O3—C12	1.333 (2)	C22—H22B	0.9600
N2—C18	1.297 (2)	C22—H22C	0.9600
N2—C20	1.503 (2)		
O3—Mn1—O1	166.75 (8)	N2—C18—C17	127.15 (17)
O3—Mn1—N1	87.70 (6)	O4—C18—C17	116.86 (17)
O1—Mn1—N1	89.36 (6)	O3—C12—C13	118.80 (18)
O3—Mn1—N2	89.14 (6)	O3—C12—C17	123.05 (17)
O1—Mn1—N2	88.96 (6)	C13—C12—C17	118.11 (18)
N1—Mn1—N2	158.90 (7)	C16—C15—C14	119.6 (2)
O3—Mn1—N3	98.25 (8)	C16—C15—H15	120.2
O1—Mn1—N3	95.00 (8)	C14—C15—H15	120.2
N1—Mn1—N3	104.43 (7)	C14—C13—C12	121.0 (2)
N2—Mn1—N3	96.67 (7)	C14—C13—H13	119.5
C23—N3—Mn1	150.12 (19)	C12—C13—H13	119.5
N3—C23—S1	178.6 (2)	C12—C17—C16	119.79 (19)
O1—C1—C2	118.27 (18)	C12—C17—C18	119.92 (17)
O1—C1—C6	123.22 (17)	C16—C17—C18	120.24 (19)
C2—C1—C6	118.49 (18)	C21—C20—N2	112.22 (18)
C1—C6—C5	119.53 (19)	C21—C20—C19	113.46 (19)
C1—C6—C7	120.16 (17)	N2—C20—C19	101.47 (16)
C5—C6—C7	120.29 (18)	C21—C20—H20	109.8
C3—C2—C1	120.6 (2)	N2—C20—H20	109.8
C3—C2—H2	119.7	C19—C20—H20	109.8
C1—C2—H2	119.7	O4—C19—C20	104.33 (16)
C4—C5—C6	120.9 (2)	O4—C19—H19A	110.9
C4—C5—H5	119.5	C20—C19—H19A	110.9
C6—C5—H5	119.5	O4—C19—H19B	110.9
C2—C3—C4	120.8 (2)	C20—C19—H19B	110.9
C2—C3—H3	119.6	H19A—C19—H19B	108.9
C4—C3—H3	119.6	C13—C14—C15	120.7 (2)
C5—C4—C3	119.5 (2)	C13—C14—H14	119.7
C5—C4—H4	120.2	C15—C14—H14	119.7
C3—C4—H4	120.2	C15—C16—C17	120.8 (2)
N1—C7—O2	115.89 (17)	C15—C16—H16	119.6
N1—C7—C6	126.91 (17)	C17—C16—H16	119.6
O2—C7—C6	117.17 (17)	C9—C10—C11	111.3 (2)
N1—C9—C10	111.78 (16)	C9—C10—H10A	109.4
N1—C9—C8	102.23 (16)	C11—C10—H10A	109.4
C10—C9—C8	113.35 (18)	C9—C10—H10B	109.4
N1—C9—H9	109.7	C11—C10—H10B	109.4
C10—C9—H9	109.7	H10A—C10—H10B	108.0
C8—C9—H9	109.7	C20—C21—C22	110.3 (2)
O2—C8—C9	105.08 (16)	C20—C21—H21A	109.6
O2—C8—H8A	110.7	C22—C21—H21A	109.6
C9—C8—H8A	110.7	C20—C21—H21B	109.6
O2—C8—H8B	110.7	C22—C21—H21B	109.6
C9—C8—H8B	110.7	H21A—C21—H21B	108.1
H8A—C8—H8B	108.8	C10—C11—H11A	109.5
C7—O2—C8	107.31 (16)	C10—C11—H11B	109.5

C7—N1—C9	108.35 (16)	H11A—C11—H11B	109.5
C7—N1—Mn1	125.88 (13)	C10—C11—H11C	109.5
C9—N1—Mn1	125.67 (12)	H11A—C11—H11C	109.5
C1—O1—Mn1	133.21 (13)	H11B—C11—H11C	109.5
C12—O3—Mn1	130.21 (12)	C21—C22—H22A	109.5
C18—N2—C20	108.37 (15)	C21—C22—H22B	109.5
C18—N2—Mn1	124.05 (13)	H22A—C22—H22B	109.5
C20—N2—Mn1	127.42 (12)	C21—C22—H22C	109.5
C18—O4—C19	106.96 (16)	H22A—C22—H22C	109.5
N2—C18—O4	115.99 (17)	H22B—C22—H22C	109.5
O3—Mn1—N3—C23	−125.7 (4)	O1—Mn1—O3—C12	−110.3 (3)
O1—Mn1—N3—C23	54.0 (4)	N1—Mn1—O3—C12	172.31 (18)
N1—Mn1—N3—C23	144.6 (4)	N2—Mn1—O3—C12	−28.56 (18)
N2—Mn1—N3—C23	−35.6 (4)	N3—Mn1—O3—C12	68.06 (19)
O1—C1—C6—C5	174.62 (19)	O3—Mn1—N2—C18	16.34 (17)
C2—C1—C6—C5	−3.9 (3)	O1—Mn1—N2—C18	−176.78 (17)
O1—C1—C6—C7	−7.0 (3)	N1—Mn1—N2—C18	97.7 (2)
C2—C1—C6—C7	174.44 (18)	N3—Mn1—N2—C18	−81.87 (17)
O1—C1—C2—C3	−175.7 (2)	O3—Mn1—N2—C20	−168.98 (17)
C6—C1—C2—C3	2.9 (3)	O1—Mn1—N2—C20	−2.10 (17)
C1—C6—C5—C4	1.7 (3)	N1—Mn1—N2—C20	−87.6 (2)
C7—C6—C5—C4	−176.6 (2)	N3—Mn1—N2—C20	92.81 (17)
C1—C2—C3—C4	0.4 (4)	C20—N2—C18—O4	4.3 (3)
C6—C5—C4—C3	1.6 (4)	Mn1—N2—C18—O4	179.85 (14)
C2—C3—C4—C5	−2.6 (4)	C20—N2—C18—C17	−176.08 (19)
C1—C6—C7—N1	−3.8 (3)	Mn1—N2—C18—C17	−0.5 (3)
C5—C6—C7—N1	174.57 (19)	C19—O4—C18—N2	7.2 (3)
C1—C6—C7—O2	178.51 (18)	C19—O4—C18—C17	−172.43 (19)
C5—C6—C7—O2	−3.1 (3)	Mn1—O3—C12—C13	−158.44 (16)
N1—C9—C8—O2	10.3 (2)	Mn1—O3—C12—C17	23.9 (3)
C10—C9—C8—O2	−110.2 (2)	O3—C12—C13—C14	−179.7 (2)
N1—C7—O2—C8	5.4 (2)	C17—C12—C13—C14	−1.9 (3)
C6—C7—O2—C8	−176.68 (18)	O3—C12—C17—C16	179.5 (2)
C9—C8—O2—C7	−9.8 (2)	C13—C12—C17—C16	1.8 (3)
O2—C7—N1—C9	1.8 (2)	O3—C12—C17—C18	2.0 (3)
C6—C7—N1—C9	−175.94 (18)	C13—C12—C17—C18	−175.69 (19)
O2—C7—N1—Mn1	−174.68 (13)	N2—C18—C17—C12	−12.8 (3)
C6—C7—N1—Mn1	7.6 (3)	O4—C18—C17—C12	166.78 (19)
C10—C9—N1—C7	113.93 (19)	N2—C18—C17—C16	169.7 (2)
C8—C9—N1—C7	−7.6 (2)	O4—C18—C17—C16	−10.7 (3)
C10—C9—N1—Mn1	−69.6 (2)	C18—N2—C20—C21	108.4 (2)
C8—C9—N1—Mn1	168.87 (14)	Mn1—N2—C20—C21	−66.9 (2)
O3—Mn1—N1—C7	165.12 (17)	C18—N2—C20—C19	−13.0 (2)
O1—Mn1—N1—C7	−1.95 (17)	Mn1—N2—C20—C19	171.63 (15)
N2—Mn1—N1—C7	83.5 (2)	C18—O4—C19—C20	−14.9 (2)
N3—Mn1—N1—C7	−96.95 (17)	C21—C20—C19—O4	−104.1 (2)
O3—Mn1—N1—C9	−10.78 (15)	N2—C20—C19—O4	16.4 (2)
O1—Mn1—N1—C9	−177.85 (16)	C12—C13—C14—C15	0.7 (4)
N2—Mn1—N1—C9	−92.4 (2)	C16—C15—C14—C13	0.7 (4)

N3—Mn1—N1—C9	87.15 (16)	C14—C15—C16—C17	−0.8 (4)
C2—C1—O1—Mn1	−167.07 (16)	C12—C17—C16—C15	−0.5 (4)
C6—C1—O1—Mn1	14.4 (3)	C18—C17—C16—C15	177.0 (2)
O3—Mn1—O1—C1	−86.1 (3)	N1—C9—C10—C11	174.2 (2)
N1—Mn1—O1—C1	−8.9 (2)	C8—C9—C10—C11	−70.9 (3)
N2—Mn1—O1—C1	−167.9 (2)	N2—C20—C21—C22	175.5 (2)
N3—Mn1—O1—C1	95.5 (2)	C19—C20—C21—C22	−70.2 (3)

Fig. 1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